W O R L D W I D E

wwPDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

May 21, 2020 – 06:34 am BST

PDB ID	:	5OVN
Title	:	Crystal Structure of FIV Reverse Transcriptase
Authors	:	Galilee, M.; Alian, A.
Deposited on	:	2017-08-29
Resolution	:	2.94 Å(reported)

The following versions of software and data (see references (i)) 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 (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.94 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	Percentile Ranks	Value
Rfree		0.267
Clashscore		17
Ramachandran outliers		0.5%
Sidechain outliers		2.7%
RSRZ outliers		7.5%

Worse   Better

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
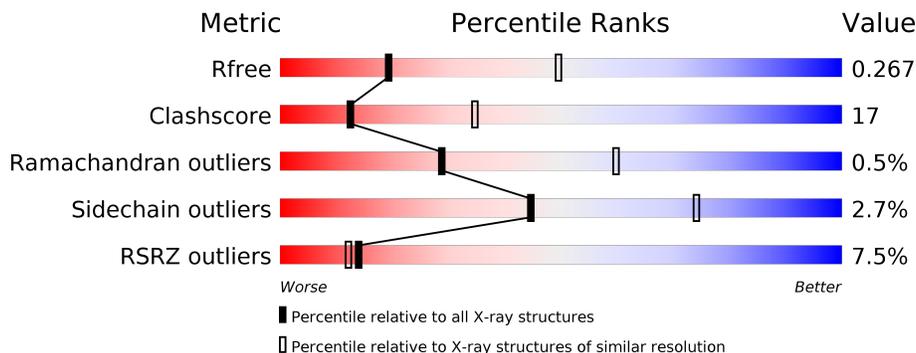
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2969 (2.98-2.90)
Clashscore	141614	3218 (2.98-2.90)
Ramachandran outliers	138981	3122 (2.98-2.90)
Sidechain outliers	138945	3124 (2.98-2.90)
RSRZ outliers	127900	2902 (2.98-2.90)

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 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 <=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	532	9% 66% 32% •
2	B	428	5% 62% 31% • 5%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7468 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 POL protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	530	Total 4175	C 2678	N 704	O 780	S 13	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	124	ALA	SER	conflict	UNP Q66972
A	466	GLN	LYS	conflict	UNP Q66972

- Molecule 2 is a protein called POL protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	405	Total 3256	C 2086	N 559	O 602	S 9	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	124	ALA	SER	conflict	UNP Q66972

- Molecule 3 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	16	Total 16	O 16	0	0
3	B	21	Total 21	O 21	0	0

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 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: POL protein

- Molecule 2: POL protein

L288 R292 Q293 K296 A305 K306 K307 A308 I309 E310 K322 E323 L324 K327 L330 P333 H334 Q335 Y338 Q339 K343 D344 P345 E346 K347 I348 Y351 G352 K353 M354 S355 R356 Q357 L369 K374 I375 R376 I381 E386 P387 R388 P392 T393 S394 R395

