



# Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2020 – 07:52 pm BST

PDB ID : 1KHV  
Title : Crystal Structure of Rabbit Hemorrhagic Disease Virus RNA-dependent RNA polymerase complexed with Lu<sup>3+</sup>  
Authors : Ng, K.K.; Cherney, M.M.; Vazquez, A.L.; Machin, A.; Alonso, J.M.; Parra, F.; James, M.N.  
Deposited on : 2001-12-01  
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

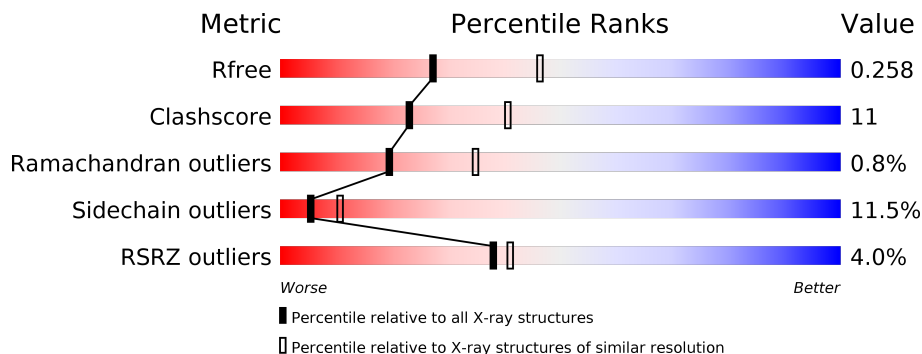
# 1 Overall quality at a glance

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	516	 % 69% 20% 5% . .
1	B	516	 7% 65% 26% 6% .

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7939 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 RNA-DIRECTED RNA POLYMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	493	3871	2464	660	719	28	0	0	0
1	B	497	3905	2486	666	725	28	0	0	0

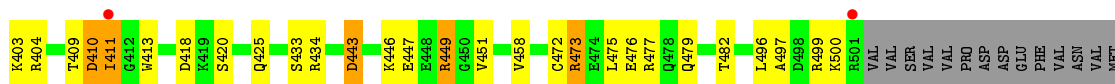
- Molecule 2 is LUTETIUM (III) ION (three-letter code: LU) (formula: Lu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Lu	0	0
			1	1		
2	A	1	Total	Lu	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	92	Total	O	0	0
			92	92		
3	B	69	Total	O	0	0
			69	69		





GLU

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.30Å 119.10Å 158.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.50 – 2.50 34.47 – 2.50	Depositor EDS
% Data completeness (in resolution range)	88.0 (34.50-2.50) 91.0 (34.47-2.50)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	0.04	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.45 (at 2.51Å)	Xtrriage
Refinement program	REFMAC 5.0, CNS	Depositor
R, $R_{free}$	0.217 , 0.265 0.212 , 0.258	Depositor DCC
$R_{free}$ test set	1306 reflections (3.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	47.5	Xtrriage
Anisotropy	0.045	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 46.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7939	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% 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:  
LU

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	0.46	0/3954	0.83	16/5356 (0.3%)
1	B	0.42	0/3989	0.81	18/5403 (0.3%)
All	All	0.44	0/7943	0.82	34/10759 (0.3%)

