



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 11:35 pm BST

PDB ID : 6J32  
Title : Crystal Structure Analysis of the Glycotransferase of kitacinnamycin  
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Deposited on : 2019-01-03  
Resolution : 2.50 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

<https://www.wwpdb.org/validation/2017/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) : 1.13  
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

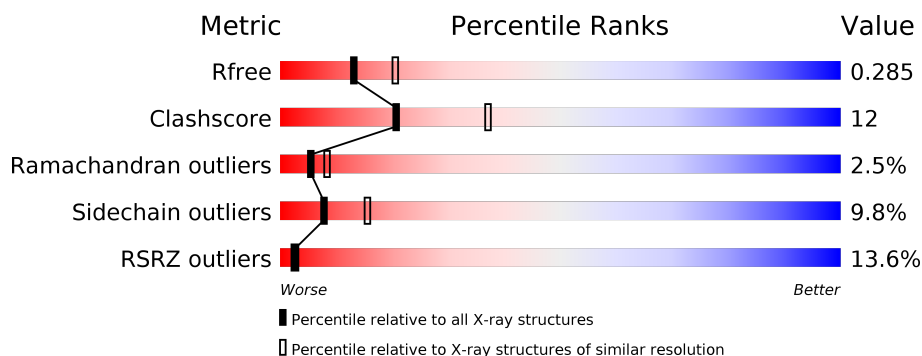
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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

Mol	Chain	Length	Quality of chain
1	A	399	<div> <div>14%</div> <div>68%</div> <div>22%</div> <div>5%</div> <div>.</div> <div>.</div> </div>
1	B	399	<div> <div>10%</div> <div>65%</div> <div>27%</div> <div>5%</div> <div>.</div> </div>
1	C	399	<div> <div>12%</div> <div>73%</div> <div>20%</div> <div>.</div> <div>.</div> </div>
1	D	399	<div> <div>18%</div> <div>69%</div> <div>21%</div> <div>6%</div> <div>.</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11972 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 Kcn28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	385	Total	C	N	O	S	0	0	0
			2953	1870	530	542	11			
1	B	386	Total	C	N	O	S	0	0	0
			2940	1861	525	544	10			
1	C	385	Total	C	N	O	S	0	0	0
			2942	1860	526	545	11			
1	D	385	Total	C	N	O	S	0	0	0
			2970	1878	534	547	11			

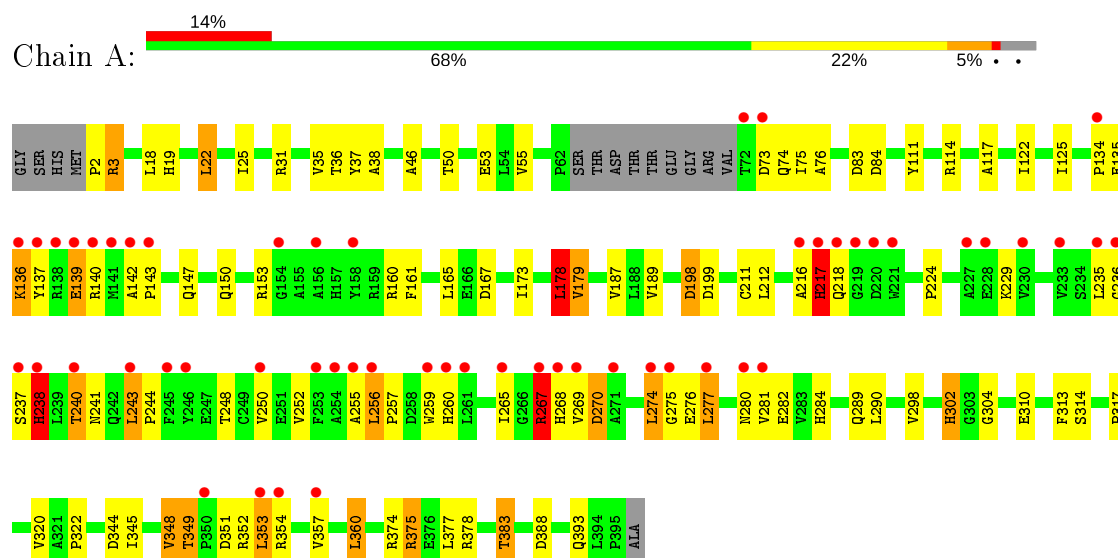
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	36	Total	O	0	0
			36	36		
2	B	54	Total	O	0	0
			54	54		
2	C	30	Total	O	0	0
			30	30		
2	D	47	Total	O	0	0
			47	47		

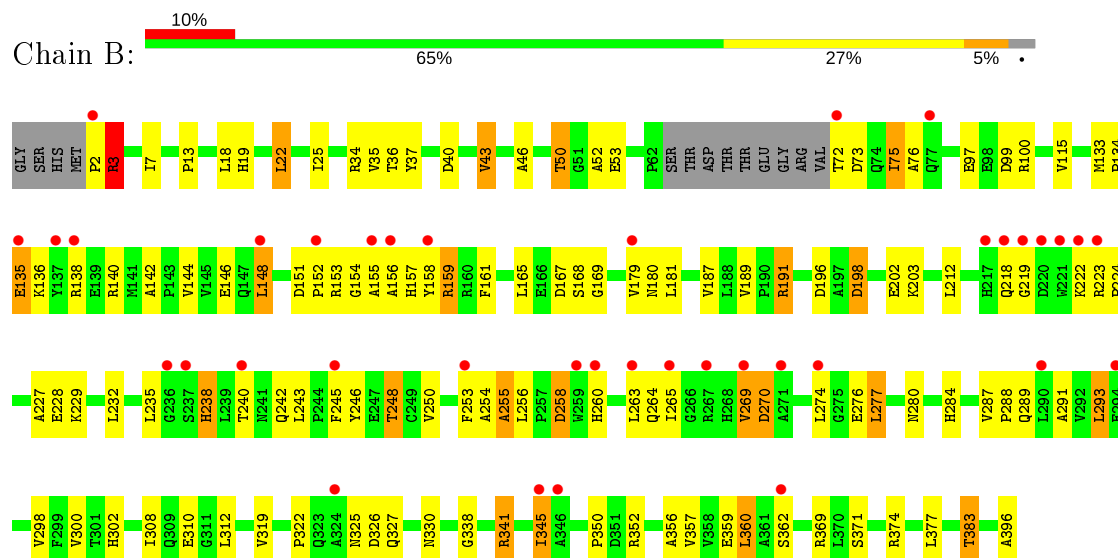
### 3 Residue-property plots [i](#)

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.

