



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:41 PM GMT

PDB ID : 1C0M  
Title : CRYSTAL STRUCTURE OF RSV TWO-DOMAIN INTEGRASE  
Authors : Yang, Z.-N.; Mueser, T.C.; Bushman, F.D.; Hyde, C.C.  
Deposited on : 1999-07-16  
Resolution : 2.53 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.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

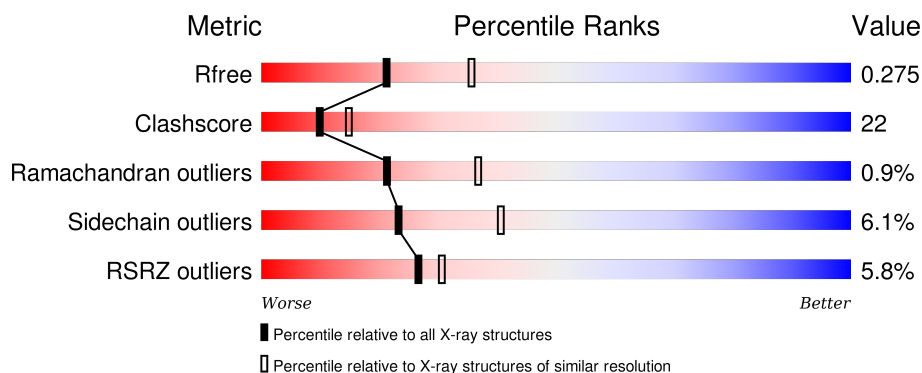
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.53 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	4241 (2.54-2.50)
Clashscore	102246	4968 (2.54-2.50)
Ramachandran outliers	100387	4873 (2.54-2.50)
Sidechain outliers	100360	4875 (2.54-2.50)
RSRZ outliers	91569	4253 (2.54-2.50)

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. 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	238	<div> <div>6%</div> <div> <div></div> <div>52%</div> <div>37%</div> <div>7%</div> </div> </div>
1	B	238	<div> <div>3%</div> <div> <div></div> <div>59%</div> <div>29%</div> <div>9%</div> </div> </div>
1	C	238	<div> <div>7%</div> <div> <div></div> <div>61%</div> <div>29%</div> <div>7%</div> </div> </div>
1	D	238	<div> <div>5%</div> <div> <div></div> <div>53%</div> <div>36%</div> <div>9%</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7034 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 PROTEIN (INTEGRASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	221	Total	C	N	O	S	0	0	0
			1740	1100	329	306	5			
1	B	216	Total	C	N	O	S	0	0	0
			1703	1078	320	300	5			
1	C	222	Total	C	N	O	S	0	0	0
			1747	1104	330	308	5			
1	D	216	Total	C	N	O	S	0	0	0
			1703	1078	320	300	5			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	199	LYS	PHE	MUTATION	UNP P03354
B	199	LYS	PHE	MUTATION	UNP P03354
C	199	LYS	PHE	MUTATION	UNP P03354
D	199	LYS	PHE	MUTATION	UNP P03354

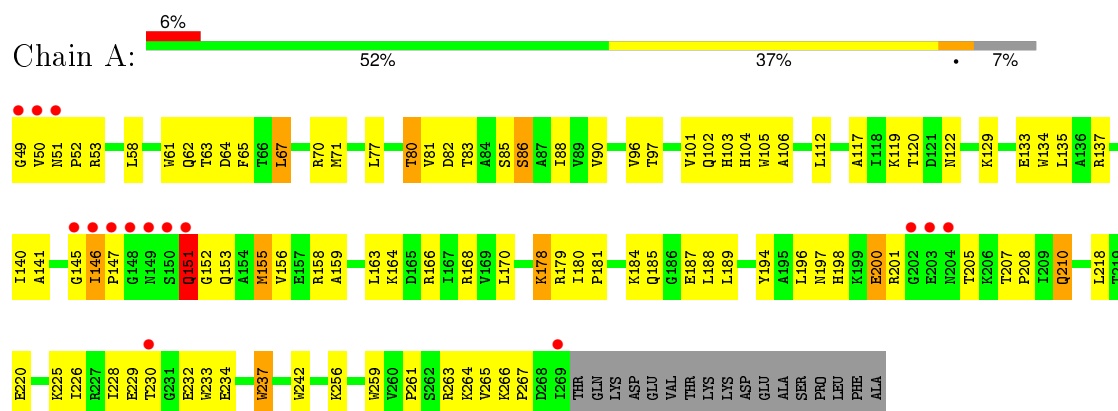
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	42	Total	O	0	0
			42	42		
2	B	33	Total	O	0	0
			33	33		
2	C	29	Total	O	0	0
			29	29		
2	D	37	Total	O	0	0
			37	37		