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	5	PHE	CB-CG-CD1	6.70	125.49	120.80
1	A	174	ASP	CB-CG-OD2	6.58	124.23	118.30
1	B	194	ASP	CB-CG-OD2	6.44	124.10	118.30
1	B	94	ASP	CB-CG-OD2	6.25	123.92	118.30
1	B	174	ASP	CB-CG-OD2	6.18	123.86	118.30
1	A	61	ASP	CB-CG-OD2	5.99	123.69	118.30
1	A	194	ASP	CB-CG-OD2	5.84	123.56	118.30
1	B	180	ASP	CB-CG-OD2	5.81	123.53	118.30
1	B	42	ASP	CB-CG-OD2	5.76	123.49	118.30
1	A	498	ASP	CB-CG-OD2	5.71	123.44	118.30
1	A	346	ASP	CB-CG-OD2	5.68	123.41	118.30
1	A	250	ASP	CB-CG-OD2	5.63	123.37	118.30
1	A	59	ASP	CB-CG-OD2	5.62	123.35	118.30
1	A	233	ASP	CB-CG-OD2	5.53	123.27	118.30
1	A	144	ASP	CB-CG-OD2	5.50	123.25	118.30
1	B	226	ASP	CB-CG-OD2	5.47	123.22	118.30
1	A	490	ASP	CB-CG-OD2	5.46	123.22	118.30
1	A	392	ASP	CB-CG-OD2	5.43	123.19	118.30
1	B	59	ASP	CB-CG-OD2	5.37	123.14	118.30
1	B	140	ASP	CB-CG-OD2	5.36	123.12	118.30
1	B	346	ASP	CB-CG-OD2	5.34	123.11	118.30
1	B	268	ASP	CB-CG-OD2	5.30	123.07	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	377	ASP	CB-CG-OD2	5.29	123.06	118.30
1	B	477	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	A	121	ASP	CB-CG-OD2	5.19	122.97	118.30
1	A	272	ASP	CB-CG-OD2	5.18	122.97	118.30
1	B	296	ASP	CB-CG-OD2	5.18	122.96	118.30
1	B	231	ASP	CB-CG-OD2	5.16	122.94	118.30
1	A	42	ASP	CB-CG-OD2	5.13	122.92	118.30
1	B	121	ASP	CB-CG-OD2	5.12	122.91	118.30
1	B	11	ASP	CB-CG-OD2	5.10	122.89	118.30
1	A	268	ASP	CB-CG-OD2	5.08	122.87	118.30
1	B	443	ASP	CB-CG-OD2	5.04	122.84	118.30
1	B	410	ASP	CB-CG-OD2	5.01	122.81	118.30