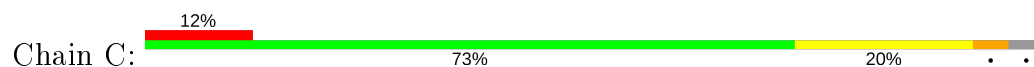
#### • Molecule 1: Kcn28

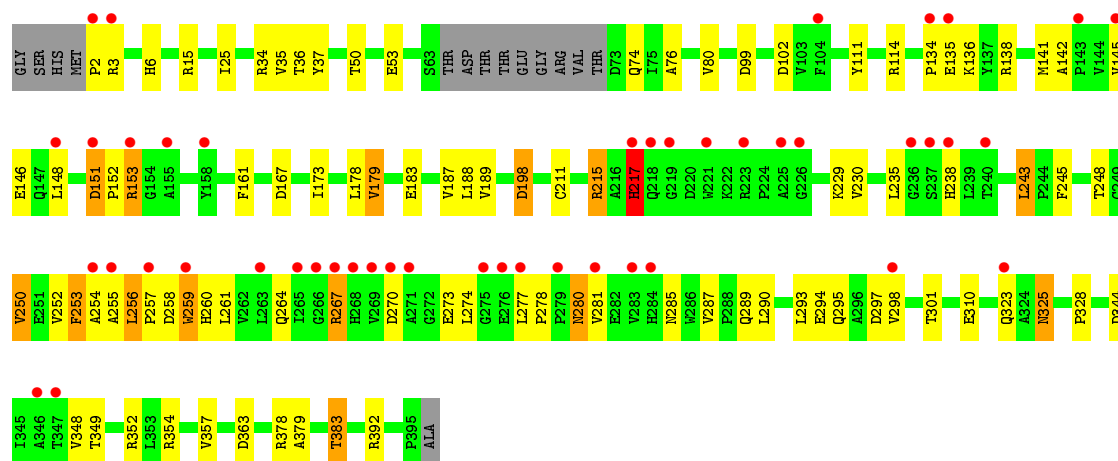


#### • Molecule 1: Kcn28

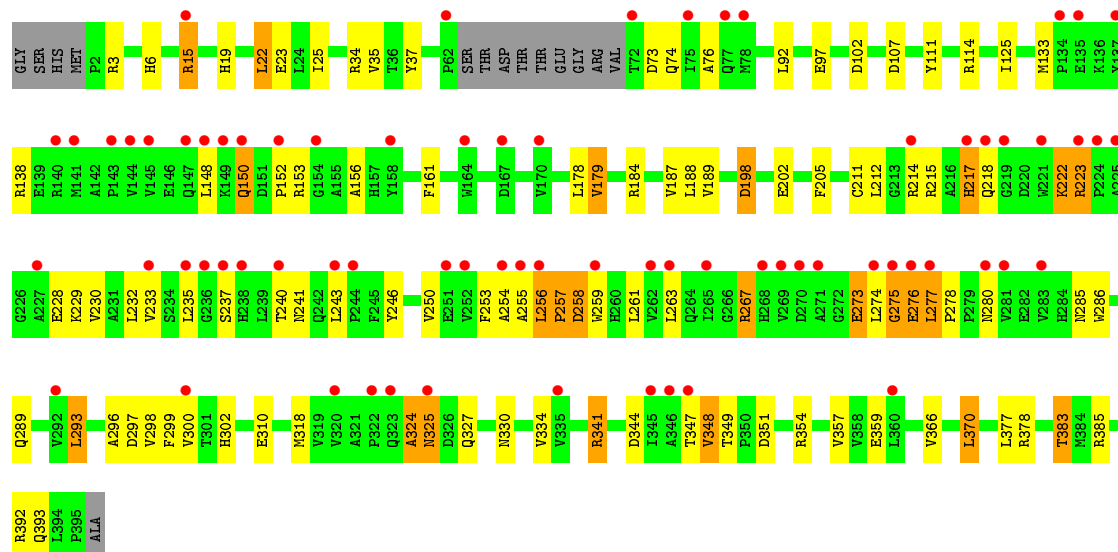


#### • Molecule 1: Kcn28





• Molecule 1: Kcn28



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	242.90 Å   242.90 Å   242.90 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	70.12 – 2.50 70.12 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.3 (70.12-2.50) 99.3 (70.12-2.50)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.72 (at 2.51 Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, $R_{free}$	0.269 , 0.285 0.269 , 0.285	Depositor DCC
$R_{free}$ test set	4090 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	59.3	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 54.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.009 for -l,-k,-h	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	11972	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.90% 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	0.27	0/3025	0.52	1/4132 (0.0%)
1	B	0.28	0/3011	0.54	1/4116 (0.0%)
1	C	0.26	0/3013	0.52	0/4117
1	D	0.29	0/3042	0.54	0/4153
All	All	0.27	0/12091	0.53	2/16518 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	178	LEU	CA-CB-CG	5.37	127.65	115.30
1	B	274	LEU	CA-CB-CG	5.02	126.85	115.30

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	2953	0	2918	70	0
1	B	2940	0	2887	86	0
1	C	2942	0	2893	63	0
1	D	2970	0	2941	75	0
2	A	36	0	0	3	0
2	B	54	0	0	5	0
2	C	30	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	47	0	0	13	0
All	All	11972	0	11639	288	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 12.