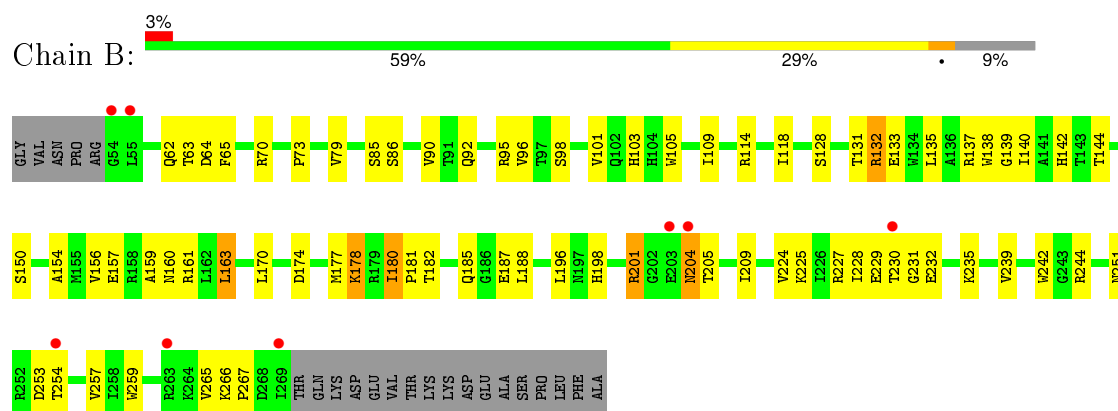
### 3 Residue-property plots

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

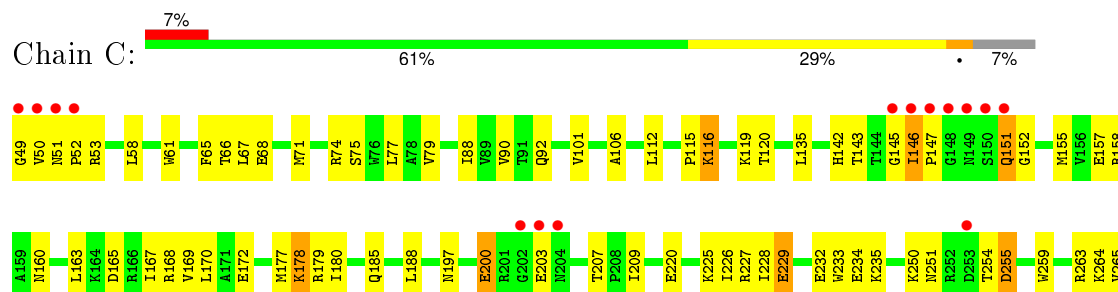
#### • Molecule 1: PROTEIN (INTEGRASE)

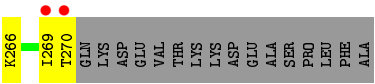


#### • Molecule 1: PROTEIN (INTEGRASE)

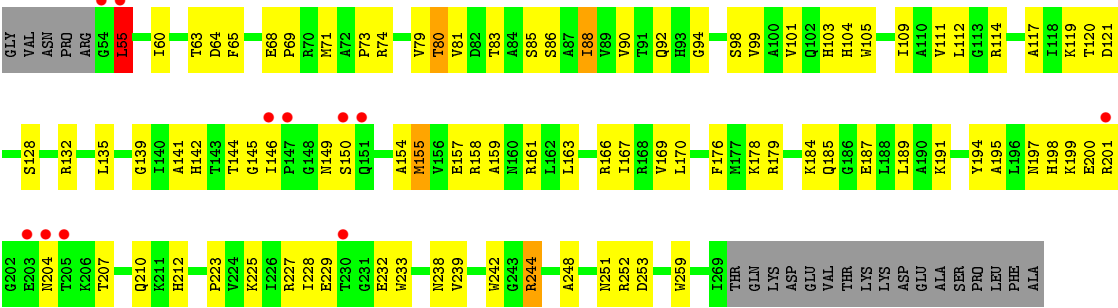


#### • Molecule 1: PROTEIN (INTEGRASE)





● Molecule 1: PROTEIN (INTEGRASE)



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	55.75Å 66.37Å 76.67Å 67.47° 78.61° 90.18°	Depositor
Resolution (Å)	15.00 – 2.53 19.82 – 2.51	Depositor EDS
% Data completeness (in resolution range)	87.6 (15.00-2.53) 75.6 (19.82-2.51)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.69 (at 2.53Å)	Xtriage
Refinement program	CNS, X-PLOR 3.851	Depositor
R, $R_{free}$	0.216 , 0.279 0.213 , 0.275	Depositor DCC
$R_{free}$ test set	1443 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	27.2	Xtriage
Anisotropy	0.261	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 54.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 29120 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	7034	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.53% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.39	0/1783	0.61	0/2422
1	B	0.37	0/1745	0.59	0/2370
1	C	0.39	0/1790	0.60	0/2432
1	D	0.37	0/1745	0.58	0/2370
All	All	0.38	0/7063	0.60	0/9594

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	1740	0	1773	98	0
1	B	1703	0	1735	63	0
1	C	1747	0	1780	71	0
1	D	1703	0	1735	82	0
2	A	42	0	0	1	0
2	B	33	0	0	2	0
2	C	29	0	0	1	0
2	D	37	0	0	0	0
All	All	7034	0	7023	307	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 22.

