



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 02:28 pm GMT

PDB ID : 1QAI  
Title : CRYSTAL STRUCTURES OF THE N-TERMINAL FRAGMENT FROM  
MOLONEY MURINE LEUKEMIA VIRUS REVERSE TRANSCRIPTASE  
COMPLEXED WITH NUCLEIC ACID: FUNCTIONAL IMPLICATIONS  
FOR TEMPLATE-PRIMER BINDING TO THE FINGERS DOMAIN  
Authors : Najmudin, S.; Cote, M.; Sun, D.; Yohannan, S.; Montano, S.P.; Gu, J.; Geor-  
giadis, M.M.  
Deposited on : 1999-03-12  
Resolution : 2.30 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  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
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) : recalc28949

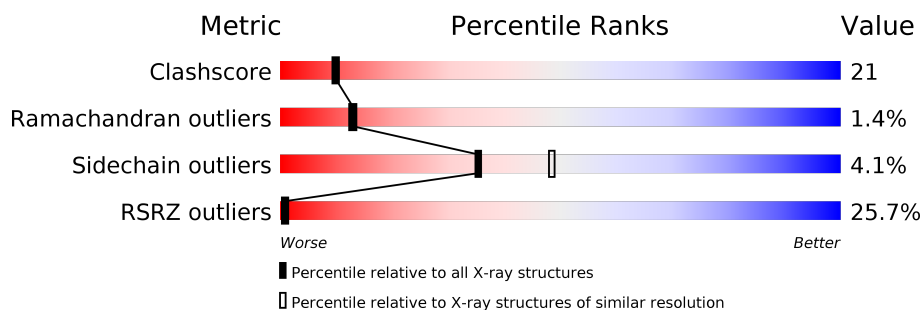
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (2.30-2.30)

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	C	8	
1	D	8	
2	A	265	
2	B	265	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4623 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 DNA chain called DNA (5'-D(\*CP\*AP\*TP\*GP\*CP\*AP\*TP\*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	8	Total	C	N	O	P	0	0	0
			161	78	30	46	7			
1	D	8	Total	C	N	O	P	0	0	0
			161	78	30	46	7			

- Molecule 2 is a protein called REVERSE TRANSCRIPTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	251	Total	C	N	O	S	0	0	0
			2008	1293	348	360	7			
2	B	251	Total	C	N	O	S	0	0	0
			2008	1293	348	360	7			

- Molecule 3 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Hg	0	0
			2	2		
3	A	2	Total	Hg	0	0
			2	2		

- Molecule 4 is water.

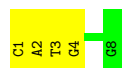
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	187	Total	O	0	0
			187	187		
4	B	79	Total	O	0	0
			79	79		
4	C	4	Total	O	0	0
			4	4		
4	D	11	Total	O	0	0
			11	11		

### 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 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: DNA (5'-D(\*CP\*AP\*TP\*GP\*CP\*AP\*TP\*G)-3')

Chain C: 



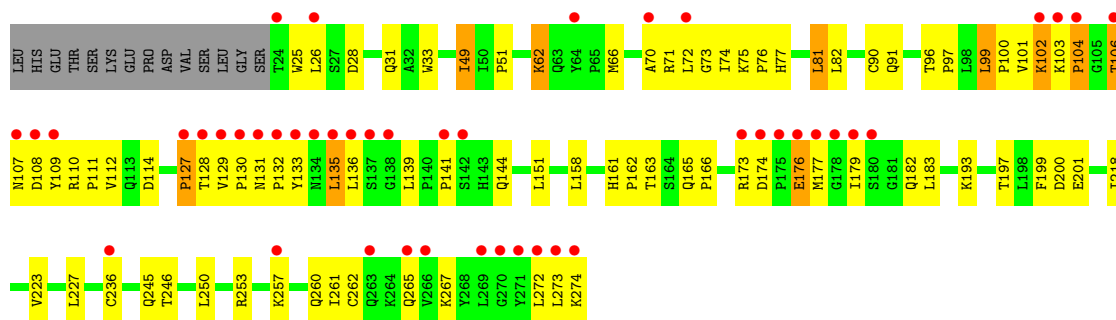
- Molecule 1: DNA (5'-D(\*CP\*AP\*TP\*GP\*CP\*AP\*TP\*G)-3')