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	3871	0	3873	91	0
1	B	3905	0	3915	87	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	92	0	0	1	0
3	B	69	0	0	2	0
All	All	7939	0	7788	177	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 (177) 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:B:20:LEU:HD13	1:B:299:ILE:HD11	1.39	1.03
1:A:49:ARG:HD2	1:A:179:LEU:HD13	1.46	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:431:THR:HG22	1:A:433:SER:H	1.34	0.93
1:A:107:ARG:HH11	1:A:107:ARG:HG2	1.33	0.91
1:A:409:THR:HG22	1:A:411:ILE:H	1.41	0.85
1:B:282:SER:O	1:B:286:THR:HG23	1.83	0.78
1:A:122:LEU:HA	1:A:134:LYS:HD3	1.67	0.77
1:A:55:ARG:HG2	1:A:437:VAL:HG13	1.65	0.76
1:B:195:VAL:O	1:B:199:VAL:HG23	1.86	0.74
1:B:75:TYR:HB3	1:B:302:THR:OG1	1.87	0.73
1:B:49:ARG:NH1	1:B:50:PRO:O	2.22	0.73
1:A:49:ARG:HD2	1:A:179:LEU:CD1	2.20	0.71
1:A:48:TYR:CD2	1:A:424:ARG:HD2	2.26	0.70
1:A:33:ARG:O	1:A:431:THR:HB	1.91	0.70
1:B:164:LEU:H	1:B:286:THR:HG22	1.57	0.70
1:A:107:ARG:NH1	1:A:107:ARG:HG2	2.05	0.69
1:B:84:VAL:HG13	1:B:88:ILE:HB	1.75	0.69
1:A:16:THR:HG22	1:A:301:GLN:HE21	1.58	0.69
1:B:164:LEU:H	1:B:286:THR:CG2	2.08	0.67
1:A:228:THR:HG23	1:A:499:ARG:HB3	1.77	0.66
1:B:122:LEU:HA	1:B:134:LYS:HD2	1.77	0.66
1:B:16:THR:H	1:B:76:GLN:HE22	1.42	0.66
1:B:150:HIS:HE1	1:B:194:ASP:OD1	1.78	0.66
1:A:5:PHE:HB3	1:A:21:VAL:O	1.96	0.66
1:B:476:GLU:HA	1:B:479:GLN:HE21	1.60	0.66
1:B:275:GLU:HG2	1:B:277:THR:HG23	1.76	0.66
1:B:240:THR:HG21	1:B:396:LEU:HD23	1.79	0.65
1:A:111:LEU:HB2	1:A:203:ALA:HA	1.79	0.65
1:A:5:PHE:CB	1:A:21:VAL:O	2.45	0.64
1:B:342:ASN:N	1:B:342:ASN:HD22	1.94	0.64
1:B:425:GLN:O	1:B:449:ARG:NH2	2.29	0.64
1:A:195:VAL:O	1:A:199:VAL:HG23	1.98	0.63
1:A:121:ASP:O	1:A:124:THR:HG23	1.98	0.63
1:B:102:LEU:HD11	1:B:211:LYS:HB3	1.80	0.63
1:B:5:PHE:N	1:B:5:PHE:CD1	2.64	0.63
1:A:55:ARG:CG	1:A:437:VAL:HG13	2.29	0.62
1:A:77:GLN:O	1:A:304:ARG:HD2	1.99	0.62
1:B:108:GLN:HG3	1:B:207:ASN:HB3	1.81	0.62
1:B:191:TRP:CZ3	1:B:293:THR:OG1	2.53	0.61
1:B:121:ASP:O	1:B:124:THR:HG23	2.01	0.61
1:A:264:ARG:NH1	1:A:288:LYS:HB3	2.15	0.61
1:A:409:THR:HG22	1:A:410:ASP:N	2.16	0.60
1:A:122:LEU:HA	1:A:134:LYS:CD	2.30	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:VAL:O	1:A:304:ARG:HD3	2.01	0.60
1:A:49:ARG:HB3	1:A:53:LEU:HD21	1.81	0.60
1:B:227:MET:HA	1:B:227:MET:CE	2.32	0.60
1:A:476:GLU:HA	1:A:479:GLN:HE21	1.66	0.59
1:A:10:ILE:HD12	1:A:298:MET:HB2	1.83	0.59
1:A:313:THR:O	1:A:317:ASN:HB2	2.03	0.59
1:A:12:TYR:OH	1:A:66:ASN:ND2	2.36	0.58
1:A:336:ILE:HG12	1:A:336:ILE:O	2.03	0.58
1:B:37:VAL:HG22	1:B:40:VAL:HG23	1.84	0.58
1:A:49:ARG:HD3	1:A:53:LEU:HD21	1.86	0.57
1:A:318:SER:O	1:A:351:THR:HG21	2.04	0.57
1:B:402:LEU:O	1:B:404:ARG:HG3	2.03	0.57