All (307) 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:A:52:PRO:HG3	1:A:152:GLY:HA2	1.12	1.07
1:C:79:VAL:HG21	1:C:160:ASN:HD21	1.18	1.05
1:C:52:PRO:HG2	1:C:152:GLY:HA2	1.43	0.97
1:C:79:VAL:HG21	1:C:160:ASN:ND2	1.79	0.96
1:A:52:PRO:CG	1:A:152:GLY:HA2	1.98	0.93
1:A:180:ILE:HD12	1:A:188:LEU:HD13	1.48	0.93
1:C:79:VAL:HG12	1:C:90:VAL:HG12	1.56	0.88
1:D:74:ARG:NH1	1:D:94:GLY:H	1.72	0.87
1:C:200:GLU:N	1:C:207:THR:HG22	1.90	0.85
1:A:52:PRO:HG3	1:A:152:GLY:CA	2.05	0.82
1:A:153:GLN:HE21	1:A:156:VAL:HG11	1.43	0.82
1:A:178:LYS:HD3	1:A:178:LYS:H	1.45	0.81
1:D:71:MET:HG3	1:D:92:GLN:NE2	1.94	0.81
1:C:229:GLU:H	1:C:229:GLU:CD	1.82	0.79
1:D:200:GLU:HG3	1:D:207:THR:HG22	1.66	0.77
1:B:90:VAL:HG21	1:B:163:LEU:HD11	1.67	0.75
1:C:52:PRO:CG	1:C:152:GLY:HA2	2.18	0.74
1:A:80:THR:HG22	1:A:104:HIS:NE2	2.02	0.74
1:A:70:ARG:O	1:A:180:ILE:HG22	1.88	0.73
1:D:155:MET:HG3	1:D:158:ARG:NH2	2.02	0.73
1:D:158:ARG:HG2	1:D:161:ARG:HH22	1.51	0.73
1:D:80:THR:HG22	1:D:104:HIS:NE2	2.04	0.73
1:A:200:GLU:N	1:A:207:THR:HG22	2.03	0.73
1:B:105:TRP:O	1:B:109:ILE:HG13	1.89	0.73
1:B:135:LEU:HD13	1:B:142:HIS:HB2	1.71	0.72
1:A:90:VAL:HG13	1:A:189:LEU:HD11	1.70	0.72
1:A:70:ARG:NH2	1:A:168:ARG:HG3	2.04	0.71
1:C:180:ILE:HD13	1:C:188:LEU:HD13	1.73	0.71
1:C:119:LYS:HD2	1:C:152:GLY:O	1.90	0.71
1:C:52:PRO:HG2	1:C:152:GLY:CA	2.20	0.71
1:C:146:ILE:HD12	1:C:147:PRO:CD	2.20	0.70
1:C:119:LYS:HZ1	1:C:145:GLY:HA3	1.56	0.70
1:B:198:HIS:ND1	1:B:209:ILE:HD13	2.06	0.70
1:A:133:GLU:HB3	1:A:137:ARG:HH21	1.56	0.69
1:C:88:ILE:H	1:C:197:ASN:HD21	1.38	0.69
1:C:135:LEU:HD13	1:C:142:HIS:HB2	1.74	0.69
1:A:88:ILE:H	1:A:197:ASN:HD21	1.41	0.69
1:D:88:ILE:H	1:D:197:ASN:HD21	1.40	0.69
1:C:200:GLU:H	1:C:207:THR:HG22	1.56	0.68
1:B:204:ASN:HD22	1:B:205:THR:H	1.41	0.68

