



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:23 PM UTC

PDB ID : 1KHV / pdb_00001khv
Title : Crystal Structure of Rabbit Hemorrhagic Disease Virus RNA-dependent RNA polymerase complexed with Lu3+
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

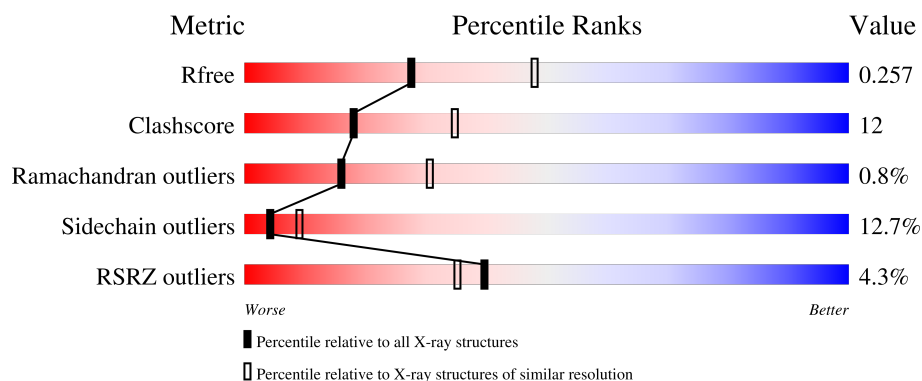
1 Overall quality at a glance

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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	2% 70% 19% 6% • • •
1	B	516	7% 65% 26% 5% •

2 Entry composition

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
1	A	493	Total	C	N	O	S	0	0	0
			3871	2464	660	719	28			
1	B	497	Total	C	N	O	S	0	0	0
			3905	2486	666	725	28			

- Molecule 2 is LUTETIUM (III) ION (CCD ID: LU) (formula: Lu).

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

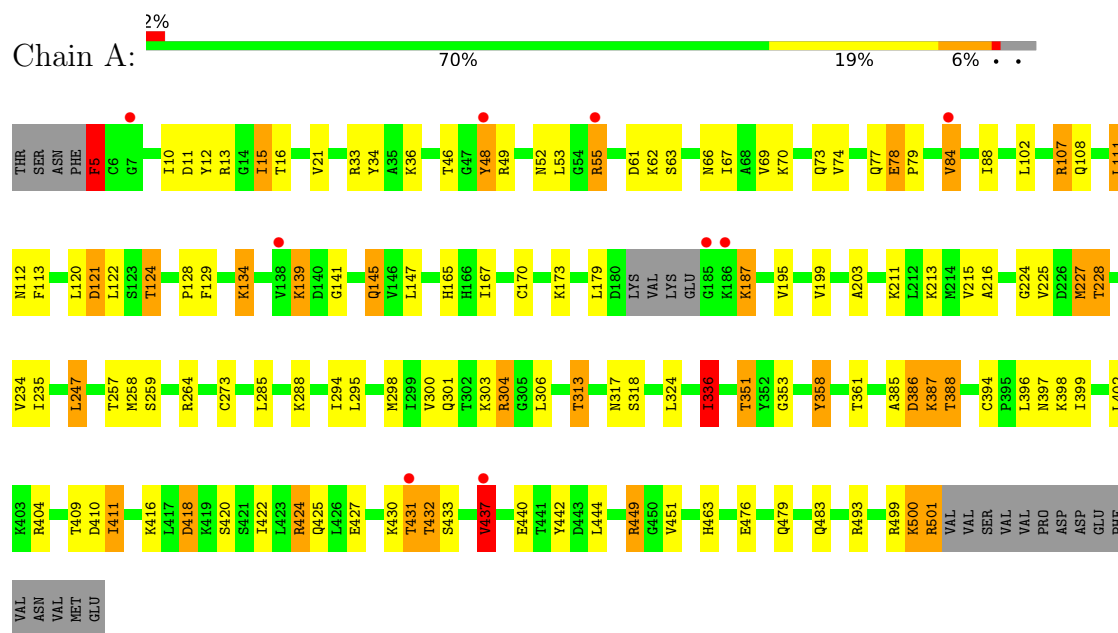
- Molecule 3 is water.