E399 S400 N401 L402 I403 N404 S405 L408 Y417 L422 N423 I424 K425 R426 A427 L428 S429
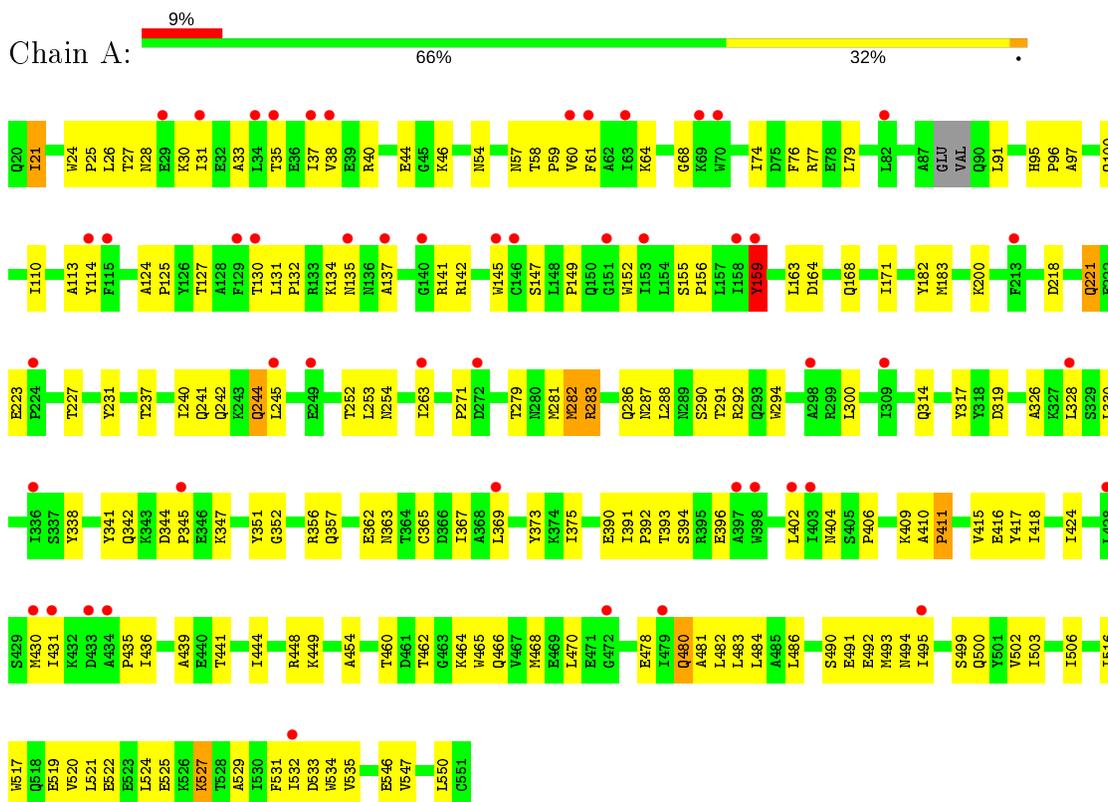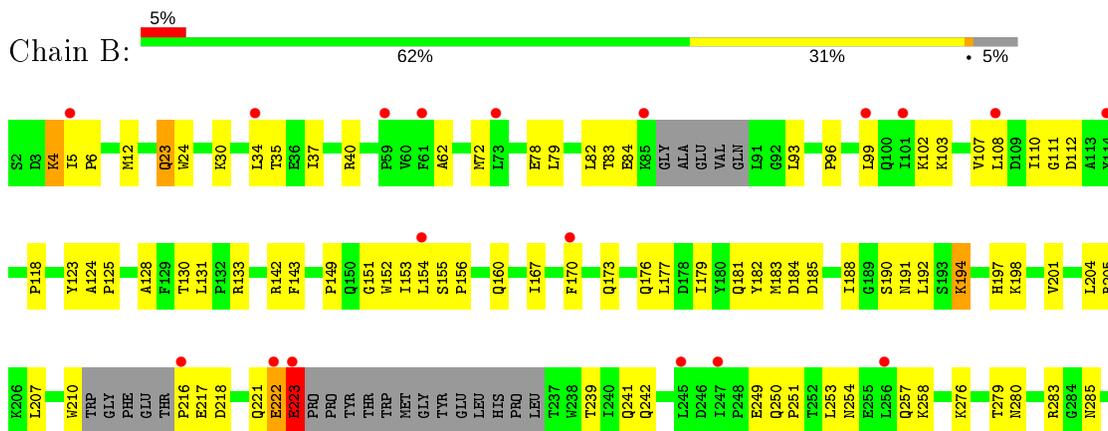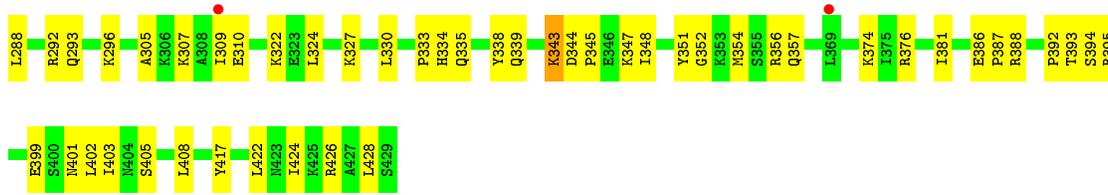
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	127.14Å 127.14Å 191.34Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	95.44 – 2.94 110.11 – 2.94	Depositor EDS
% Data completeness (in resolution range)	96.7 (95.44-2.94) 96.7 (110.11-2.94)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.24 (at 2.96Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.219 , 0.266 0.221 , 0.267	Depositor DCC
R_{free} test set	1828 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å^2)	83.9	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 85.2	EDS
L-test for twinning [2]	$<|L|> = 0.48$, $<L^2> = 0.31$	Xtriage
Estimated twinning fraction	0.026 for -h,-k,l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	7468	wwPDB-VP
Average B, all atoms (Å^2)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $<|L|>$, $<L^2>$ 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)