1:B:102:LEU:CD1	1:B:211:LYS:HB3	2.35	0.57
1:A:67:ILE:HG21	1:A:187:LYS:HE2	1.87	0.56
1:B:344:TYR:H	1:B:344:TYR:HD1	1.54	0.56
1:A:78:GLU:HG3	1:A:79:PRO:HD2	1.87	0.56
1:B:13:ARG:NH2	3:B:533:HOH:O	2.31	0.56
1:A:112:ASN:ND2	1:B:296:ASP:OD1	2.38	0.55
1:B:333:CYS:O	1:B:338:LEU:N	2.39	0.55
1:A:52:ASN:C	1:A:52:ASN:HD22	2.10	0.55
1:B:411:ILE:HG12	1:B:411:ILE:O	2.06	0.55
1:B:228:THR:HG23	1:B:499:ARG:HD3	1.89	0.55
1:A:5:PHE:HE1	1:A:167:ILE:HD12	1.72	0.55
1:B:122:LEU:HB3	1:B:135:ILE:HB	1.89	0.54
1:B:25:PRO:O	1:B:27:PRO:HD3	2.07	0.54
1:B:411:ILE:HG13	1:B:497:ALA:HA	1.89	0.54
1:B:476:GLU:HA	1:B:479:GLN:NE2	2.22	0.54
1:B:342:ASN:H	1:B:342:ASN:HD22	1.54	0.53
1:A:386:ASP:O	1:A:388:THR:N	2.42	0.53
1:B:386:ASP:HB2	1:B:388:THR:HG22	1.91	0.52
1:A:15:ILE:HG22	1:A:73:GLN:HG2	1.91	0.52
1:B:472:CYS:O	1:B:476:GLU:HG3	2.10	0.52
1:A:409:THR:CG2	1:A:410:ASP:N	2.72	0.52
1:A:431:THR:CG2	1:A:432:THR:N	2.72	0.51
1:B:177:ARG:NH1	1:B:186:LYS:O	2.43	0.51
1:A:145:GLN:HA	1:A:145:GLN:HE21	1.75	0.51
1:A:402:LEU:O	1:A:404:ARG:NH1	2.44	0.51
1:A:15:ILE:HG21	1:A:69:VAL:HG13	1.92	0.51
1:A:36:LYS:O	1:A:440:GLU:HA	2.11	0.51
1:B:342:ASN:ND2	1:B:342:ASN:N	2.59	0.51
1:A:425:GLN:O	1:A:449:ARG:NH2	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:PHE:HB2	1:A:21:VAL:O	2.11	0.50
1:A:170:CYS:HB3	1:A:295:LEU:HA	1.93	0.50
1:A:84:VAL:HG22	1:A:88:ILE:HG21	1.93	0.50
1:B:231:ASP:O	1:B:235:ILE:HG23	2.11	0.50
1:B:164:LEU:N	1:B:286:THR:HG22	2.24	0.50
1:B:236:ILE:HG21	1:B:413:TRP:CE2	2.47	0.50
1:A:49:ARG:HH11	1:A:179:LEU:HD11	1.77	0.50
1:A:225:VAL:HG21	1:A:235:ILE:HD11	1.94	0.50
1:A:5:PHE:CZ	1:A:129:PHE:CZ	3.00	0.50
1:A:36:LYS:NZ	1:A:427:GLU:OE2	2.27	0.49
1:A:128:PRO:HB2	1:A:294:ILE:HD12	1.94	0.49
1:A:258:MET:HE1	1:A:324:LEU:HD11	1.93	0.49
1:B:95:VAL:HG22	1:B:322:TRP:CE2	2.48	0.49
1:A:396:LEU:C	1:A:398:LYS:H	2.16	0.49
1:A:318:SER:HB3	1:A:351:THR:HG22	1.95	0.49
1:A:394:CYS:HB2	1:A:398:LYS:HD3	1.95	0.49
1:B:110:ASN:ND2	3:B:540:HOH:O	2.41	0.49
1:A:61:ASP:O	1:A:63:SER:N	2.38	0.48
1:B:458:VAL:HG13	1:B:496:LEU:HD13	1.95	0.48
1:B:228:THR:CG2	1:B:499:ARG:HD3	2.44	0.48
1:B:33:ARG:HG3	1:B:434:ARG:HH11	1.78	0.47
1:A:107:ARG:NH1	1:A:107:ARG:CG	2.69	0.47
1:A:213:LYS:HG3	1:A:224:GLY:HA3	1.97	0.47
1:B:449:ARG:HB3	1:B:482:THR:HG21	1.96	0.47
1:B:398:LYS:HG2	1:B:398:LYS:O	2.14	0.47
1:B:322:TRP:O	1:B:326:SER:HB3	2.14	0.46
1:A:63:SER:O	1:A:67:ILE:HG13	2.14	0.46
1:B:108:GLN:HG3	1:B:207:ASN:CB	2.46	0.46
1:A:34:TYR:CZ	1:A:430:LYS:HE3	2.51	0.46
1:A:5:PHE:CZ	1:A:129:PHE:CE1	3.04	0.46
1:A:10:ILE:CD1	1:A:298:MET:HB2	2.46	0.46
1:A:500:LYS:HE2	1:A:500:LYS:HB3	1.59	0.46
1:A:500:LYS:O	1:A:501:ARG:O	2.33	0.46
1:A:16:THR:HG22	1:A:301:GLN:NE2	2.26	0.46
1:A:108:GLN:OE1	1:A:211:LYS:HE3	2.14	0.46