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:135:LEU:HD13	1:D:142:HIS:HB2	1.74	0.68
1:D:111:VAL:HG12	1:D:112:LEU:HD12	1.76	0.68
1:C:178:LYS:HZ2	1:C:178:LYS:C	1.96	0.68
1:B:228:ILE:HG12	1:B:229:GLU:N	2.09	0.68
1:B:224:VAL:HG21	1:B:265:VAL:CG1	2.24	0.67
1:C:71:MET:HE3	1:C:180:ILE:HD12	1.75	0.67
1:A:51:ASN:HA	1:A:151:GLN:OE1	1.95	0.66
1:B:227:ARG:HH11	1:B:231:GLY:HA2	1.59	0.66
1:B:228:ILE:HG12	1:B:229:GLU:H	1.61	0.65
1:B:204:ASN:HD22	1:B:205:THR:N	1.94	0.65
1:C:119:LYS:HD3	1:C:120:THR:N	2.12	0.65
1:D:244:ARG:HA	1:D:244:ARG:HE	1.61	0.65
1:B:170:LEU:HB2	1:B:188:LEU:HD21	1.78	0.64
1:A:62:GLN:NE2	1:A:156:VAL:H	1.95	0.64
1:A:207:THR:H	1:A:210:GLN:NE2	1.96	0.64
1:D:132:ARG:HH11	1:D:132:ARG:HG3	1.61	0.64
1:C:146:ILE:HD12	1:C:147:PRO:HD2	1.79	0.64
1:B:85:SER:O	1:B:86:SER:OG	2.17	0.63
1:A:200:GLU:H	1:A:207:THR:HG22	1.63	0.63
1:B:70:ARG:O	1:B:180:ILE:HG23	1.98	0.63
1:A:146:ILE:HD13	1:A:147:PRO:N	2.14	0.63
1:D:90:VAL:HG21	1:D:163:LEU:HD11	1.81	0.63
1:A:230:THR:HG23	1:A:232:GLU:H	1.62	0.62
1:A:180:ILE:HD12	1:A:188:LEU:CD1	2.27	0.62
1:D:65:PHE:CE1	1:D:101:VAL:HG12	2.36	0.61
1:D:111:VAL:HG12	1:D:112:LEU:CD1	2.31	0.61
1:D:55:LEU:N	1:D:55:LEU:HD23	2.14	0.61
1:C:71:MET:CE	1:C:180:ILE:HD12	2.30	0.61
1:D:85:SER:O	1:D:86:SER:HB2	2.01	0.61
1:D:55:LEU:H	1:D:55:LEU:HD23	1.65	0.61
1:D:128:SER:O	1:D:132:ARG:HG2	2.01	0.60
1:A:85:SER:O	1:A:86:SER:HB3	1.99	0.60
1:A:83:THR:HA	1:A:155:MET:CE	2.32	0.60
1:B:161:ARG:HH21	1:B:161:ARG:HG3	1.67	0.60
1:B:180:ILE:HD12	1:B:181:PRO:HD2	1.83	0.60
1:D:81:VAL:HG21	1:D:159:ALA:HB2	1.84	0.59
1:D:81:VAL:HG13	1:D:88:ILE:HG22	1.84	0.59
1:B:254:THR:HG22	1:B:254:THR:O	2.03	0.59
1:B:128:SER:OG	1:B:131:THR:HG22	2.02	0.59
1:A:119:LYS:HD3	1:A:120:THR:N	2.17	0.59
1:A:67:LEU:O	1:A:164:LYS:NZ	2.34	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:155:MET:HG3	1:D:158:ARG:HH21	1.66	0.58
1:C:269:ILE:O	1:C:269:ILE:HG12	2.03	0.58
1:A:228:ILE:HG22	1:A:229:GLU:N	2.19	0.58
1:D:200:GLU:HG3	1:D:207:THR:CG2	2.33	0.58
1:B:98:SER:O	1:B:101:VAL:HG22	2.04	0.58
1:C:90:VAL:HG11	1:C:163:LEU:HD22	1.87	0.57
1:A:83:THR:HA	1:A:155:MET:HE2	1.85	0.57
1:A:197:ASN:O	1:A:208:PRO:HD2	2.05	0.56
1:A:180:ILE:HD13	1:A:185:GLN:HA	1.87	0.56
1:D:85:SER:OG	1:D:212:HIS:HD2	1.87	0.56
1:A:51:ASN:HA	1:A:151:GLN:CD	2.25	0.56
1:C:233:TRP:CD2	1:C:266:LYS:HE2	2.41	0.56
1:D:251:ASN:OD1	1:D:253:ASP:HB2	2.06	0.56
1:D:99:VAL:HG22	1:D:103:HIS:CE1	2.40	0.56
1:A:234:GLU:CD	1:A:237:TRP:HZ3	2.08	0.56
1:D:74:ARG:HH11	1:D:94:GLY:H	1.46	0.56
1:C:65:PHE:HE2	1:C:101:VAL:HG23	1.69	0.56
1:D:227:ARG:HA	1:D:232:GLU:O	2.05	0.56
1:A:81:VAL:HG21	1:A:159:ALA:HB2	1.87	0.55
1:A:261:PRO:HD2	1:A:264:LYS:HD2	1.87	0.55
1:D:223:PRO:HB3	1:D:252:ARG:NH2	2.20	0.55
1:C:227:ARG:HB3	1:C:264:LYS:HG3	1.87	0.55
1:C:90:VAL:HG11	1:C:163:LEU:CD2	2.37	0.55
1:D:98:SER:O	1:D:101:VAL:HG22	2.07	0.55
1:B:150:SER:HA	1:B:154:ALA:HB2	1.89	0.55
1:A:53:ARG:HB3	1:A:259:TRP:CZ2	2.41	0.55
1:C:163:LEU:O	1:C:167:ILE:HG12	2.07	0.54