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

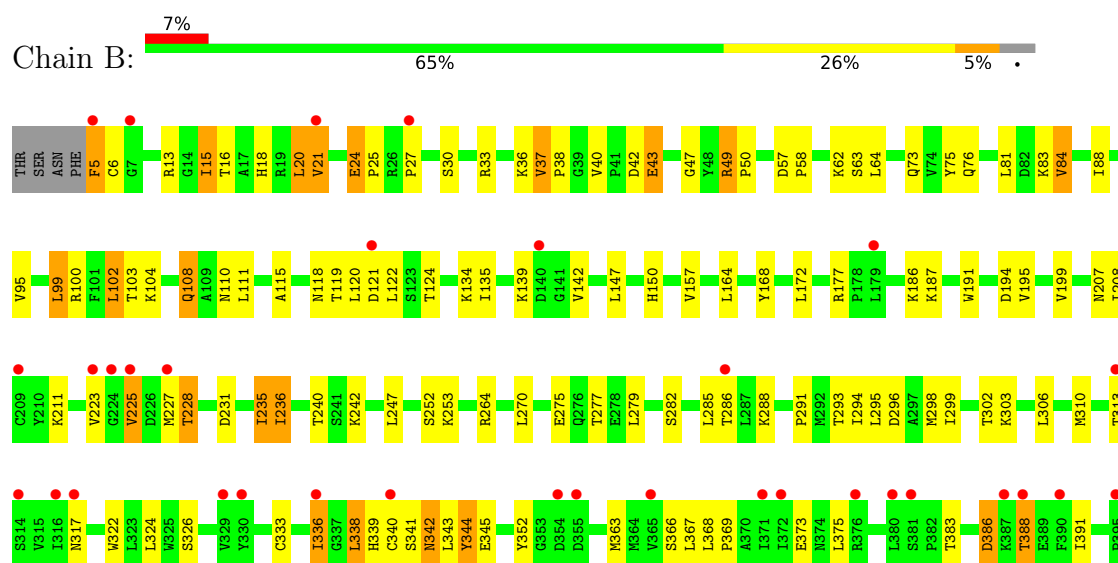
3 Residue-property plots

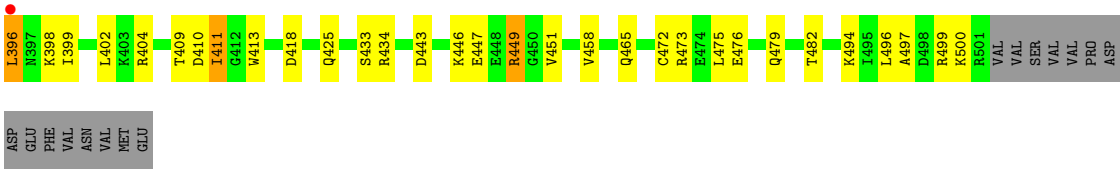
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: RNA-DIRECTED RNA POLYMERASE



• Molecule 1: RNA-DIRECTED RNA POLYMERASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	70.30Å 119.10Å 158.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.50 – 2.50 34.50 – 2.50	Depositor EDS
% Data completeness (in resolution range)	88.0 (34.50-2.50) 90.9 (34.50-2.50)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.45 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.0, CNS	Depositor
R, R_{free}	0.217 , 0.265 0.212 , 0.257	Depositor DCC
R_{free} test set	1306 reflections (3.06%)	wwPDB-VP
Wilson B-factor (Å ²)	47.5	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 52.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7939	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

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	0.59	1/3954 (0.0%)	1.00	8/5356 (0.1%)
1	B	0.55	0/3989	0.98	2/5403 (0.0%)
All	All	0.57	1/7943 (0.0%)	0.99	10/10759 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	227	MET	SD-CE	-7.05	1.61	1.79

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	5	PHE	CA-CB-CG	9.82	123.62	113.80
1	A	336	ILE	N-CA-C	-6.33	106.16	112.17
1	A	399	ILE	N-CA-C	5.80	116.77	110.21
1	B	465	GLN	N-CA-C	5.60	117.06	111.07
1	A	216	ALA	N-CA-C	5.57	118.11	111.71
1	A	5	PHE	CA-C-N	-5.53	115.31	123.05
1	A	5	PHE	C-N-CA	-5.53	115.31	123.05
1	A	437	VAL	CB-CA-C	-5.48	102.30	111.29
1	B	47	GLY	N-CA-C	5.11	120.29	114.67
1	A	113	PHE	N-CA-C	5.01	117.13	111.11