Chain D: 



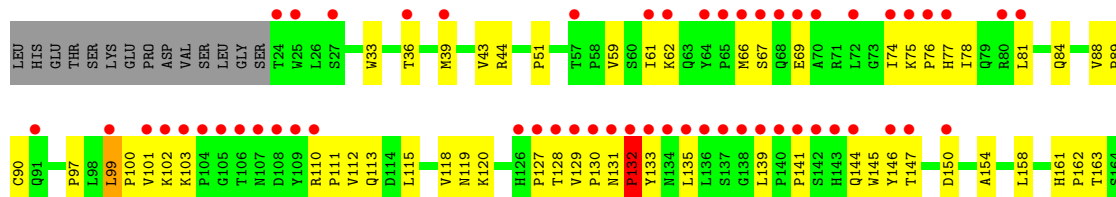
- Molecule 2: REVERSE TRANSCRIPTASE

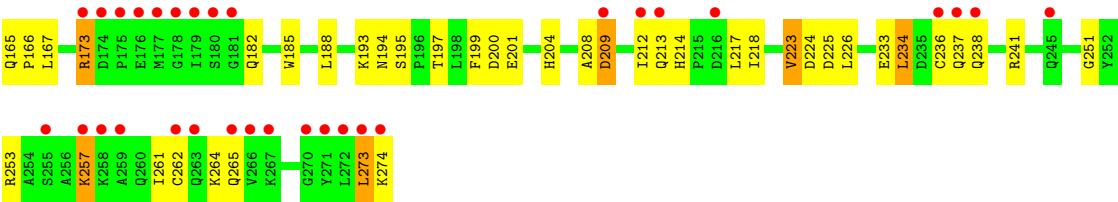
Chain A: 



- Molecule 2: REVERSE TRANSCRIPTASE

Chain B: 





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	61.14Å 38.43Å 129.75Å 90.00° 100.58° 90.00°	Depositor
Resolution (Å)	10.00 – 2.30 9.99 – 2.30	Depositor EDS
% Data completeness (in resolution range)	90.0 (10.00-2.30) 91.2 (9.99-2.30)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.37 (at 2.31Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.233 , 0.296 0.234 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	26.4	Xtriage
Anisotropy	0.640	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 78.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	4623	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: HG

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	C	0.27	0/180	0.62	0/276
1	D	0.31	0/180	0.65	0/276
2	A	0.39	0/2064	0.67	0/2815
2	B	0.30	0/2064	0.60	0/2815
All	All	0.35	0/4488	0.64	0/6182

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	C	161	0	92	9	0
1	D	161	0	92	3	0
2	A	2008	0	2024	79	0
2	B	2008	0	2025	89	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	187	0	0	10	0
4	B	79	0	0	5	0
4	C	4	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	11	0	0	1	0
All	All	4623	0	4233	180	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 21.