All (288) 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:257:PRO:O	1:D:259:TRP:N	1.85	1.08
1:D:256:LEU:HD21	1:D:354:ARG:HH12	1.24	1.00
1:C:352:ARG:NH1	2:C:401:HOH:O	1.94	0.99
1:B:158:TYR:H	1:B:159:ARG:NH1	1.62	0.98
1:B:229:LYS:NZ	2:B:401:HOH:O	1.97	0.96
1:D:73:ASP:OD2	1:D:153:ARG:NH1	2.01	0.94
1:B:158:TYR:HB2	1:B:159:ARG:HE	1.36	0.90
1:D:6:HIS:N	1:D:102:ASP:OD2	2.05	0.88
1:D:258:ASP:OD1	2:D:401:HOH:O	1.95	0.83
1:D:107:ASP:OD1	2:D:402:HOH:O	1.96	0.82
1:D:215:ARG:NH1	2:D:407:HOH:O	2.14	0.81
1:A:19:HIS:HA	1:A:22:LEU:HD22	1.61	0.80
1:A:84:ASP:OD2	2:A:401:HOH:O	2.00	0.80
1:C:253:PHE:HA	1:C:256:LEU:HD12	1.65	0.79
1:C:294:GLU:OE1	2:C:403:HOH:O	2.01	0.78
1:D:97:GLU:OE1	2:D:403:HOH:O	2.01	0.77
1:D:359:GLU:OE2	2:D:404:HOH:O	2.01	0.77
1:B:158:TYR:CD2	1:B:159:ARG:NH1	2.53	0.77
1:B:156:ALA:N	1:B:159:ARG:HH21	1.82	0.76
1:A:360:LEU:O	2:A:402:HOH:O	2.03	0.76
1:B:158:TYR:HD2	1:B:159:ARG:HH11	1.29	0.76
1:D:385:ARG:NH1	2:D:406:HOH:O	2.10	0.75
1:B:167:ASP:OD2	1:D:217:HIS:ND1	2.19	0.75
1:C:298:VAL:HG11	1:C:357:VAL:HG13	1.68	0.74
1:A:267:ARG:HG2	1:A:268:HIS:H	1.50	0.74
1:B:19:HIS:HA	1:B:22:LEU:HD22	1.67	0.74
1:C:183:GLU:OE2	2:C:404:HOH:O	2.05	0.73
1:D:19:HIS:HA	1:D:22:LEU:HD22	1.70	0.73
1:D:215:ARG:O	2:D:405:HOH:O	2.07	0.73
1:B:158:TYR:H	1:B:159:ARG:CZ	2.01	0.72
1:C:289:GLN:NE2	1:C:310:GLU:OE1	2.22	0.72
1:A:348:VAL:HG21	1:A:353:LEU:HD23	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:ASP:N	1:B:258:ASP:OD1	2.18	0.71
1:C:229:LYS:HB2	1:C:259:TRP:CD1	2.25	0.71
1:A:83:ASP:OD1	1:A:160:ARG:NH2	2.23	0.71
1:B:298:VAL:HG11	1:B:357:VAL:HG13	1.72	0.70
1:A:289:GLN:NE2	1:A:310:GLU:OE1	2.23	0.70
1:C:301:THR:OG1	2:C:405:HOH:O	2.09	0.70
1:A:256:LEU:O	1:A:280:ASN:ND2	2.24	0.70
1:C:2:PRO:HG2	1:C:3:ARG:NH1	2.06	0.70
1:D:341:ARG:NH2	1:D:359:GLU:OE1	2.22	0.70
1:C:34:ARG:NH2	1:C:99:ASP:OD2	2.20	0.69
1:A:236:GLY:H	1:A:302:HIS:H	1.38	0.69
1:C:114:ARG:NH1	1:C:178:LEU:HA	2.07	0.69
1:B:158:TYR:HD2	1:B:159:ARG:NH1	1.88	0.69
1:A:298:VAL:HG11	1:A:357:VAL:HG13	1.75	0.68
1:D:240:THR:OG1	1:D:246:TYR:OH	2.08	0.68
1:B:235:LEU:HD22	1:B:240:THR:HB	1.76	0.68
1:D:256:LEU:HD21	1:D:354:ARG:NH1	2.05	0.68
1:C:258:ASP:O	2:C:406:HOH:O	2.12	0.67
1:B:168:SER:OG	2:B:402:HOH:O	2.14	0.66
1:D:184:ARG:NH1	2:D:410:HOH:O	2.24	0.65
1:A:75:ILE:HG21	1:A:153:ARG:HB3	1.78	0.65
1:D:222:LYS:NZ	1:D:222:LYS:HB2	2.12	0.64
1:C:15:ARG:N	2:C:402:HOH:O	2.30	0.64
1:B:269:VAL:HG13	1:B:270:ASP:H	1.63	0.64
1:B:191:ARG:NH2	1:B:202:GLU:OE2	2.31	0.64
1:C:256:LEU:HD13	1:C:259:TRP:HE3	1.63	0.64
1:A:237:SER:HB2	1:A:304:GLY:HA3	1.78	0.63
1:A:235:LEU:HD22	1:A:240:THR:HB	1.81	0.63
1:D:156:ALA:O	2:D:408:HOH:O	2.15	0.63
1:D:325:ASN:N	1:D:325:ASN:OD1	2.31	0.63
1:A:198:ASP:N	1:A:198:ASP:OD1	2.30	0.62
1:B:223:ARG:NH1	1:B:227:ALA:O	2.32	0.62
1:B:253:PHE:O	1:B:255:ALA:N	2.29	0.62
1:A:136:LYS:HA	1:A:139:GLU:OE2	2.01	0.61
1:C:135:GLU:HG3	1:C:135:GLU:O	2.01	0.61
1:A:143:PRO:O	1:A:147:GLN:N	2.25	0.61
1:A:349:THR:HG22	1:A:352:ARG:H	1.65	0.60
1:B:157:HIS:H	1:B:159:ARG:NH2	1.99	0.60
1:A:265:ILE:HG12	1:A:284:HIS:O	2.02	0.59
1:B:169:GLY:O	2:B:403:HOH:O	2.17	0.59
1:C:267:ARG:HA	1:C:285:ASN:HB3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:253:PHE:O	1:D:280:ASN:ND2	2.35	0.59