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	99	0
1	B	3905	0	3915	92	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	190	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 (190) 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
1:B:227:MET:HA	1:B:227:MET:HE2	1.49	0.95
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:A:258:MET:HE1	1:A:324:LEU:HD11	1.72	0.70
1:B:164:LEU:H	1:B:286:THR:HG22	1.57	0.70
1:A:107:ARG:HG2	1:A:107:ARG:NH1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD22	1:B:342:ASN:N	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:5:PHE:N	1:B:5:PHE:CD1	2.64	0.63
1:B:102:LEU:HD11	1:B:211:LYS:HB3	1.80	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:122:LEU:HA	1:A:134:LYS:CD	2.30	0.60
1:A:49:ARG:HB3	1:A:53:LEU:HD21	1.81	0.60
1:A:74:VAL:O	1:A:304:ARG:HD3	2.01	0.60
1:A:409:THR:HG22	1:A:410:ASP:N	2.16	0.60
1:A:52:ASN:HD22	1:A:52:ASN:C	2.10	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: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:A:336:ILE:HG12	1:A:336:ILE:O	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:HD1	1:B:344:TYR:H	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:258:MET:HE3	1:A:259:SER:H	1.72	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:A:396:LEU:C	1:A:398:LYS:H	2.16	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:HD22	1:B:342:ASN:H	1.54	0.53
1:A:386:ASP:O	1:A:388:THR:N	2.42	0.53
1:B:227:MET:HA	1:B:227:MET:CE	2.32	0.52
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:HE21	1:A:145:GLN:HA	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:N	1:B:342:ASN:ND2	2.59	0.51
1:A:425:GLN:O	1:A:449:ARG:NH2	2.41	0.51
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:164:LEU:N	1:B:286:THR:HG22	2.24	0.50
1:B:231:ASP:O	1:B:235:ILE:HG23	2.11	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:B:95:VAL:HG22	1:B:322:TRP:CE2	2.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:301:GLN:CD	1:A:301:GLN:N	2.72	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:306:LEU:HD11	1:B:310:MET:HE2	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:298:MET:HE3	1:A:300:VAL:HG22	1.96	0.46
1:A:500:LYS:HB3	1:A:500:LYS:HE2	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:43:GLU:H	1:B:43:GLU:HG3	1.54	0.45
1:B:242:LYS:NZ	1:B:345:GLU:O	2.50	0.45
1:B:473:ARG:C	1:B:473:ARG:HD3	2.41	0.45
1:B:225:VAL:HG13	1:B:227:MET:HE3	1.98	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
1:B:15:ILE:HD11	1:B:73:GLN:N	2.31	0.45
1:B:120:LEU:HB3	1:B:124:THR:HG21	1.97	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:386:ASP:C	1:A:388:THR:H	2.25	0.44
1:A:225:VAL:CG1	1:A:227:MET:HE3	2.47	0.44
1:A:424:ARG:HH11	1:A:424:ARG:HG2	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:227:MET:HE1	1:A:235:ILE:HD12	1.99	0.44
1:B:24:GLU:CD	1:B:24:GLU:H	2.25	0.44
1:A:5:PHE:CE1	1:A:167:ILE:HD12	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:409:THR:HG21	1:A:411:ILE:HG22	1.99	0.44
1:B:363:MET:HE2	1:B:367:LEU:HD22	1.98	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:HD12	1:B:336:ILE:HA	1.75	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:52:ASN:C	1:A:52:ASN:ND2	2.76	0.43
1:A:424:ARG:HH11	1:A:424:ARG:CG	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:49:ARG:HD3	1:A:53:LEU:CD2	2.48	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:NH1	1:B:49:ARG:HG3	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:A:227:MET:HA	1:A:227:MET:HE2	2.01	0.42
1:A:257:THR:O	1:A:258:MET:C	2.63	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:B:227:MET:HE1	1:B:235:ILE:HD13	2.02	0.42
1:A:431:THR:HG22	1:A:432:THR:N	2.35	0.41
1:B:118:ASN:HD22	1:B:118:ASN:HA	1.58	0.41
1:A:211:LYS:HE2	1:A:211:LYS:HB2	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
1:A:258:MET:HE3	1:A:258:MET:HA	2.03	0.40
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:HD3	1:B:473:ARG:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:ASP:HA	1:B:58:PRO:HD3	1.81	0.40
1:B:104:LYS:HD3	1:B:104:LYS:HA	1.88	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%)	9	17
1	B	495/516 (96%)	475 (96%)	19 (4%)	1 (0%)	43	63
All	All	984/1032 (95%)	938 (95%)	38 (4%)	8 (1%)	16	31

