Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 08:29 PM GMT

PDB ID	:	1KHV
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

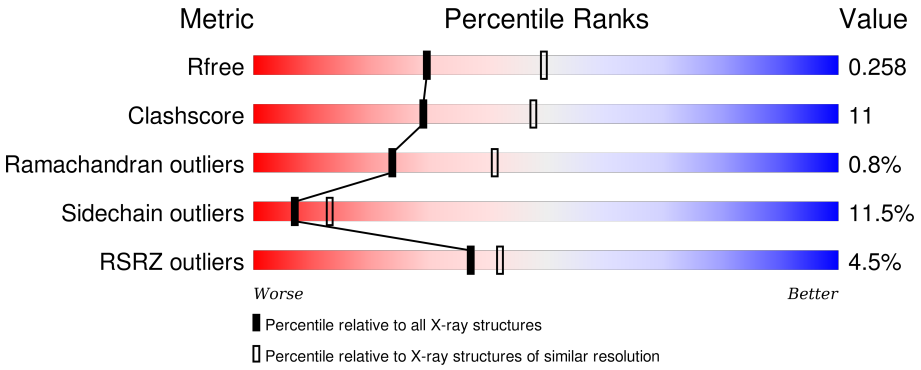
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (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 >=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 <=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% 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
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 (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.

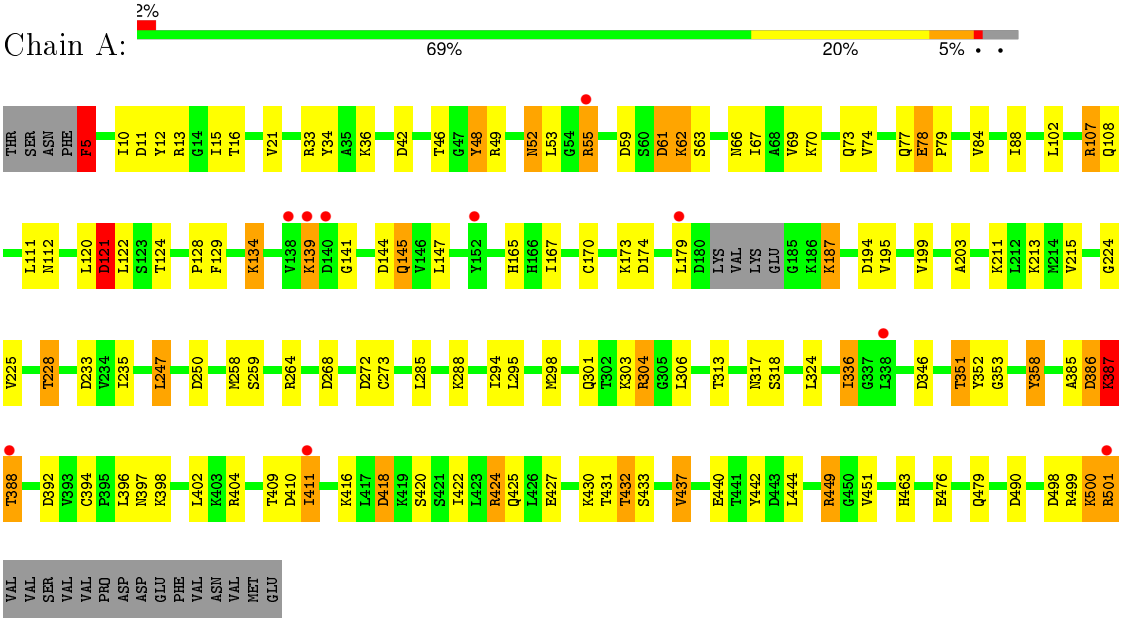
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	92	Total	O	0	0
			92	92		
3	B	69	Total	O	0	0
			69	69		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