1:A:317:ASN:HB3	1:A:353:GLY:HA2	1.98	0.45
1:B:409:THR:OG1	1:B:411:ILE:HG22	2.16	0.45
1:B:242:LYS:NZ	1:B:345:GLU:O	2.50	0.45
1:B:43:GLU:HG3	1:B:43:GLU:H	1.54	0.45
1:A:165:HIS:HB3	1:A:167:ILE:HG13	1.99	0.45
1:A:53:LEU:HD23	1:A:53:LEU:HA	1.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:120:LEU:HB3	1:B:124:THR:HG21	1.97	0.45
1:B:15:ILE:HD11	1:B:73:GLN:N	2.31	0.45
1:A:107:ARG:HA	1:A:273:CYS:O	2.17	0.44
1:A:385:ALA:O	1:A:387:LYS:N	2.50	0.44
1:A:424:ARG:HG2	1:A:424:ARG:HH11	1.81	0.44
1:B:5:PHE:HA	1:B:18:HIS:CG	2.53	0.44
1:A:55:ARG:HG2	1:A:437:VAL:CG1	2.44	0.44
1:A:5:PHE:CE1	1:A:167:ILE:HD12	2.51	0.44
1:A:409:THR:HG21	1:A:411:ILE:HG22	1.99	0.44
1:B:6:CYS:SG	1:B:21:VAL:HG23	2.58	0.44
1:A:247:LEU:HB3	1:A:358:TYR:HD2	1.83	0.43
1:B:172:LEU:HB3	1:B:187:LYS:HE2	2.00	0.43
1:B:336:ILE:HA	1:B:336:ILE:HD12	1.75	0.43
1:A:258:MET:HE2	1:A:259:SER:H	1.83	0.43
1:B:37:VAL:HA	1:B:38:PRO:HD3	1.84	0.43
1:B:24:GLU:HA	1:B:25:PRO:HD2	1.90	0.43
1:A:424:ARG:CG	1:A:424:ARG:HH11	2.30	0.43
1:B:108:GLN:CG	1:B:207:ASN:HB3	2.48	0.43
1:A:303:LYS:NZ	3:A:578:HOH:O	2.52	0.43
1:B:15:ILE:CD1	1:B:73:GLN:HG2	2.49	0.43
1:A:301:GLN:N	1:A:301:GLN:CD	2.72	0.43
1:A:49:ARG:HD3	1:A:53:LEU:CD2	2.48	0.43
1:B:227:MET:HE2	1:B:227:MET:HA	2.01	0.43
1:A:418:ASP:OD1	1:A:420:SER:HB2	2.18	0.43
1:A:387:LYS:HD2	1:A:387:LYS:H	1.84	0.42
1:B:49:ARG:HG3	1:B:49:ARG:NH1	2.35	0.42
1:A:34:TYR:OH	1:A:430:LYS:HE3	2.20	0.42
1:A:416:LYS:HB3	1:A:463:HIS:CE1	2.54	0.42
1:B:368:LEU:N	1:B:369:PRO:HD2	2.35	0.42
1:B:168:TYR:CD2	1:B:191:TRP:HB3	2.54	0.42
1:B:49:ARG:HH11	1:B:49:ARG:CG	2.33	0.42
1:A:431:THR:HG22	1:A:432:THR:N	2.35	0.41
1:B:118:ASN:HA	1:B:118:ASN:HD22	1.58	0.41
1:A:211:LYS:HB2	1:A:211:LYS:HE2	1.87	0.41
1:B:313:THR:O	1:B:317:ASN:HB2	2.21	0.41
1:B:223:VAL:HA	1:B:352:TYR:CE2	2.56	0.41
1:A:409:THR:CG2	1:A:410:ASP:H	2.33	0.41
1:B:291:PRO:HD2	1:B:302:THR:CG2	2.50	0.41
1:B:472:CYS:HA	1:B:475:LEU:HB2	2.02	0.41
1:B:324:LEU:HD23	1:B:324:LEU:HA	1.84	0.41
1:B:111:LEU:HB3	1:B:115:ALA:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:TYR:O	1:A:444:LEU:N	2.54	0.40
1:B:264:ARG:HA	1:B:288:LYS:HG2	2.02	0.40
1:B:294:ILE:HA	1:B:298:MET:O	2.20	0.40
1:B:339:HIS:O	1:B:339:HIS:CG	2.74	0.40
1:B:473:ARG:O	1:B:473:ARG:HD3	2.21	0.40
1:B:104:LYS:HD3	1:B:104:LYS:HA	1.88	0.40
1:B:473:ARG:C	1:B:473:ARG:HD3	2.41	0.40
1:B:57:ASP:HA	1:B:58:PRO:HD3	1.81	0.40
1:B:252:SER:OG	1:B:253:LYS:HE2	2.21	0.40
1:B:443:ASP:OD1	1:B:446:LYS:HE2	2.21	0.40
1:B:99:LEU:O	1:B:103:THR:HG23	2.22	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	489/516 (95%)	463 (95%)	19 (4%)	7 (1%)	11	20
1	B	495/516 (96%)	475 (96%)	19 (4%)	1 (0%)	47	68
All	All	984/1032 (95%)	938 (95%)	38 (4%)	8 (1%)	19	35