All (180) 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)
2:B:74:ILE:HG23	2:B:111:PRO:HG3	1.32	1.05
2:B:102:LYS:H	2:B:102:LYS:HD2	1.28	0.97
2:A:179:ILE:HD12	2:A:183:LEU:HD21	1.49	0.93
2:B:62:LYS:HD2	2:B:62:LYS:H	1.31	0.92
2:A:127:PRO:HG3	2:A:197:THR:CG2	2.00	0.92
2:A:128:THR:O	2:A:130:PRO:HD3	1.71	0.88
2:A:127:PRO:HG3	2:A:197:THR:HG23	1.56	0.86
2:B:103:LYS:HG3	2:B:110:ARG:HD2	1.58	0.86
2:A:74:ILE:HG23	2:A:111:PRO:HG3	1.59	0.84
2:A:236:CYS:HG	2:A:262:CYS:HG	0.87	0.82
2:A:161:HIS:CD2	2:A:163:THR:HG23	2.14	0.81
2:A:71:ARG:NH2	2:A:173:ARG:H	1.78	0.81
2:B:236:CYS:HG	2:B:262:CYS:HG	1.28	0.80
2:A:71:ARG:HH21	2:A:173:ARG:H	1.31	0.76
2:B:173:ARG:HE	2:B:173:ARG:N	1.82	0.76
2:A:139:LEU:HD23	2:A:218:ILE:HG21	1.67	0.76
2:B:223:VAL:HG22	4:B:949:HOH:O	1.86	0.75
2:A:161:HIS:HD2	2:A:163:THR:H	1.32	0.75
2:A:102:LYS:N	2:A:102:LYS:HD2	2.01	0.74
1:D:1:DC:H2''	1:D:2:DA:H5'	1.71	0.73
1:C:1:DC:H2''	1:C:2:DA:H5'	1.69	0.73
2:B:161:HIS:CD2	2:B:163:THR:HG23	2.25	0.72
2:B:173:ARG:HE	2:B:173:ARG:H	1.37	0.72
2:A:101:VAL:HG11	2:A:110:ARG:HH21	1.56	0.71
2:A:102:LYS:HE2	2:A:109:TYR:HE1	1.55	0.70
2:B:188:LEU:HD22	2:B:195:SER:OG	1.91	0.70
2:B:158:LEU:HD12	2:B:188:LEU:HD12	1.72	0.70
2:B:146:TYR:O	2:B:262:CYS:HA	1.91	0.70
2:A:102:LYS:HD2	2:A:102:LYS:H	1.57	0.69
2:A:77:HIS:O	2:A:81:LEU:HD22	1.93	0.68
2:A:128:THR:O	2:A:130:PRO:CD	2.40	0.68
1:D:1:DC:H2''	1:D:2:DA:C5'	2.23	0.68