1:D:132:ARG:NH1	1:D:132:ARG:HG3	2.23	0.54
1:B:224:VAL:HG21	1:B:265:VAL:HG12	1.89	0.54
1:D:223:PRO:HB3	1:D:252:ARG:HH22	1.72	0.54
1:B:142:HIS:CE1	1:B:144:THR:HG22	2.43	0.54
1:D:81:VAL:HG21	1:D:159:ALA:CB	2.38	0.54
1:C:178:LYS:NZ	1:C:179:ARG:O	2.41	0.54
1:D:150:SER:HA	1:D:154:ALA:HB2	1.90	0.53
1:C:65:PHE:CE2	1:C:101:VAL:HG23	2.42	0.53
1:A:135:LEU:HD12	1:A:140:ILE:HB	1.91	0.53
1:B:73:PRO:HD2	2:B:310:HOH:O	2.07	0.53
1:A:97:THR:O	1:A:101:VAL:HG23	2.07	0.53
1:D:120:THR:OG1	1:D:142:HIS:HE1	1.91	0.53
1:B:180:ILE:HG13	1:B:185:GLN:HG2	1.91	0.53
1:D:60:ILE:HG21	1:D:119:LYS:HE2	1.90	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:ARG:CZ	1:A:168:ARG:HG3	2.39	0.52
1:A:122:ASN:OD1	1:A:145:GLY:O	2.28	0.52
1:B:227:ARG:HA	1:B:232:GLU:O	2.09	0.52
1:D:114:ARG:NH2	1:D:139:GLY:O	2.41	0.52
1:A:194:TYR:CD1	1:A:198:HIS:CD2	2.97	0.52
1:C:178:LYS:H	1:C:178:LYS:NZ	2.07	0.52
1:B:161:ARG:HG3	1:B:161:ARG:NH2	2.24	0.52
1:D:238:ASN:HD21	1:D:252:ARG:HE	1.58	0.52
1:B:62:GLN:NE2	1:B:156:VAL:H	2.08	0.52
1:A:146:ILE:HD13	1:A:147:PRO:CD	2.40	0.51
1:A:146:ILE:HD13	1:A:147:PRO:HD2	1.92	0.51
1:A:158:ARG:HG3	1:A:158:ARG:HH11	1.75	0.51
1:A:178:LYS:HG2	1:A:179:ARG:N	2.26	0.51
1:D:74:ARG:NH1	1:D:94:GLY:N	2.51	0.51
1:A:218:LEU:HD12	1:A:218:LEU:N	2.25	0.51
1:A:81:VAL:HG21	1:A:159:ALA:CB	2.41	0.51
1:A:51:ASN:HD22	1:A:151:GLN:HG2	1.76	0.51
1:C:168:ARG:O	1:C:172:GLU:HG3	2.10	0.51
1:A:51:ASN:CG	1:A:52:PRO:HD2	2.31	0.51
1:C:229:GLU:OE1	1:C:229:GLU:N	2.41	0.50
1:B:65:PHE:CE2	1:B:96:VAL:HG13	2.46	0.50
1:D:88:ILE:HD12	1:D:88:ILE:C	2.32	0.50
1:B:225:LYS:HE3	1:B:267:PRO:O	2.11	0.50
1:C:251:ASN:HD22	1:C:254:THR:H	1.58	0.50
1:B:180:ILE:HD12	1:B:181:PRO:CD	2.41	0.50
1:C:226:ILE:HA	1:C:264:LYS:O	2.10	0.50
1:A:228:ILE:HG23	1:A:229:GLU:OE1	2.11	0.50
1:B:265:VAL:O	1:B:266:LYS:HG3	2.12	0.50
1:A:225:LYS:HA	1:A:234:GLU:O	2.11	0.50
1:A:218:LEU:CD1	1:A:218:LEU:N	2.74	0.50
1:B:251:ASN:OD1	1:B:253:ASP:HB2	2.12	0.49
1:A:178:LYS:CD	1:A:178:LYS:H	2.22	0.49
1:D:80:THR:HG22	1:D:104:HIS:CE1	2.46	0.49
1:B:114:ARG:NH2	1:B:139:GLY:O	2.35	0.49
1:A:180:ILE:HD11	1:A:184:LYS:O	2.13	0.49
1:D:80:THR:CG2	1:D:104:HIS:NE2	2.74	0.49
1:B:188:LEU:O	1:B:188:LEU:HD23	2.13	0.49
1:A:58:LEU:HD21	1:A:112:LEU:O	2.11	0.49
1:A:228:ILE:CG2	1:A:229:GLU:N	2.75	0.49
1:D:225:LYS:HD3	1:D:233:TRP:HB3	1.94	0.49
1:D:90:VAL:CG2	1:D:163:LEU:HD11	2.43	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:239:VAL:HG21	1:D:242:TRP:CE2	2.48	0.48
1:B:156:VAL:O	1:B:159:ALA:HB3	2.12	0.48
1:D:65:PHE:HE1	1:D:101:VAL:HG12	1.77	0.48
1:B:65:PHE:CD2	1:B:96:VAL:HG13	2.48	0.48
1:B:64:ASP:OD2	1:B:64:ASP:C	2.52	0.48
1:C:225:LYS:HA	1:C:234:GLU:O	2.12	0.48
1:B:239:VAL:HG11	1:B:242:TRP:CE2	2.48	0.48
1:C:71:MET:HE1	1:C:185:GLN:HG2	1.95	0.48
1:A:207:THR:H	1:A:210:GLN:HE21	1.60	0.48
1:D:195:ALA:O	1:D:199:LYS:HB2	2.13	0.48
1:D:74:ARG:HH11	1:D:94:GLY:N	2.11	0.48
1:D:92:GLN:HE22	1:D:185:GLN:NE2	2.12	0.48
1:C:116:LYS:HD2	2:C:302:HOH:O	2.14	0.47