1:C:254:ALA:HA	1:C:280:ASN:HD21	1.69	0.57
1:C:243:LEU:HD22	1:C:243:LEU:H	1.69	0.57
1:A:374:ARG:HH21	1:A:378:ARG:HH22	1.52	0.57
1:B:75:ILE:HG21	1:B:153:ARG:HD3	1.86	0.56
1:B:341:ARG:NH2	1:B:359:GLU:OE1	2.36	0.56
1:C:261:LEU:HB3	1:C:281:VAL:HG22	1.85	0.56
1:B:245:PHE:CD1	1:B:345:ILE:HG12	2.40	0.56
1:A:344:ASP:O	1:A:348:VAL:HG12	2.04	0.56
1:B:157:HIS:N	1:B:159:ARG:NH2	2.53	0.56
1:B:138:ARG:NH1	1:B:180:ASN:HD22	2.03	0.56
1:D:215:ARG:HB3	2:D:405:HOH:O	2.05	0.56
1:B:34:ARG:NH2	1:B:99:ASP:OD2	2.30	0.55
1:C:278:PRO:HB2	1:C:280:ASN:ND2	2.21	0.55
1:C:250:VAL:HG21	1:C:274:LEU:HD12	1.88	0.55
1:C:280:ASN:H	1:C:280:ASN:HD22	1.52	0.55
1:A:25:ILE:HG23	1:A:35:VAL:HG11	1.88	0.54
1:A:217:HIS:O	1:A:218:GLN:HG2	2.08	0.54
1:B:154:GLY:C	1:B:159:ARG:NH2	2.60	0.54
1:B:156:ALA:N	1:B:159:ARG:NH2	2.52	0.54
1:A:136:LYS:O	1:A:139:GLU:HG2	2.08	0.54
1:B:338:GLY:O	1:B:369:ARG:NH1	2.41	0.54
1:B:158:TYR:N	1:B:159:ARG:CZ	2.70	0.54
1:D:230:VAL:HB	1:D:296:ALA:HA	1.89	0.54
1:C:6:HIS:N	1:C:102:ASP:OD2	2.29	0.54
1:B:362:SER:HA	2:B:401:HOH:O	2.08	0.53
1:B:159:ARG:H	1:B:159:ARG:NE	2.07	0.53
1:B:218:GLN:HB3	1:B:288:PRO:HB3	1.89	0.53
1:D:229:LYS:HA	1:D:297:ASP:OD2	2.07	0.53
1:D:289:GLN:NE2	1:D:310:GLU:OE1	2.38	0.53
1:B:155:ALA:C	1:B:159:ARG:HH21	2.12	0.53
1:B:224:PRO:HG2	1:B:260:HIS:CD2	2.44	0.53
1:C:151:ASP:C	1:C:153:ARG:H	2.11	0.53
1:B:3:ARG:NH2	2:B:412:HOH:O	2.41	0.52
1:C:363:ASP:OD2	2:C:407:HOH:O	2.19	0.52
1:C:256:LEU:HD13	1:C:259:TRP:CE3	2.44	0.52
1:D:302:HIS:HD2	1:D:327:GLN:HE21	1.56	0.52
1:D:302:HIS:HD2	1:D:327:GLN:NE2	2.06	0.52
1:B:25:ILE:HG23	1:B:35:VAL:HG11	1.90	0.52
1:C:245:PHE:HE2	1:C:348:VAL:HG21	1.75	0.52
1:D:198:ASP:N	1:D:198:ASP:OD1	2.29	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:246:TYR:CD1	1:D:263:LEU:HD11	2.45	0.52
1:C:229:LYS:HA	1:C:297:ASP:OD2	2.11	0.51
1:C:215:ARG:HG3	1:C:217:HIS:H	1.76	0.51
1:A:114:ARG:NH1	1:A:178:LEU:HA	2.26	0.51
1:A:73:ASP:OD1	1:A:74:GLN:N	2.38	0.51
1:C:280:ASN:ND2	1:C:281:VAL:HG23	2.26	0.51
1:B:265:ILE:HG12	1:B:284:HIS:O	2.11	0.51
1:C:260:HIS:ND1	1:C:280:ASN:O	2.44	0.51
1:B:3:ARG:NH1	1:B:396:ALA:O	2.40	0.50
1:D:73:ASP:OD1	1:D:74:GLN:N	2.44	0.50
1:C:280:ASN:N	1:C:280:ASN:HD22	2.08	0.50
1:A:139:GLU:HA	1:A:142:ALA:HB2	1.93	0.50
1:B:50:THR:HG22	1:B:52:ALA:H	1.75	0.50
1:D:378:ARG:NH2	2:D:417:HOH:O	2.43	0.50
1:B:158:TYR:HB2	1:B:159:ARG:NE	2.14	0.50
1:A:313:PHE:O	2:A:403:HOH:O	2.19	0.50
1:D:187:VAL:HG12	1:D:189:VAL:HG22	1.93	0.50
1:A:2:PRO:HB2	1:A:3:ARG:HD2	1.93	0.50
1:B:245:PHE:CG	1:B:345:ILE:HG12	2.47	0.50
1:D:256:LEU:O	1:D:280:ASN:ND2	2.32	0.49
1:B:289:GLN:NE2	1:B:310:GLU:OE1	2.39	0.49
1:D:324:ALA:N	1:D:327:GLN:OE1	2.37	0.49
1:B:151:ASP:OD1	1:B:152:PRO:HD2	2.12	0.49
1:D:25:ILE:HG23	1:D:35:VAL:HG11	1.95	0.49
1:D:237:SER:HB2	1:D:302:HIS:HE2	1.77	0.49
1:A:236:GLY:N	1:A:302:HIS:HB2	2.27	0.49
1:B:133:MET:HE3	1:B:138:ARG:HD3	1.95	0.49
1:B:269:VAL:HG13	1:B:270:ASP:N	2.27	0.49
1:C:141:MET:O	1:C:145:VAL:HG13	2.12	0.49
1:A:224:PRO:HG2	1:A:260:HIS:CD2	2.48	0.49
1:B:248:THR:HG22	1:B:350:PRO:HG3	1.93	0.49
1:D:15:ARG:CZ	1:D:19:HIS:HB2	2.43	0.49
1:B:284:HIS:HB2	1:B:287:VAL:HG12	1.95	0.48
1:A:135:GLU:HB3	1:A:199:ASP:O	2.13	0.48