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:245:GLN:HG2	4:A:1039:HOH:O	1.93	0.67
2:A:99:LEU:HD21	2:A:114:ASP:HB2	1.76	0.66
2:A:274:LYS:O	2:A:274:LYS:HD2	1.96	0.66
2:B:197:THR:O	2:B:201:GLU:HG3	1.97	0.65
1:C:2:DA:H1'	1:C:3:DT:H5''	1.79	0.65
2:A:127:PRO:HG3	2:A:197:THR:HG21	1.78	0.64
2:A:129:VAL:HG13	4:A:1026:HOH:O	1.97	0.64
2:B:161:HIS:HD2	2:B:163:THR:H	1.46	0.64
1:C:2:DA:H2''	1:C:3:DT:C5'	2.29	0.63
2:B:193:LYS:HG3	2:B:194:ASN:N	2.14	0.62
2:A:132:PRO:HA	2:A:135:LEU:HB3	1.82	0.61
2:B:62:LYS:CD	2:B:62:LYS:H	2.09	0.61
2:A:127:PRO:HB3	4:A:1026:HOH:O	2.00	0.61
2:A:129:VAL:HA	4:A:1046:HOH:O	2.00	0.61
2:B:67:SER:HB2	2:B:69:GLU:HG2	1.83	0.61
2:B:33:TRP:HH2	2:B:261:ILE:HD11	1.66	0.60
2:B:75:LYS:HG3	4:B:910:HOH:O	2.01	0.60
2:B:200:ASP:HB2	4:B:949:HOH:O	2.02	0.59
2:B:61:ILE:HB	2:B:97:PRO:HD3	1.83	0.59
2:B:75:LYS:N	2:B:76:PRO:HD2	2.17	0.59
2:A:136:LEU:O	2:A:136:LEU:HD13	2.02	0.58
2:B:77:HIS:O	2:B:81:LEU:HD13	2.03	0.58
2:A:176:GLU:CD	2:A:176:GLU:H	2.07	0.58
2:A:103:LYS:HB2	2:A:104:PRO:HD2	1.85	0.58
1:C:3:DT:H2''	1:C:4:DG:C8	2.39	0.58
2:A:49:ILE:HG23	4:A:1008:HOH:O	2.02	0.58
2:B:102:LYS:HD2	2:B:102:LYS:N	2.10	0.57
2:B:43:VAL:HG23	2:B:44:ARG:HG3	1.87	0.57
2:B:66:MET:CE	2:B:100:PRO:HD2	2.34	0.57
2:B:214:HIS:HB3	2:B:217:LEU:HD12	1.86	0.57
2:B:90:CYS:O	2:B:182:GLN:HB2	2.04	0.57
2:B:74:ILE:CG2	2:B:111:PRO:HG3	2.23	0.56
2:B:273:LEU:HD13	2:B:273:LEU:N	2.20	0.56
2:A:129:VAL:O	2:A:129:VAL:HG23	2.06	0.56
2:A:179:ILE:CD1	2:A:183:LEU:HD21	2.31	0.55
2:A:174:ASP:OD1	2:A:177:MET:HB2	2.07	0.55
2:B:131:ASN:N	2:B:132:PRO:CD	2.70	0.54
2:B:101:VAL:HB	2:B:112:VAL:HG21	1.90	0.54
2:A:161:HIS:CD2	2:A:162:PRO:HD2	2.42	0.54
2:A:25:TRP:CE2	2:A:261:ILE:HG21	2.43	0.54
4:D:180:HOH:O	2:B:120:LYS:HE3	2.08	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:66:MET:HE2	2:B:100:PRO:HD2	1.90	0.53
2:A:90:CYS:O	2:A:182:GLN:HB2	2.07	0.53
2:B:234:LEU:O	2:B:238:GLN:HG2	2.07	0.53
2:B:51:PRO:HD2	4:B:973:HOH:O	2.07	0.53
2:A:197:THR:O	2:A:201:GLU:HG3	2.08	0.53
2:B:62:LYS:HD2	2:B:62:LYS:N	2.13	0.53
1:C:2:DA:C2'	1:C:3:DT:H5''	2.39	0.53
2:B:74:ILE:HG22	2:B:78:ILE:HG12	1.91	0.53
2:A:158:LEU:HD11	2:A:199:PHE:HA	1.90	0.52
1:C:2:DA:H2''	1:C:3:DT:H5'	1.91	0.52
2:A:161:HIS:HD2	2:A:163:THR:HG23	1.73	0.52
2:B:129:VAL:HG11	2:B:204:HIS:NE2	2.25	0.52
2:B:88:VAL:HG13	2:B:89:PRO:HD2	1.92	0.52
2:A:75:LYS:HB3	2:A:76:PRO:HD3	1.91	0.51
2:B:77:HIS:NE2	2:B:110:ARG:NH1	2.58	0.51
2:B:233:GLU:O	2:B:237:GLN:HG3	2.09	0.51
2:A:131:ASN:OD1	2:A:133:TYR:HB3	2.11	0.51
2:A:106:THR:HG22	2:A:107:ASN:N	2.26	0.50
2:A:227:LEU:C	2:A:227:LEU:HD23	2.31	0.50
1:C:2:DA:H2''	1:C:3:DT:H5''	1.94	0.50
2:A:101:VAL:HG21	2:A:112:VAL:HG21	1.94	0.49
2:B:59:VAL:HG13	2:B:59:VAL:O	2.12	0.49
2:A:129:VAL:HG12	2:A:200:ASP:OD2	2.11	0.49
2:B:257:LYS:HZ3	2:B:257:LYS:HB2	1.76	0.49
2:A:132:PRO:O	2:A:136:LEU:N	2.44	0.49
2:B:118:VAL:HG13	2:B:167:LEU:HD11	1.95	0.49
1:C:2:DA:C1'	1:C:3:DT:H5''	2.43	0.49
2:B:173:ARG:HB3	4:B:981:HOH:O	2.13	0.49
2:A:106:THR:C	2:A:108:ASP:H	2.17	0.48
2:B:237:GLN:O	2:B:241:ARG:HG3	2.13	0.48
2:B:141:PRO:O	2:B:144:GLN:HG3	2.14	0.48
2:A:103:LYS:HB2	2:A:104:PRO:CD	2.45	0.47
2:B:131:ASN:H	2:B:132:PRO:CD	2.27	0.47
2:B:133:TYR:C	2:B:135:LEU:H	2.17	0.47
2:B:89:PRO:O	2:B:90:CYS:HB3	2.14	0.47
2:A:26:LEU:HA	2:A:33:TRP:CD1	2.50	0.47
2:A:141:PRO:O	2:A:144:GLN:HG3	2.15	0.47
2:B:110:ARG:HH11	2:B:110:ARG:HG2	1.80	0.47
2:A:101:VAL:HG11	2:A:110:ARG:NH2	2.26	0.47
2:A:31:GLN:O	2:A:253:ARG:NH1	2.48	0.47
2:B:128:THR:O	2:B:128:THR:HG22	2.15	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:139:LEU:CD2	2:B:218:ILE:HG21	2.45	0.46
1:D:1:DC:H1'	1:D:2:DA:H5''	1.98	0.46
2:B:257:LYS:HA	2:B:257:LYS:NZ	2.30	0.46
2:B:158:LEU:HD11	2:B:199:PHE:HA	1.96	0.46
2:B:36:THR:O	2:B:36:THR:HG22	2.17	0.45
2:A:260:GLN:NE2	2:A:267:LYS:O	2.49	0.45
2:A:272:LEU:HD23	2:A:273:LEU:N	2.31	0.45
2:B:165:GLN:N	2:B:166:PRO:CD	2.79	0.45
2:A:66:MET:CE	2:A:100:PRO:HG3	2.46	0.45
2:B:39:MET:HG3	2:B:84:GLN:CD	2.37	0.45
2:A:71:ARG:HH21	2:A:173:ARG:N	2.06	0.45
2:A:99:LEU:HD22	2:A:99:LEU:N	2.30	0.45
2:B:131:ASN:N	2:B:132:PRO:HD2	2.32	0.44
2:B:257:LYS:HA	2:B:257:LYS:HZ2	1.81	0.44
2:B:88:VAL:HG12	2:B:89:PRO:O	2.17	0.44
2:B:208:ALA:O	2:B:212:ILE:HD13	2.17	0.44
2:A:82:LEU:HD11	2:A:179:ILE:HD11	1.99	0.44
2:A:73:GLY:O	2:A:76:PRO:HD2	2.18	0.44
2:A:81:LEU:HD13	4:A:925:HOH:O	2.17	0.44
2:A:132:PRO:O	2:A:136:LEU:HB2	2.17	0.44
2:B:99:LEU:N	2:B:99:LEU:HD23	2.33	0.44
2:A:265:GLN:HA	2:A:273:LEU:O	2.18	0.44
2:A:151:LEU:HD12	2:A:199:PHE:HZ	1.83	0.43
2:B:119:ASN:O	2:B:193:LYS:NZ	2.46	0.43
2:B:101:VAL:HG12	2:B:102:LYS:O	2.17	0.43
2:B:66:MET:HE3	2:B:100:PRO:HD2	2.01	0.43
2:A:193:LYS:HD2	4:A:951:HOH:O	2.18	0.43
2:B:225:ASP:C	2:B:226:LEU:HD12	2.39	0.43
2:B:161:HIS:CD2	2:B:163:THR:H	2.32	0.43
2:B:150:ASP:HA	2:B:224:ASP:O	2.18	0.43
2:A:70:ALA:HA	2:A:109:TYR:CD2	2.54	0.42
2:A:99:LEU:HA	2:A:100:PRO:HD3	1.89	0.42
2:B:251:GLY:O	2:B:253:ARG:NH1	2.53	0.42
2:B:241:ARG:HG2	2:B:241:ARG:HH11	1.84	0.42
2:B:265:GLN:CD	2:B:274:LYS:HB3	2.40	0.42
2:B:273:LEU:HD13	2:B:273:LEU:H	1.81	0.42
2:A:51:PRO:HD2	4:A:954:HOH:O	2.19	0.42
2:A:272:LEU:C	2:A:272:LEU:HD23	2.40	0.42
2:A:62:LYS:CA	2:A:62:LYS:HE3	2.50	0.42
2:B:139:LEU:C	2:B:139:LEU:HD13	2.40	0.42
2:A:49:ILE:HG13	2:A:49:ILE:O	2.16	0.42