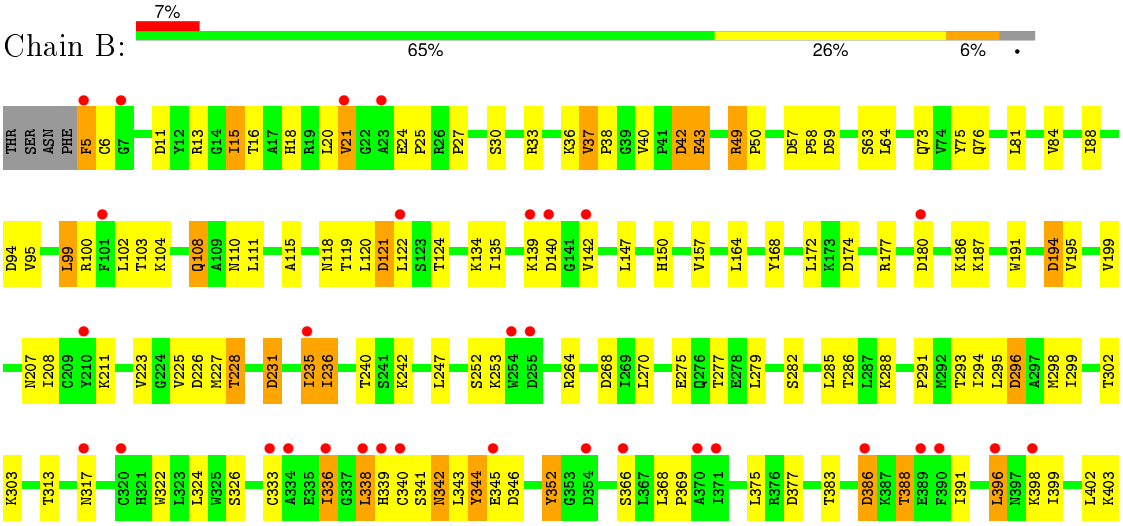
- Molecule 1: RNA-DIRECTED RNA POLYMERASE

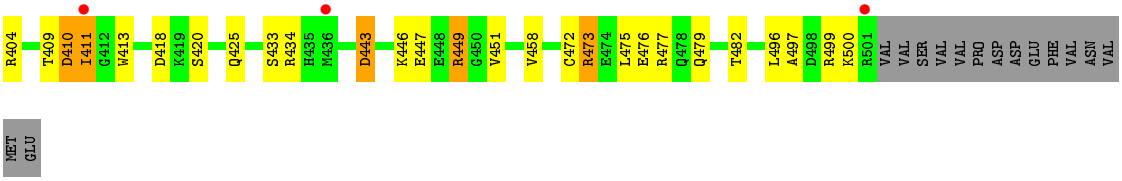
Chain A:



- Molecule 1: RNA-DIRECTED RNA POLYMERASE

Chain B:




R404
T409
D410
I411
G412
W413
D418
K419
S420
Q425
S433
R434
H435
M436
D443
K446
E447
E448
R449
G450
V451
V458
C472
R473
E474
L475
E476
R477
Q478
Q479
T482
L496
A497
D498
R499
K500
R501
VAL
VAL
SER
VAL
VAL
PRO
ASP
ASP
GLU
PHE
VAL
ASN
VAL
MET
GLU