1:A:229:LYS:HB2	1:A:259:TRP:NE1	2.27	0.48
1:D:211:CYS:HA	1:D:383:THR:HG22	1.95	0.48
1:D:125:ILE:HD11	1:D:393:GLN:HG3	1.95	0.48
1:A:349:THR:HG23	1:A:351:ASP:H	1.78	0.48
1:B:223:ARG:NH1	1:B:228:GLU:O	2.46	0.48
1:B:224:PRO:HG2	1:B:260:HIS:NE2	2.28	0.48
1:B:325:ASN:O	1:B:326:ASP:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:252:VAL:HG13	1:C:354:ARG:HB3	1.94	0.48
1:D:289:GLN:O	1:D:293:LEU:HB2	2.14	0.48
1:C:258:ASP:OD1	1:C:258:ASP:N	2.47	0.48
1:A:117:ALA:HB1	1:A:122:ILE:O	2.13	0.48
1:B:232:LEU:HD23	1:B:293:LEU:HD13	1.95	0.48
1:B:73:ASP:HB3	1:B:76:ALA:HB3	1.96	0.48
1:D:237:SER:HB2	1:D:302:HIS:NE2	2.29	0.48
1:A:173:ILE:HG21	1:A:178:LEU:HB3	1.96	0.47
1:A:257:PRO:C	1:A:259:TRP:H	2.17	0.47
1:C:173:ILE:HD13	1:C:178:LEU:HB2	1.94	0.47
1:C:253:PHE:O	1:C:255:ALA:N	2.40	0.47
1:C:198:ASP:OD1	1:C:198:ASP:N	2.32	0.47
1:A:229:LYS:HB2	1:A:259:TRP:CD1	2.48	0.47
1:D:232:LEU:HD23	1:D:293:LEU:HD13	1.96	0.47
1:B:264:GLN:HB2	1:B:287:VAL:HG13	1.97	0.47
1:A:375:ARG:HD2	1:C:379:ALA:HA	1.95	0.47
1:A:187:VAL:HG12	1:A:189:VAL:HG22	1.96	0.47
1:D:150:GLN:OE1	1:D:150:GLN:N	2.25	0.47
1:A:211:CYS:HA	1:A:383:THR:HG22	1.96	0.47
1:A:75:ILE:HD13	1:A:153:ARG:HB2	1.96	0.47
1:D:178:LEU:O	1:D:179:VAL:HB	2.15	0.47
1:C:142:ALA:O	1:C:146:GLU:HG3	2.16	0.46
1:A:216:ALA:O	1:A:218:GLN:N	2.48	0.46
1:C:142:ALA:O	1:C:145:VAL:HG22	2.15	0.46
1:A:36:THR:HG22	1:A:53:GLU:HB3	1.96	0.46
1:B:308:ILE:HD12	1:B:330:ASN:HB3	1.97	0.46
1:C:325:ASN:O	1:C:328:PRO:HD2	2.15	0.46
1:B:97:GLU:OE1	1:B:100:ARG:NH2	2.40	0.46
1:C:151:ASP:N	1:C:152:PRO:HD3	2.30	0.46
1:C:25:ILE:HB	1:C:50:THR:HG21	1.98	0.46
1:B:159:ARG:CD	1:B:159:ARG:H	2.24	0.46
1:B:300:VAL:HG22	1:B:319:VAL:HB	1.98	0.46
1:D:351:ASP:HA	1:D:354:ARG:HG2	1.97	0.46
1:A:160:ARG:HA	1:B:219:GLY:HA2	1.97	0.46
1:A:73:ASP:H	1:A:76:ALA:HB3	1.80	0.46
1:D:178:LEU:HD13	1:D:179:VAL:HG23	1.98	0.46
1:D:228:GLU:HB2	1:D:258:ASP:HB2	1.97	0.46
1:B:18:LEU:HD21	1:B:46:ALA:HB3	1.98	0.45
1:A:153:ARG:HA	1:B:284:HIS:HE2	1.80	0.45
1:C:245:PHE:O	1:C:248:THR:OG1	2.29	0.45
1:A:282:GLU:HB2	1:D:152:PRO:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:111:TYR:CG	1:D:179:VAL:HG22	2.50	0.45
1:A:250:VAL:HG21	1:A:274:LEU:HD21	1.97	0.45
1:D:240:THR:HG1	1:D:246:TYR:HH	1.35	0.45
1:C:111:TYR:CD1	1:C:179:VAL:HG22	2.52	0.45
1:C:187:VAL:HG12	1:C:189:VAL:HG22	1.98	0.45
1:D:298:VAL:HG11	1:D:357:VAL:HG13	1.98	0.45
1:B:148:LEU:O	1:B:154:GLY:HA3	2.16	0.45
1:C:2:PRO:HG2	1:C:3:ARG:HH12	1.81	0.44
1:D:347:THR:OG1	1:D:348:VAL:N	2.50	0.44
1:C:229:LYS:HB2	1:C:259:TRP:HD1	1.80	0.44
1:C:25:ILE:HG23	1:C:35:VAL:HG11	1.99	0.44
1:B:276:GLU:O	1:B:277:LEU:HB2	2.18	0.44
1:C:211:CYS:HA	1:C:383:THR:HG22	1.99	0.44
1:B:187:VAL:HG12	1:B:189:VAL:HG22	2.00	0.44
1:D:344:ASP:O	1:D:348:VAL:HG13	2.18	0.44
1:B:256:LEU:O	1:B:280:ASN:ND2	2.51	0.44
1:A:267:ARG:HD2	1:A:267:ARG:N	2.33	0.44
1:B:36:THR:HG22	1:B:53:GLU:HB3	1.99	0.44
1:B:151:ASP:O	1:B:154:GLY:N	2.51	0.43
1:D:76:ALA:HB2	1:D:153:ARG:HH22	1.83	0.43
1:A:268:HIS:O	1:A:270:ASP:N	2.52	0.43
1:A:250:VAL:HG22	1:A:281:VAL:HG11	1.99	0.43
1:B:212:LEU:O	1:B:383:THR:HG21	2.18	0.43
1:C:270:ASP:HA	1:C:285:ASN:OD1	2.19	0.43
1:C:36:THR:HG22	1:C:53:GLU:HB2	2.01	0.43