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:39:MET:HG3	2:B:84:GLN:OE1	2.20	0.42
2:A:128:THR:O	2:A:128:THR:HG22	2.20	0.41
2:A:132:PRO:HA	2:A:135:LEU:CB	2.50	0.41
2:B:162:PRO:HA	2:B:165:GLN:HG3	2.02	0.41
2:A:165:GLN:N	2:A:166:PRO:CD	2.83	0.41
2:B:135:LEU:C	2:B:135:LEU:HD13	2.40	0.41
2:B:214:HIS:CB	2:B:217:LEU:HD12	2.49	0.41
2:B:74:ILE:HG23	2:B:111:PRO:CG	2.24	0.41
2:A:110:ARG:NH1	4:A:1035:HOH:O	2.53	0.41
2:A:26:LEU:HD12	2:A:26:LEU:N	2.36	0.41
2:A:96:THR:HA	2:A:97:PRO:HD3	1.86	0.41
2:B:145:TRP:CZ3	2:B:233:GLU:HB2	2.55	0.41
2:B:154:ALA:HB1	2:B:199:PHE:CZ	2.56	0.41
2:A:99:LEU:HD21	2:A:114:ASP:CB	2.48	0.41
2:B:129:VAL:HA	2:B:130:PRO:HD3	1.86	0.41
1:C:1:DC:H2''	1:C:2:DA:C5'	2.45	0.41
2:B:113:GLN:HG2	2:B:115:LEU:HG	2.03	0.40
2:A:246:THR:HG22	2:A:250:LEU:CD1	2.51	0.40
2:B:147:THR:OG1	2:B:262:CYS:SG	2.77	0.40
2:B:209:ASP:O	2:B:213:GLN:HG3	2.21	0.40
2:B:81:LEU:HD23	2:B:185:TRP:CZ3	2.57	0.40
2:A:62:LYS:HA	2:A:62:LYS:HE3	2.03	0.40
2:B:131:ASN:O	2:B:132:PRO:C	2.59	0.40
2:B:173:ARG:H	2:B:173:ARG:NE	2.14	0.40
2:A:91:GLN:NE2	4:A:978:HOH:O	2.54	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
2	A	249/265 (94%)	227 (91%)	18 (7%)	4 (2%)	<b>11</b> <b>10</b>