1:C:142:HIS:CD2	1:C:143:THR:N	2.82	0.47
1:D:163:LEU:CD2	1:D:167:ILE:HD11	2.45	0.47
1:C:228:ILE:HG22	1:C:232:GLU:O	2.15	0.47
1:D:117:ALA:HB2	1:D:141:ALA:HB3	1.95	0.47
1:A:189:LEU:O	1:A:189:LEU:HD13	2.15	0.47
1:D:55:LEU:H	1:D:55:LEU:CD2	2.26	0.47
1:D:71:MET:CE	1:D:189:LEU:HD13	2.45	0.47
1:A:226:ILE:HA	1:A:264:LYS:O	2.14	0.47
1:B:178:LYS:HD2	1:B:178:LYS:C	2.35	0.47
1:B:135:LEU:HD13	1:B:142:HIS:CB	2.42	0.46
1:D:244:ARG:HG3	1:D:244:ARG:O	2.16	0.46
1:C:74:ARG:HB2	1:C:92:GLN:HE21	1.80	0.46
1:B:157:GLU:CD	1:B:161:ARG:HH22	2.17	0.46
1:D:201:ARG:HB3	1:D:204:ASN:OD1	2.15	0.46
1:B:198:HIS:CE1	1:B:209:ILE:HG21	2.51	0.46
1:C:225:LYS:HG2	1:C:235:LYS:HG2	1.97	0.46
1:D:194:TYR:O	1:D:198:HIS:HB2	2.16	0.46
1:C:92:GLN:HE22	1:C:185:GLN:NE2	2.13	0.46
1:C:74:ARG:CB	1:C:92:GLN:HE21	2.29	0.46
1:A:188:LEU:HD23	1:A:188:LEU:O	2.16	0.45
1:C:92:GLN:HE22	1:C:185:GLN:HE22	1.64	0.45
1:C:188:LEU:O	1:C:188:LEU:HD23	2.17	0.45
1:A:88:ILE:HG23	1:A:201:ARG:HH22	1.81	0.45
1:A:63:THR:HG22	1:A:64:ASP:N	2.31	0.45
1:A:51:ASN:ND2	1:A:151:GLN:HG2	2.32	0.45
1:C:53:ARG:CZ	1:C:155:MET:HE1	2.46	0.45
1:A:180:ILE:HG13	1:A:181:PRO:HD2	1.98	0.45
1:A:153:GLN:HE21	1:A:156:VAL:CG1	2.21	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:248:ALA:HB2	1:D:259:TRP:CH2	2.51	0.45
1:A:119:LYS:HE2	1:A:152:GLY:HA3	1.98	0.45
1:C:178:LYS:HZ2	1:C:178:LYS:CA	2.29	0.45
1:A:77:LEU:HD13	1:A:163:LEU:HD21	1.99	0.45
1:C:178:LYS:HB2	1:C:179:ARG:H	1.52	0.45
1:A:230:THR:HG23	1:A:232:GLU:HB2	1.98	0.45
1:A:71:MET:HE3	1:A:185:GLN:HB3	1.99	0.45
1:D:178:LYS:HB3	1:D:179:ARG:H	1.53	0.45
1:C:61:TRP:CE2	1:C:115:PRO:HB3	2.52	0.45
1:C:165:ASP:O	1:C:169:VAL:HG23	2.17	0.45
1:D:120:THR:O	1:D:144:THR:HA	2.17	0.44
1:A:65:PHE:CE2	1:A:101:VAL:HG22	2.52	0.44
1:C:79:VAL:HG12	1:C:90:VAL:CG1	2.39	0.44
1:C:106:ALA:HB2	1:D:187:GLU:HG3	1.99	0.44
1:A:65:PHE:CE2	1:A:96:VAL:HG13	2.53	0.44
1:A:106:ALA:CB	1:B:187:GLU:HG3	2.47	0.44
1:B:132:ARG:HH11	1:B:132:ARG:HG2	1.83	0.44
1:A:166:ARG:HD3	1:A:166:ARG:HA	1.79	0.44
1:A:129:LYS:HE2	1:A:133:GLU:OE2	2.18	0.44
1:A:226:ILE:HD11	1:A:237:TRP:CZ3	2.52	0.44
1:D:105:TRP:O	1:D:109:ILE:HG13	2.17	0.44
1:C:71:MET:CE	1:C:185:GLN:HG2	2.47	0.44
1:D:112:LEU:O	1:D:212:HIS:HE1	2.01	0.44
1:A:119:LYS:HD2	1:A:152:GLY:O	2.18	0.43
1:B:65:PHE:CE2	1:B:101:VAL:HG12	2.53	0.43
1:B:133:GLU:O	1:B:137:ARG:HG3	2.17	0.43
1:B:182:THR:HA	1:B:185:GLN:HG3	2.00	0.43
1:A:49:GLY:C	1:A:51:ASN:H	2.21	0.43
1:A:180:ILE:HD11	1:A:184:LYS:C	2.38	0.43
1:C:269:ILE:O	1:C:270:THR:C	2.56	0.43
1:D:228:ILE:HD11	1:D:232:GLU:HB2	1.99	0.43
1:C:209:ILE:HA	1:C:209:ILE:HD12	1.90	0.43
1:A:263:ARG:HG3	1:A:263:ARG:H	1.64	0.43
1:A:106:ALA:HB2	1:B:187:GLU:HG3	2.01	0.43
1:D:83:THR:HA	1:D:155:MET:CE	2.48	0.43
1:B:180:ILE:HD12	1:B:181:PRO:N	2.34	0.43
1:A:65:PHE:HE2	1:A:101:VAL:HG22	1.83	0.43
1:A:178:LYS:HD3	1:A:178:LYS:N	2.24	0.43
1:A:65:PHE:CD2	1:A:96:VAL:HG13	2.53	0.43
1:A:233:TRP:CD2	1:A:266:LYS:HE2	2.53	0.43