1:A:276:GLU:O	1:A:277:LEU:HB2	2.19	0.43
1:C:259:TRP:CH2	1:C:357:VAL:HG12	2.53	0.43
1:A:125:ILE:HD11	1:A:393:GLN:HG3	2.00	0.43
1:A:317:PRO:HB2	1:A:360:LEU:HG	2.00	0.43
1:B:198:ASP:N	1:B:198:ASP:OD2	2.47	0.43
1:D:274:LEU:O	1:D:276:GLU:N	2.51	0.43
1:D:275:GLY:O	1:D:276:GLU:HB2	2.19	0.43
1:B:138:ARG:NH1	1:B:180:ASN:ND2	2.67	0.42
1:C:267:ARG:CA	1:C:285:ASN:HB3	2.48	0.42
1:C:344:ASP:O	1:C:348:VAL:HG13	2.19	0.42
1:B:142:ALA:O	1:B:146:GLU:HG3	2.19	0.42
1:D:212:LEU:O	1:D:383:THR:HG21	2.18	0.42
1:A:111:TYR:CD2	1:A:179:VAL:HG22	2.54	0.42
1:A:212:LEU:O	1:A:383:THR:HG21	2.18	0.42
1:D:366:VAL:O	1:D:370:LEU:HD22	2.20	0.42
1:A:255:ALA:O	1:A:257:PRO:HD3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:299:PHE:O	1:D:318:MET:HA	2.19	0.42
1:D:253:PHE:CG	1:D:261:LEU:HB2	2.54	0.42
1:D:202:GLU:HA	1:D:205:PHE:O	2.19	0.42
1:A:250:VAL:HG11	1:A:274:LEU:HD21	2.00	0.42
1:A:31:ARG:NH1	1:A:388:ASP:OD1	2.41	0.42
1:C:134:PRO:C	1:C:136:LYS:H	2.23	0.42
1:D:277:LEU:HA	1:D:278:PRO:HD3	1.92	0.42
1:C:76:ALA:O	1:C:80:VAL:HG23	2.19	0.42
1:D:254:ALA:C	1:D:256:LEU:H	2.22	0.42
1:B:134:PRO:HG2	1:B:196:ASP:HB2	2.01	0.42
1:C:230:VAL:HB	1:C:295:GLN:O	2.19	0.42
1:D:233:VAL:HG22	1:D:300:VAL:HB	2.01	0.42
1:D:23:GLU:OE1	2:D:409:HOH:O	2.21	0.42
1:B:167:ASP:OD2	1:D:217:HIS:CE1	2.73	0.41
1:B:13:PRO:HG3	1:B:40:ASP:HB3	2.01	0.41
1:D:133:MET:HE3	1:D:138:ARG:HD3	2.01	0.41
1:C:111:TYR:CG	1:C:179:VAL:HG22	2.55	0.41
1:C:392:ARG:HA	1:C:392:ARG:HD2	1.89	0.41
1:D:255:ALA:O	1:D:257:PRO:HD3	2.20	0.41
1:B:115:VAL:HG11	1:B:168:SER:HB3	2.02	0.41
1:B:2:PRO:HB2	1:B:3:ARG:H	1.70	0.41
1:D:114:ARG:HD3	1:D:178:LEU:CD2	2.50	0.41
1:A:252:VAL:HG21	1:A:353:LEU:HB3	2.02	0.41
1:B:158:TYR:CB	1:B:159:ARG:HH11	2.34	0.41
1:B:7:ILE:O	1:B:35:VAL:HA	2.21	0.41
1:B:356:ALA:O	1:B:360:LEU:HB2	2.21	0.41
1:A:114:ARG:HH11	1:A:178:LEU:HA	1.86	0.41
1:B:302:HIS:O	1:B:327:GLN:HB3	2.21	0.41
1:A:243:LEU:N	1:A:244:PRO:HD2	2.35	0.41
1:B:135:GLU:OE2	1:B:181:LEU:HD13	2.21	0.41
1:B:288:PRO:HB2	1:B:291:ALA:HB3	2.02	0.41
1:B:13:PRO:HG3	1:B:40:ASP:CB	2.50	0.41
1:C:135:GLU:OE1	1:C:138:ARG:HG3	2.20	0.41
1:A:136:LYS:HB2	1:A:136:LYS:HE2	1.62	0.41
1:A:229:LYS:HB2	1:A:259:TRP:HE1	1.86	0.41
1:A:38:ALA:HA	1:A:55:VAL:O	2.21	0.41
1:D:330:ASN:O	1:D:334:VAL:HG22	2.21	0.41
1:D:34:ARG:HA	2:D:432:HOH:O	2.21	0.41
1:A:257:PRO:HA	1:A:280:ASN:HD21	1.86	0.40
1:B:302:HIS:O	1:B:322:PRO:HA	2.21	0.40
1:A:134:PRO:HD2	1:A:137:TYR:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:SER:O	1:A:238:HIS:HB2	2.22	0.40
1:B:246:TYR:CD1	1:B:263:LEU:HD11	2.55	0.40
1:A:320:VAL:HG12	1:A:322:PRO:HD3	2.03	0.40
1:D:223:ARG:HG3	1:D:230:VAL:HG21	2.03	0.40
1:A:18:LEU:HD21	1:A:46:ALA:HB3	2.03	0.40
1:B:18:LEU:HD22	1:B:43:VAL:HG21	2.03	0.40
1:C:148:LEU:HA	1:C:148:LEU:HD23	1.84	0.40
1:D:111:TYR:CD2	1:D:179:VAL:HG22	2.56	0.40
1:D:235:LEU:HG	1:D:302:HIS:HB3	2.03	0.40
1:D:257:PRO:HB2	1:D:258:ASP:H	1.60	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	381/399 (96%)	354 (93%)	20 (5%)	7 (2%)	8	14
1	B	382/399 (96%)	355 (93%)	20 (5%)	7 (2%)	8	14
1	C	381/399 (96%)	345 (91%)	26 (7%)	10 (3%)	5	8
1	D	381/399 (96%)	351 (92%)	16 (4%)	14 (4%)	3	4
All	All	1525/1596 (96%)	1405 (92%)	82 (5%)	38 (2%)	5	8