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	249/265 (94%)	221 (89%)	25 (10%)	3 (1%)	15	16
All	All	498/530 (94%)	448 (90%)	43 (9%)	7 (1%)	13	13

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	106	THR
2	A	104	PRO
2	A	127	PRO
2	A	223	VAL
2	B	127	PRO
2	B	223	VAL
2	B	132	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	
2	A	221/234 (94%)	211 (96%)	10 (4%)	32	44
2	B	221/234 (94%)	213 (96%)	8 (4%)	40	55
All	All	442/468 (94%)	424 (96%)	18 (4%)	35	48

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	28	ASP
2	A	49	ILE
2	A	62	LYS
2	A	72	LEU
2	A	81	LEU
2	A	99	LEU
2	A	102	LYS
2	A	135	LEU
2	A	176	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	A	257	LYS
2	B	99	LEU
2	B	132	PRO
2	B	173	ARG
2	B	209	ASP
2	B	234	LEU
2	B	257	LYS
2	B	264	LYS
2	B	273	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	68	GLN
2	A	84	GLN
2	A	91	GLN
2	A	107	ASN
2	A	134	ASN
2	A	161	HIS
2	A	190	GLN
2	A	237	GLN
2	A	249	ASN
2	B	131	ASN
2	B	134	ASN
2	B	144	GLN
2	B	161	HIS
2	B	237	GLN
2	B	245	GLN
2	B	249	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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	C	8/8 (100%)	0.82	0 100 100	38, 45, 52, 57	0
1	D	8/8 (100%)	0.98	1 (12%) 4 6	27, 49, 63, 75	0
2	A	251/265 (94%)	0.75	45 (17%) 2 2	5, 25, 81, 98	0
2	B	251/265 (94%)	1.83	87 (34%) 0 0	18, 48, 97, 100	0
All	All	518/546 (94%)	1.28	133 (25%) 1 1	5, 37, 94, 100	0

All (133) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	135	LEU	11.3
2	B	134	ASN	10.8
2	B	174	ASP	10.3
2	B	128	THR	9.9
2	B	179	ILE	9.8
2	A	130	PRO	8.6
2	B	178	GLY	8.6
2	A	178	GLY	8.5
2	B	105	GLY	8.0
2	B	131	ASN	7.9
2	A	132	PRO	7.7
2	A	131	ASN	7.6
2	B	106	THR	7.5
2	A	135	LEU	7.0
2	B	137	SER	7.0
2	B	67	SER	6.8
2	A	128	THR	6.6
2	B	132	PRO	6.5
2	B	109	TYR	6.3
2	A	106	THR	6.2
2	A	177	MET	6.1