1:B:228:ILE:HG23	1:B:230:THR:H	1.83	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:THR:HG22	1:A:104:HIS:CE1	2.53	0.43
1:D:158:ARG:HG2	1:D:161:ARG:NH2	2.26	0.43
1:D:55:LEU:CD2	1:D:55:LEU:N	2.82	0.43
1:D:63:THR:HG22	1:D:64:ASP:N	2.34	0.43
1:D:71:MET:HG3	1:D:92:GLN:HE22	1.78	0.43
1:C:178:LYS:HZ1	1:C:178:LYS:H	1.65	0.43
1:B:257:VAL:HG23	1:B:257:VAL:O	2.18	0.43
1:D:68:GLU:HA	1:D:69:PRO:HD2	1.86	0.43
1:C:74:ARG:HB2	1:C:92:GLN:NE2	2.34	0.42
1:B:157:GLU:O	1:B:160:ASN:HB2	2.18	0.42
1:B:103:HIS:HB3	2:B:309:HOH:O	2.18	0.42
1:A:187:GLU:OE2	1:B:103:HIS:HD2	2.02	0.42
1:D:63:THR:HA	1:D:79:VAL:O	2.18	0.42
1:A:62:GLN:HE21	1:A:156:VAL:H	1.65	0.42
1:A:188:LEU:C	1:A:188:LEU:HD23	2.40	0.42
1:A:242:TRP:CZ2	1:B:244:ARG:HG2	2.54	0.42
1:D:99:VAL:HG22	1:D:103:HIS:NE2	2.34	0.42
1:D:248:ALA:HB2	1:D:259:TRP:CZ3	2.55	0.42
1:C:49:GLY:C	1:C:51:ASN:H	2.21	0.42
1:B:177:MET:H	1:B:178:LYS:NZ	2.18	0.42
1:A:166:ARG:NH1	2:A:304:HOH:O	2.52	0.42
1:C:220:GLU:OE2	1:C:250:LYS:NZ	2.51	0.42
1:C:53:ARG:HB3	1:C:259:TRP:CE2	2.54	0.42
1:A:256:LYS:HB3	1:A:256:LYS:HE2	1.83	0.42
1:D:88:ILE:H	1:D:197:ASN:ND2	2.13	0.42
1:A:163:LEU:HA	1:A:196:LEU:HD11	2.00	0.42
1:C:255:ASP:O	1:C:255:ASP:CG	2.58	0.42
1:C:151:GLN:H	1:C:151:GLN:CD	2.23	0.42
1:A:102:GLN:HG2	1:A:134:TRP:CG	2.54	0.42
1:D:121:ASP:HA	1:D:145:GLY:O	2.20	0.42
1:D:163:LEU:HD22	1:D:167:ILE:HD11	2.02	0.41
1:C:106:ALA:CB	1:D:187:GLU:HG3	2.50	0.41
1:A:267:PRO:HB3	1:B:259:TRP:CD2	2.55	0.41
1:C:79:VAL:CG2	1:C:160:ASN:HD21	2.08	0.41
1:B:105:TRP:CZ2	1:B:118:ILE:HG21	2.55	0.41
1:C:88:ILE:HD11	1:C:163:LEU:HD13	2.03	0.41
1:A:166:ARG:O	1:A:170:LEU:HG	2.20	0.41
1:B:63:THR:HA	1:B:79:VAL:O	2.20	0.41
1:C:119:LYS:C	1:C:119:LYS:HD3	2.41	0.41
1:B:170:LEU:CB	1:B:188:LEU:HD21	2.48	0.41
1:D:65:PHE:CZ	1:D:101:VAL:HG12	2.55	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:ALA:HB2	1:A:141:ALA:HB3	2.02	0.41
1:A:234:GLU:OE1	1:A:237:TRP:HZ3	2.04	0.41
1:D:176:PHE:CZ	1:D:184:LYS:HD3	2.56	0.41
1:D:244:ARG:CA	1:D:244:ARG:HE	2.27	0.41
1:A:61:TRP:CD1	1:A:82:ASP:HA	2.56	0.41
1:D:146:ILE:HG13	1:D:149:ASN:HB3	2.03	0.41
1:C:229:GLU:CD	1:C:229:GLU:N	2.61	0.40
1:B:163:LEU:HA	1:B:196:LEU:HD11	2.03	0.40
1:C:178:LYS:HZ2	1:C:179:ARG:N	2.18	0.40
1:B:181:PRO:O	1:B:185:GLN:HG3	2.21	0.40
1:A:105:TRP:CZ3	1:A:135:LEU:HD21	2.56	0.40
1:A:220:GLU:HA	1:A:220:GLU:OE1	2.21	0.40
1:C:68:GLU:O	1:C:75:SER:HB2	2.20	0.40
1:B:201:ARG:HG3	1:B:201:ARG:HH11	1.86	0.40
1:D:207:THR:OG1	1:D:210:GLN:HG3	2.22	0.40
1:C:146:ILE:HD12	1:C:147:PRO:N	2.35	0.40
1:D:170:LEU:HD13	1:D:191:LYS:HB3	2.04	0.40
1:C:58:LEU:HD21	1:C:112:LEU:O	2.22	0.40
1:D:166:ARG:HA	1:D:169:VAL:HG22	2.03	0.40
1:B:138:TRP:HB3	1:B:140:ILE:HG13	2.02	0.40
1:A:233:TRP:CG	1:A:266:LYS:HE2	2.57	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	219/238 (92%)	202 (92%)	14 (6%)	3 (1%)	14	23
1	B	214/238 (90%)	200 (94%)	14 (6%)	0	100	100
1	C	220/238 (92%)	201 (91%)	16 (7%)	3 (1%)	14	23
1	D	214/238 (90%)	201 (94%)	11 (5%)	2 (1%)	21	37