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	387	LYS
1	B	21	VAL
1	A	62	LYS
1	A	139	LYS
1	A	397	ASN
1	A	386	ASP
1	A	48	TYR

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Mol	Chain	Res	Type
1	A	141	GLY

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	423/446 (95%)	382 (90%)	41 (10%)	8 16
1	B	427/446 (96%)	370 (87%)	57 (13%)	4 7
All	All	850/892 (95%)	752 (88%)	98 (12%)	5 11

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	PHE
1	A	11	ASP
1	A	13	ARG
1	A	46	THR
1	A	52	ASN
1	A	55	ARG
1	A	62	LYS
1	A	70	LYS
1	A	78	GLU
1	A	102	LEU
1	A	107	ARG
1	A	120	LEU
1	A	121	ASP
1	A	134	LYS
1	A	139	LYS
1	A	145	GLN
1	A	147	LEU
1	A	173	LYS
1	A	187	LYS
1	A	215	VAL
1	A	228	THR
1	A	247	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	285	LEU
1	A	304	ARG
1	A	306	LEU
1	A	336	ILE
1	A	351	THR
1	A	352	TYR
1	A	358	TYR
1	A	387	LYS
1	A	388	THR
1	A	411	ILE
1	A	418	ASP
1	A	422	ILE
1	A	424	ARG
1	A	432	THR
1	A	437	VAL
1	A	449	ARG
1	A	451	VAL
1	A	500	LYS
1	A	501	ARG
1	B	5	PHE
1	B	15	ILE
1	B	30	SER
1	B	36	LYS
1	B	37	VAL
1	B	42	ASP
1	B	43	GLU
1	B	49	ARG
1	B	63	SER
1	B	64	LEU
1	B	81	LEU
1	B	99	LEU
1	B	100	ARG
1	B	108	GLN
1	B	119	THR
1	B	139	LYS
1	B	142	VAL
1	B	147	LEU
1	B	157	VAL
1	B	208	ILE
1	B	225	VAL
1	B	228	THR
1	B	235	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	236	ILE
1	B	247	LEU
1	B	270	LEU
1	B	279	LEU
1	B	285	LEU
1	B	295	LEU
1	B	303	LYS
1	B	336	ILE
1	B	338	LEU
1	B	340	CYS
1	B	341	SER
1	B	342	ASN
1	B	343	LEU
1	B	344	TYR
1	B	352	TYR
1	B	366	SER
1	B	375	LEU
1	B	383	THR
1	B	386	ASP
1	B	388	THR
1	B	391	ILE
1	B	396	LEU
1	B	399	ILE
1	B	403	LYS
1	B	410	ASP
1	B	411	ILE
1	B	418	ASP
1	B	420	SER
1	B	433	SER
1	B	447	GLU
1	B	449	ARG
1	B	451	VAL
1	B	473	ARG
1	B	500	LYS

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

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	18	HIS
1	A	52	ASN
1	A	66	ASN
1	A	118	ASN

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Mol	Chain	Res	Type
1	A	145	GLN
1	A	206	HIS
1	A	301	GLN
1	A	479	GLN
1	B	76	GLN
1	B	118	ASN
1	B	150	HIS
1	B	237	ASN
1	B	342	ASN
1	B	374	ASN
1	B	465	GLN
1	B	479	GLN

### 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](#)

Of 2 ligands modelled in this entry, 2 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	A	493/516 (95%)	0.03	6 (1%) 79 80	16, 26, 50, 66	0
1	B	497/516 (96%)	0.35	34 (6%) 17 17	14, 28, 47, 64	0
All	All	990/1032 (95%)	0.19	40 (4%) 38 41	14, 27, 48, 66	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	5	PHE	5.4
1	B	336	ILE	4.6
1	A	140	ASP	4.5
1	B	333	CYS	4.4
1	B	21	VAL	4.1
1	B	339	HIS	3.9
1	B	142	VAL	3.9
1	A	138	VAL	3.7
1	B	340	CYS	3.6
1	B	366	SER	3.5
1	B	254	TRP	3.4
1	B	411	ILE	3.4
1	B	140	ASP	3.3
1	B	389	GLU	3.2
1	B	390	PHE	3.2
1	B	398	LYS	3.1
1	B	338	LEU	3.1
1	B	139	LYS	3.1
1	B	371	ILE	3.0
1	B	23	ALA	3.0
1	A	55	ARG	3.0
1	B	370	ALA	3.0
1	B	334	ALA	2.7
1	A	501	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	179	LEU	2.5
1	B	317	ASN	2.5
1	B	396	LEU	2.5
1	B	320	CYS	2.5
1	B	501	ARG	2.4
1	B	255	ASP	2.4
1	B	122	LEU	2.4
1	A	411	ILE	2.4
1	B	386	ASP	2.3
1	B	354	ASP	2.3
1	B	101	PHE	2.2
1	B	180	ASP	2.1
1	B	7	GLY	2.1
1	B	365	VAL	2.1
1	B	374	ASN	2.1
1	B	235	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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
2	LU	A	517	1/1	0.83	0.27	60,60,60,60	1
2	LU	B	517	1/1	0.94	0.25	55,55,55,55	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.