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	179	VAL
1	A	238	HIS
1	A	267	ARG
1	A	275	GLY
1	B	179	VAL

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Mol	Chain	Res	Type
1	B	254	ALA
1	B	255	ALA
1	C	179	VAL
1	C	217	HIS
1	C	325	ASN
1	D	179	VAL
1	D	218	GLN
1	D	258	ASP
1	D	267	ARG
1	D	275	GLY
1	D	276	GLU
1	D	348	VAL
1	B	269	VAL
1	C	153	ARG
1	D	241	ASN
1	D	257	PRO
1	D	273	GLU
1	A	277	LEU
1	C	257	PRO
1	D	277	LEU
1	B	238	HIS
1	C	74	GLN
1	C	151	ASP
1	D	3	ARG
1	D	214	ARG
1	D	324	ALA
1	A	217	HIS
1	B	3	ARG
1	B	277	LEU
1	C	238	HIS
1	A	269	VAL
1	C	253	PHE
1	C	277	LEU

### 5.3.2 Protein sidechains ⓘ

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	308/323 (95%)	273 (89%)	35 (11%)	5	11
1	B	304/323 (94%)	268 (88%)	36 (12%)	5	10
1	C	307/323 (95%)	284 (92%)	23 (8%)	13	26
1	D	312/323 (97%)	285 (91%)	27 (9%)	10	20
All	All	1231/1292 (95%)	1110 (90%)	121 (10%)	8	15

All (121) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	22	LEU
1	A	37	TYR
1	A	50	THR
1	A	136	LYS
1	A	139	GLU
1	A	140	ARG
1	A	150	GLN
1	A	161	PHE
1	A	165	LEU
1	A	167	ASP
1	A	178	LEU
1	A	198	ASP
1	A	217	HIS
1	A	238	HIS
1	A	240	THR
1	A	241	ASN
1	A	243	LEU
1	A	248	THR
1	A	256	LEU
1	A	267	ARG
1	A	270	ASP
1	A	274	LEU
1	A	290	LEU
1	A	302	HIS
1	A	314	SER
1	A	345	ILE
1	A	348	VAL
1	A	349	THR
1	A	353	LEU
1	A	354	ARG
1	A	360	LEU
1	A	375	ARG

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Mol	Chain	Res	Type
1	A	377	LEU
1	A	383	THR
1	B	3	ARG
1	B	22	LEU
1	B	37	TYR
1	B	43	VAL
1	B	50	THR
1	B	72	THR
1	B	75	ILE
1	B	135	GLU
1	B	136	LYS
1	B	140	ARG
1	B	144	VAL
1	B	148	LEU
1	B	159	ARG
1	B	161	PHE
1	B	165	LEU
1	B	191	ARG
1	B	198	ASP
1	B	203	LYS
1	B	222	LYS
1	B	238	HIS
1	B	242	GLN
1	B	243	LEU
1	B	248	THR
1	B	250	VAL
1	B	258	ASP
1	B	270	ASP
1	B	293	LEU
1	B	312	LEU
1	B	341	ARG
1	B	345	ILE
1	B	352	ARG
1	B	360	LEU
1	B	371	SER
1	B	374	ARG
1	B	377	LEU
1	B	383	THR
1	C	37	TYR
1	C	161	PHE
1	C	167	ASP
1	C	188	LEU

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Mol	Chain	Res	Type
1	C	198	ASP
1	C	215	ARG
1	C	217	HIS
1	C	235	LEU
1	C	243	LEU
1	C	250	VAL
1	C	256	LEU
1	C	259	TRP
1	C	264	GLN
1	C	267	ARG
1	C	273	GLU
1	C	280	ASN
1	C	287	VAL
1	C	290	LEU
1	C	293	LEU
1	C	323	GLN
1	C	349	THR
1	C	378	ARG
1	C	383	THR
1	D	15	ARG
1	D	22	LEU
1	D	37	TYR
1	D	92	LEU
1	D	148	LEU
1	D	150	GLN
1	D	161	PHE
1	D	188	LEU
1	D	198	ASP
1	D	217	HIS
1	D	222	LYS
1	D	223	ARG
1	D	243	LEU
1	D	250	VAL
1	D	256	LEU
1	D	267	ARG
1	D	273	GLU
1	D	285	ASN
1	D	286	TRP
1	D	293	LEU
1	D	325	ASN
1	D	341	ARG
1	D	349	THR

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Mol	Chain	Res	Type
1	D	370	LEU
1	D	377	LEU
1	D	383	THR
1	D	392	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	268	HIS
1	B	180	ASN
1	B	295	GLN
1	C	280	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 [i](#)

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	385/399 (96%)	1.02	54 (14%) <b>2</b> <b>2</b>	42, 74, 146, 207	0
1	B	386/399 (96%)	0.87	38 (9%) <b>7</b> <b>7</b>	41, 72, 142, 224	0
1	C	385/399 (96%)	0.90	46 (11%) <b>4</b> <b>4</b>	52, 82, 150, 216	0
1	D	385/399 (96%)	1.18	72 (18%) <b>1</b> <b>1</b>	42, 77, 148, 197	0
All	All	1541/1596 (96%)	0.99	210 (13%) <b>3</b> <b>2</b>	41, 77, 148, 224	0

All (210) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	255	ALA	21.1
1	A	219	GLY	10.3
1	B	219	GLY	9.7
1	A	255	ALA	9.6
1	D	236	GLY	8.6
1	A	72	THR	8.5
1	C	275	GLY	8.3
1	C	255	ALA	8.2
1	D	346	ALA	7.8
1	C	238	HIS	7.8
1	C	271	ALA	7.6
1	A	254	ALA	7.1
1	D	237	SER	7.1
1	D	265	ILE	6.6
1	A	216	ALA	6.6
1	D	275	GLY	6.5
1	C	254	ALA	6.5
1	B	156	ALA	6.3
1	D	218	GLN	6.2
1	A	238	HIS	5.9
1	C	277	LEU	5.9