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	867/952 (91%)	804 (93%)	55 (6%)	8 (1%)	21	37

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	50	VAL
1	A	151	GLN
1	C	50	VAL
1	C	151	GLN
1	A	200	GLU
1	C	200	GLU
1	D	55	LEU
1	D	73	PRO

### 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	183/198 (92%)	171 (93%)	12 (7%)	21	36
1	B	179/198 (90%)	169 (94%)	10 (6%)	26	45
1	C	184/198 (93%)	169 (92%)	15 (8%)	14	26
1	D	179/198 (90%)	172 (96%)	7 (4%)	39	64
All	All	725/792 (92%)	681 (94%)	44 (6%)	23	40

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	LEU
1	A	80	THR
1	A	86	SER
1	A	103	HIS
1	A	146	ILE
1	A	151	GLN
1	A	155	MET

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	178	LYS
1	A	205	THR
1	A	210	GLN
1	A	237	TRP
1	A	265	VAL
1	B	92	GLN
1	B	95	ARG
1	B	132	ARG
1	B	163	LEU
1	B	174	ASP
1	B	178	LYS
1	B	180	ILE
1	B	201	ARG
1	B	204	ASN
1	B	235	LYS
1	C	66	THR
1	C	67	LEU
1	C	77	LEU
1	C	116	LYS
1	C	146	ILE
1	C	157	GLU
1	C	158	ARG
1	C	170	LEU
1	C	177	MET
1	C	178	LYS
1	C	203	GLU
1	C	229	GLU
1	C	255	ASP
1	C	263	ARG
1	C	265	VAL
1	D	55	LEU
1	D	80	THR
1	D	88	ILE
1	D	155	MET
1	D	157	GLU
1	D	229	GLU
1	D	244	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	92	GLN
1	A	153	GLN
1	A	197	ASN
1	A	198	HIS
1	A	210	GLN
1	A	251	ASN
1	B	62	GLN
1	B	92	GLN
1	B	103	HIS
1	B	160	ASN
1	B	204	ASN
1	C	92	GLN
1	C	153	GLN
1	C	160	ASN
1	C	185	GLN
1	C	197	ASN
1	C	251	ASN
1	D	92	GLN
1	D	142	HIS
1	D	160	ASN
1	D	185	GLN
1	D	197	ASN
1	D	212	HIS
1	D	238	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

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	221/238 (92%)	0.16	15 (6%) 20 23	10, 26, 51, 60	0
1	B	216/238 (90%)	0.13	8 (3%) 45 51	18, 29, 47, 55	0
1	C	222/238 (93%)	0.18	17 (7%) 16 18	10, 26, 51, 59	0
1	D	216/238 (90%)	0.11	11 (5%) 32 37	18, 29, 47, 50	0
All	All	875/952 (91%)	0.15	51 (5%) 26 30	10, 28, 48, 60	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	50	VAL	7.7
1	A	202	GLY	6.6
1	A	147	PRO	6.4
1	D	54	GLY	6.4
1	C	150	SER	6.1
1	C	202	GLY	6.0
1	A	150	SER	5.9
1	C	50	VAL	5.7
1	C	149	ASN	5.7
1	C	148	GLY	4.9
1	C	147	PRO	4.8
1	C	146	ILE	4.6
1	B	230	THR	4.5
1	A	203	GLU	4.4
1	A	204	ASN	4.4
1	D	55	LEU	4.2
1	C	151	GLN	4.2
1	D	201	ARG	4.1
1	A	146	ILE	4.0
1	A	149	ASN	3.9
1	C	204	ASN	3.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	203	GLU	3.7
1	C	203	GLU	3.7
1	B	269	ILE	3.5
1	A	145	GLY	3.5
1	A	269	ILE	3.5
1	C	49	GLY	3.5
1	C	270	THR	3.5
1	D	204	ASN	3.4
1	B	55	LEU	3.4
1	A	230	THR	3.3
1	D	205	THR	3.2
1	D	203	GLU	3.2
1	C	269	ILE	3.2
1	C	52	PRO	3.1
1	A	151	GLN	3.1
1	B	54	GLY	3.1
1	D	146	ILE	3.0
1	D	150	SER	3.0
1	A	49	GLY	2.8
1	C	253	ASP	2.8
1	A	51	ASN	2.5
1	A	148	GLY	2.5
1	B	263	ARG	2.4
1	D	230	THR	2.4
1	C	145	GLY	2.3
1	C	51	ASN	2.2
1	D	147	PRO	2.1
1	B	204	ASN	2.1
1	D	151	GLN	2.1
1	B	254	THR	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 ⓘ

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.