4 Data and refinement statistics (i)

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 34.47 – 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
$< I/\sigma(I) >$ [1]	3.45 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, R_{free}	0.217 , 0.265 0.212 , 0.258	Depositor DCC
R_{free} test set	1306 reflections (3.16%)	DCC
Wilson B-factor (Å^2)	47.5	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 46.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 42667 reflections	Xtriage
F_o,F_c correlation	0.94	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.46	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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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:B:108:GLN:HG3	1:B:207:ASN:HB3	1.81	0.62
1:A:77:GLN:O	1:A:304:ARG:HD2	1.99	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: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: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:B:344:TYR:H	1:B:344:TYR:HD1	1.54	0.56
1:A:67:ILE:HG21	1:A:187:LYS:HE2	1.87	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:B:333:CYS:O	1:B:338:LEU:N	2.39	0.55
1:A:112:ASN:ND2	1:B:296:ASP:OD1	2.38	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:476:GLU:HA	1:B:479:GLN:NE2	2.22	0.54
1:B:411:ILE:HG13	1:B:497:ALA:HA	1.89	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:B:472:CYS:O	1:B:476:GLU:HG3	2.10	0.52
1:A:15:ILE:HG22	1:A:73:GLN:HG2	1.91	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: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:B:164:LEU:N	1:B:286:THR:HG22	2.24	0.50
1:A:84:VAL:HG22	1:A:88:ILE:HG21	1.93	0.50
1:B:236:ILE:HG21	1:B:413:TRP:CE2	2.47	0.50
1:B:231:ASP:O	1:B:235:ILE:HG23	2.11	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:258:MET:HE1	1:A:324:LEU:HD11	1.93	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:B:449:ARG:HB3	1:B:482:THR:HG21	1.96	0.47
1:A:213:LYS:HG3	1:A:224:GLY:HA3	1.97	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: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: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: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:409:THR:HG21	1:A:411:ILE:HG22	1.99	0.44
1:A:5:PHE:CE1	1:A:167:ILE:HD12	2.51	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:B:37:VAL:HA	1:B:38:PRO:HD3	1.84	0.43
1:A:258:MET:HE2	1:A:259:SER:H	1.83	0.43
1:B:24:GLU:HA	1:B:25:PRO:HD2	1.90	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:B:15:ILE:CD1	1:B:73:GLN:HG2	2.49	0.43
1:A:303:LYS:NZ	3:A:578:HOH:O	2.52	0.43
1:A:49:ARG:HD3	1:A:53:LEU:CD2	2.48	0.43
1:A:301:GLN:N	1:A:301:GLN:CD	2.72	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:B:49:ARG:HG3	1:B:49:ARG:NH1	2.35	0.42
1:A:387:LYS:HD2	1:A:387:LYS:H	1.84	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: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: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: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:104:LYS:HA	1:B:104:LYS:HD3	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%)	14 24
1	B	495/516 (96%)	475 (96%)	19 (4%)	1 (0%)	52 75
All	All	984/1032 (95%)	938 (95%)	38 (4%)	8 (1%)	24 41

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

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%)	10 19
1	B	427/446 (96%)	370 (87%)	57 (13%)	5 9
All	All	850/892 (95%)	752 (88%)	98 (12%)	7 13

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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Mol	Chain	Res	Type
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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Mol	Chain	Res	Type
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:

Mol	Chain	Res	Type
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

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

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

There are no such residues in this entry.

5.8 Polymer linkage issues

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^{th} 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	10 (2%)	68	72	16, 26, 50, 66	0
1	B	497/516 (96%)	0.40	35 (7%)	19	22	14, 28, 47, 64	0
All	All	990/1032 (95%)	0.24	45 (4%)	37	42	14, 27, 48, 66	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	5	PHE	5.4
1	B	336	ILE	4.8
1	B	21	VAL	4.4
1	B	333	CYS	4.4
1	A	140	ASP	4.3
1	B	142	VAL	4.1
1	B	339	HIS	4.0
1	A	138	VAL	3.9
1	B	340	CYS	3.8
1	B	411	ILE	3.7
1	B	366	SER	3.7
1	B	139	LYS	3.5
1	B	389	GLU	3.3
1	B	371	ILE	3.3
1	B	23	ALA	3.3
1	B	390	PHE	3.3
1	B	254	TRP	3.3
1	B	398	LYS	3.3
1	B	370	ALA	3.2
1	B	140	ASP	3.2
1	B	338	LEU	3.1
1	A	55	ARG	3.0
1	B	320	CYS	2.7
1	B	317	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	179	LEU	2.6
1	B	255	ASP	2.6
1	B	396	LEU	2.6
1	B	334	ALA	2.6
1	A	501	ARG	2.5
1	A	411	ILE	2.5
1	B	354	ASP	2.5
1	B	122	LEU	2.5
1	B	501	ARG	2.4
1	A	388	THR	2.4
1	B	101	PHE	2.3
1	B	7	GLY	2.3
1	B	386	ASP	2.3
1	B	180	ASP	2.2
1	B	235	ILE	2.1
1	A	139	LYS	2.1
1	B	210	TYR	2.1
1	B	345	GLU	2.1
1	A	338	LEU	2.1
1	A	152	TYR	2.0
1	B	436	MET	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^{th} 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^2)	Q<0.9
2	LU	B	517	1/1	0.92	0.26	1.97	55,55,55,55	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	LU	A	517	1/1	0.84	0.26	-	60,60,60,60	1

6.5 Other polymers (i)

There are no such residues in this entry.