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Mol	Chain	Res	Type	RSRZ
1	A	259	TRP	5.8
1	C	219	GLY	5.7
1	A	271	ALA	5.7
1	C	145	VAL	5.5
1	A	73	ASP	5.5
1	A	274	LEU	5.5
1	D	158	TYR	5.4
1	D	283	VAL	5.3
1	D	263	LEU	5.3
1	A	137	TYR	5.2
1	C	218	GLN	5.2
1	D	271	ALA	5.2
1	D	274	LEU	5.1
1	D	72	THR	5.0
1	A	281	VAL	5.0
1	A	275	GLY	5.0
1	D	269	VAL	4.8
1	D	219	GLY	4.7
1	D	144	VAL	4.7
1	A	142	ALA	4.6
1	D	259	TRP	4.6
1	D	347	THR	4.6
1	B	155	ALA	4.6
1	D	238	HIS	4.5
1	A	265	ILE	4.5
1	A	243	LEU	4.5
1	A	141	MET	4.5
1	B	152	PRO	4.2
1	A	253	PHE	4.2
1	B	236	GLY	4.2
1	A	230	VAL	4.1
1	B	346	ALA	4.1
1	C	266	GLY	4.1
1	B	221	TRP	4.1
1	A	218	GLN	4.1
1	D	217	HIS	4.0
1	D	225	ALA	4.0
1	A	236	GLY	4.0
1	A	260	HIS	4.0
1	C	259	TRP	3.9
1	B	345	ILE	3.9
1	A	353	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	246	TYR	3.9
1	D	145	VAL	3.9
1	D	150	GLN	3.8
1	A	267	ARG	3.8
1	A	217	HIS	3.8
1	A	156	ALA	3.7
1	C	3	ARG	3.7
1	A	235	LEU	3.7
1	D	322	PRO	3.7
1	C	148	LEU	3.6
1	A	269	VAL	3.6
1	C	284	HIS	3.5
1	D	148	LEU	3.5
1	B	218	GLN	3.5
1	D	141	MET	3.5
1	D	135	GLU	3.4
1	B	271	ALA	3.4
1	A	237	SER	3.4
1	A	228	GLU	3.4
1	D	233	VAL	3.4
1	C	217	HIS	3.4
1	B	72	THR	3.4
1	A	139	GLU	3.4
1	B	148	LEU	3.4
1	D	252	VAL	3.4
1	A	245	PHE	3.3
1	D	77	GLN	3.3
1	D	75	ILE	3.3
1	B	137	TYR	3.2
1	D	325	ASN	3.2
1	B	237	SER	3.2
1	D	15	ARG	3.2
1	B	240	THR	3.1
1	B	265	ILE	3.1
1	C	281	VAL	3.1
1	A	350	PRO	3.1
1	D	170	VAL	3.1
1	C	221	TRP	3.0
1	C	267	ARG	3.0
1	A	154	GLY	3.0
1	D	323	GLN	3.0
1	C	279	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	62	PRO	3.0
1	C	158	TYR	3.0
1	C	346	ALA	3.0
1	A	357	VAL	3.0
1	B	158	TYR	2.9
1	A	221	TRP	2.9
1	C	155	ALA	2.9
1	C	257	PRO	2.9
1	C	268	HIS	2.9
1	B	259	TRP	2.9
1	A	143	PRO	2.9
1	C	2	PRO	2.9
1	C	283	VAL	2.9
1	C	226	GLY	2.9
1	D	143	PRO	2.9
1	D	223	ARG	2.8
1	D	277	LEU	2.8
1	D	281	VAL	2.8
1	C	276	GLU	2.8
1	A	233	VAL	2.7
1	D	280	ASN	2.7
1	A	158	TYR	2.7
1	D	240	THR	2.7
1	B	135	GLU	2.7
1	A	220	ASP	2.7
1	B	138	ARG	2.7
1	D	251	GLU	2.7
1	D	270	ASP	2.7
1	C	223	ARG	2.7
1	D	167	ASP	2.7
1	A	354	ARG	2.6
1	C	153	ARG	2.6
1	D	224	PRO	2.6
1	A	277	LEU	2.6
1	D	235	LEU	2.6
1	D	147	GLN	2.6
1	C	236	GLY	2.6
1	D	276	GLU	2.6
1	C	237	SER	2.6
1	D	268	HIS	2.6
1	D	152	PRO	2.6
1	D	243	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	240	THR	2.6
1	D	227	ALA	2.6
1	D	320	VAL	2.5
1	B	2	PRO	2.5
1	A	261	LEU	2.5
1	B	263	LEU	2.5
1	D	149	LYS	2.5
1	D	256	LEU	2.5
1	D	78	MET	2.5
1	B	77	GLN	2.5
1	C	135	GLU	2.5
1	C	263	LEU	2.4
1	D	221	TRP	2.4
1	A	134	PRO	2.4
1	B	253	PHE	2.4
1	B	217	HIS	2.4
1	B	223	ARG	2.4
1	A	250	VAL	2.4
1	B	222	LYS	2.4
1	D	164	TRP	2.4
1	A	256	LEU	2.4
1	C	323	GLN	2.3
1	D	254	ALA	2.3
1	D	154	GLY	2.3
1	D	244	PRO	2.3
1	B	274	LEU	2.3
1	C	143	PRO	2.3
1	D	262	VAL	2.3
1	D	335	VAL	2.3
1	C	265	ILE	2.3
1	B	267	ARG	2.3
1	A	268	HIS	2.3
1	B	220	ASP	2.3
1	B	260	HIS	2.3
1	D	345	ILE	2.3
1	A	227	ALA	2.3
1	C	269	VAL	2.3
1	A	280	ASN	2.3
1	B	324	ALA	2.2
1	D	140	ARG	2.2
1	D	292	VAL	2.2
1	C	134	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	134	PRO	2.2
1	C	347	THR	2.2
1	B	290	LEU	2.1
1	A	140	ARG	2.1
1	D	300	VAL	2.1
1	C	104	PHE	2.1
1	C	270	ASP	2.1
1	D	214	ARG	2.1
1	B	269	VAL	2.1
1	B	294	GLU	2.1
1	B	362	SER	2.1
1	C	225	ALA	2.1
1	D	137	TYR	2.1
1	A	240	THR	2.0
1	B	245	PHE	2.0
1	A	136	LYS	2.0
1	A	138	ARG	2.0
1	B	179	VAL	2.0
1	C	151	ASP	2.0
1	C	298	VAL	2.0
1	D	360	LEU	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.