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	A	129	VAL	6.0
2	B	180	SER	5.7
2	B	104	PRO	5.7
2	A	174	ASP	5.6
2	A	104	PRO	5.6
2	A	133	TYR	5.5
2	B	133	TYR	5.5
2	A	271	TYR	5.5
2	B	138	GLY	5.5
2	B	130	PRO	5.4
2	B	216	ASP	5.4
2	B	262	CYS	5.4
2	A	134	ASN	5.3
2	A	103	LYS	5.2
2	B	74	ILE	5.0
2	B	66	MET	5.0
2	B	69	GLU	4.8
2	B	274	LYS	4.8
2	B	177	MET	4.7
2	A	179	ILE	4.7
2	A	274	LYS	4.6
2	B	65	PRO	4.6
2	B	129	VAL	4.6
2	B	266	VAL	4.6
2	A	107	ASN	4.4
2	B	271	TYR	4.4
2	B	139	LEU	4.1
2	B	176	GLU	4.1
2	B	175	PRO	4.1
2	A	102	LYS	3.9
2	B	259	ALA	3.8
2	B	91	GLN	3.8
2	B	140	PRO	3.8
2	B	64	TYR	3.8
2	B	181	GLY	3.7
2	B	272	LEU	3.7
2	B	107	ASN	3.6
2	B	110	ARG	3.6
2	B	76	PRO	3.6
2	B	267	LYS	3.6
2	B	273	LEU	3.6
2	B	102	LYS	3.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	B	77	HIS	3.5
2	B	27	SER	3.5
2	B	70	ALA	3.5
2	B	75	LYS	3.5
2	A	109	TYR	3.4
2	B	143	HIS	3.4
2	B	68	GLN	3.4
2	A	70	ALA	3.4
2	B	173	ARG	3.4
2	B	24	THR	3.3
2	B	147	THR	3.3
2	B	127	PRO	3.2
2	B	144	GLN	3.2
2	B	136	LEU	3.2
2	B	108	ASP	3.2
2	B	142	SER	3.2
2	B	141	PRO	3.1
2	A	137	SER	3.1
2	B	209	ASP	3.1
2	A	127	PRO	3.1
2	A	272	LEU	3.1
2	A	265	GLN	3.0
2	B	80	ARG	3.0
2	B	36	THR	2.9
2	A	138	GLY	2.9
2	B	257	LYS	2.9
2	B	263	GLN	2.8
2	A	173	ARG	2.7
2	B	103	LYS	2.7
2	A	141	PRO	2.6
2	B	72	LEU	2.6
2	A	257	LYS	2.6
2	A	175	PRO	2.6
2	A	270	GLY	2.5
2	B	126	HIS	2.5
2	A	236	CYS	2.5
2	A	266	VAL	2.5
2	B	212	ILE	2.5
2	A	180	SER	2.4
2	A	269	LEU	2.4
2	B	265	GLN	2.4
2	B	258	LYS	2.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	B	62	LYS	2.4
2	B	245	GLN	2.4
2	A	136	LEU	2.4
2	B	81	LEU	2.4
2	A	64	TYR	2.3
2	B	39	MET	2.3
2	A	72	LEU	2.3
2	B	57	THR	2.3
2	B	213	GLN	2.2
2	A	142	SER	2.2
1	D	1	DC	2.2
2	A	176	GLU	2.2
2	B	99	LEU	2.2
2	B	150	ASP	2.2
2	B	101	VAL	2.1
2	B	238	GLN	2.1
2	B	146	TYR	2.1
2	A	24	THR	2.1
2	B	270	GLY	2.1
2	B	255	SER	2.1
2	A	26	LEU	2.1
2	A	273	LEU	2.1
2	B	237	GLN	2.1
2	A	263	GLN	2.1
2	B	236	CYS	2.1
2	A	108	ASP	2.0
2	B	25	TRP	2.0
2	B	61	ILE	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	HG	B	902	1/1	0.99	0.16	-0.30	52,52,52,52	1
3	HG	A	901	1/1	0.99	0.11	-0.39	27,27,27,27	1
3	HG	B	904	1/1	0.87	0.09	-1.10	61,61,61,61	1
3	HG	A	903	1/1	0.97	0.08	-1.44	45,45,45,45	1

## 6.5 Other polymers

There are no such residues in this entry.