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
1	A	141	GLY

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	423/446 (95%)	376 (89%)	47 (11%)	6	12
1	B	427/446 (96%)	366 (86%)	61 (14%)	3	6
All	All	850/892 (95%)	742 (87%)	108 (13%)	4	9

All (108) 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	15	ILE
1	A	46	THR
1	A	55	ARG
1	A	70	LYS
1	A	78	GLU
1	A	84	VAL
1	A	102	LEU
1	A	107	ARG
1	A	111	LEU
1	A	120	LEU
1	A	121	ASP
1	A	124	THR
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	234	VAL
1	A	247	LEU
1	A	285	LEU
1	A	304	ARG

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Mol	Chain	Res	Type
1	A	306	LEU
1	A	313	THR
1	A	336	ILE
1	A	351	THR
1	A	358	TYR
1	A	361	THR
1	A	388	THR
1	A	411	ILE
1	A	418	ASP
1	A	422	ILE
1	A	424	ARG
1	A	431	THR
1	A	432	THR
1	A	437	VAL
1	A	449	ARG
1	A	451	VAL
1	A	483	GLN
1	A	493	ARG
1	A	500	LYS
1	A	501	ARG
1	B	5	PHE
1	B	15	ILE
1	B	20	LEU
1	B	24	GLU
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	62	LYS
1	B	63	SER
1	B	64	LEU
1	B	81	LEU
1	B	83	LYS
1	B	84	VAL
1	B	99	LEU
1	B	100	ARG
1	B	102	LEU
1	B	108	GLN
1	B	119	THR
1	B	139	LYS

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Mol	Chain	Res	Type
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
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	366	SER
1	B	373	GLU
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	410	ASP
1	B	411	ILE
1	B	418	ASP
1	B	433	SER
1	B	447	GLU
1	B	449	ARG
1	B	451	VAL
1	B	494	LYS
1	B	500	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	52	ASN
1	A	66	ASN
1	A	118	ASN
1	A	145	GLN
1	A	206	HIS
1	A	301	GLN
1	A	342	ASN
1	A	479	GLN
1	B	76	GLN
1	B	118	ASN
1	B	150	HIS
1	B	237	ASN
1	B	238	ASN
1	B	342	ASN
1	B	374	ASN
1	B	425	GLN
1	B	452	GLN
1	B	465	GLN
1	B	479	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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, 95th 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 ²)	Q<0.9
1	A	493/516 (95%)	0.08	9 (1%) 67 64	16, 26, 50, 66	0
1	B	497/516 (96%)	0.53	34 (6%) 23 20	14, 28, 47, 64	0
All	All	990/1032 (95%)	0.31	43 (4%) 40 35	14, 27, 48, 66	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	336	ILE	4.2
1	B	390	PHE	3.9
1	B	371	ILE	3.9
1	B	313	THR	3.4
1	A	138	VAL	3.3
1	B	225	VAL	3.1
1	B	316	ILE	2.9
1	B	395	PRO	2.9
1	B	380	LEU	2.9
1	B	5	PHE	2.8
1	B	314	SER	2.8
1	B	121	ASP	2.8
1	B	330	TYR	2.7
1	B	140	ASP	2.7
1	B	286	THR	2.7
1	B	388	THR	2.6
1	B	227	MET	2.6
1	B	223	VAL	2.5
1	A	7	GLY	2.5
1	B	224	GLY	2.5
1	A	84	VAL	2.5
1	A	48	TYR	2.4
1	B	317	ASN	2.4
1	A	55	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	355	ASP	2.3
1	A	437	VAL	2.3
1	B	381	SER	2.2
1	A	186	LYS	2.2
1	A	185	GLY	2.2
1	A	431	THR	2.2
1	B	209	CYS	2.2
1	B	387	LYS	2.2
1	B	7	GLY	2.1
1	B	340	CYS	2.1
1	B	354	ASP	2.1
1	B	365	VAL	2.1
1	B	396	LEU	2.1
1	B	329	VAL	2.1
1	B	179	LEU	2.1
1	B	27	PRO	2.1
1	B	376	ARG	2.0
1	B	372	ILE	2.0
1	B	21	VAL	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 oligosaccharides 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, 95th 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($\text{\AA}^2$)	Q<0.9
2	LU	A	517	1/1	0.79	0.14	60,60,60,60	1
2	LU	B	517	1/1	0.92	0.07	55,55,55,55	1

6.5 Other polymers [i](#)

There are no such residues in this entry.