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	0.33	1/4279 (0.0%)	0.59	1/5830 (0.0%)
2	B	0.48	3/3333 (0.1%)	0.76	7/4528 (0.2%)
All	All	0.41	4/7612 (0.1%)	0.67	8/10358 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
2	B	0	4
All	All	0	7

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	222	GLU	C-N	19.46	1.78	1.34
2	B	223	GLU	C-N	-7.19	1.17	1.34
2	B	221	GLN	C-N	6.16	1.48	1.34
1	A	159	TYR	CD2-CE2	-5.09	1.31	1.39

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	222	GLU	O-C-N	-21.73	87.93	122.70
2	B	223	GLU	O-C-N	-16.30	96.62	122.70
2	B	222	GLU	CA-C-N	14.66	149.44	117.20
2	B	222	GLU	C-N-CA	10.63	148.28	121.70
2	B	223	GLU	CA-C-N	10.17	139.57	117.20
2	B	408	LEU	CB-CG-CD1	-6.42	100.09	111.00
2	B	408	LEU	CA-CB-CG	6.01	129.12	115.30
1	A	21	ILE	CG1-CB-CG2	-5.60	99.07	111.40

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	182	TYR	Peptide
1	A	223	GLU	Peptide
1	A	344	ASP	Peptide
2	B	182	TYR	Peptide
2	B	223	GLU	Mainchain
2	B	343	LYS	Peptide
2	B	357	GLN	Peptide

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	4175	0	4064	152	0
2	B	3256	0	3241	103	0
3	A	16	0	0	2	0
3	B	21	0	0	0	0
All	All	7468	0	7305	248	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 17.

All (248) 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:222:GLU:C	2:B:223:GLU:N	1.78	1.36
2:B:23:GLN:NE2	2:B:24:TRP:O	1.64	1.29
1:A:522:GLU:C	1:A:525:GLU:OE2	1.94	1.05
1:A:21:ILE:HD11	1:A:58:THR:HA	1.36	1.03
1:A:522:GLU:O	1:A:525:GLU:OE2	1.80	0.99
1:A:21:ILE:HD12	1:A:21:ILE:O	1.68	0.91
1:A:127:THR:HG21	1:A:145:TRP:HB2	1.54	0.89
1:A:127:THR:HG21	1:A:145:TRP:H	1.40	0.86
1:A:522:GLU:HA	1:A:525:GLU:OE2	1.76	0.86
1:A:522:GLU:CA	1:A:525:GLU:OE2	2.24	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:VAL:HG23	1:A:74:ILE:HG13	1.59	0.84
2:B:222:GLU:O	2:B:223:GLU:N	2.13	0.81
1:A:506:ILE:HG21	1:A:532:ILE:HG21	1.63	0.81
1:A:441:THR:HA	1:A:494:ASN:HB2	1.64	0.79
1:A:522:GLU:HA	1:A:525:GLU:CD	2.02	0.79
1:A:54:ASN:HB3	1:A:142:ARG:HH21	1.49	0.75
1:A:21:ILE:HD12	1:A:21:ILE:C	2.04	0.74
2:B:23:GLN:NE2	2:B:24:TRP:N	2.36	0.73
1:A:127:THR:CG2	1:A:145:TRP:H	2.02	0.72
1:A:21:ILE:HD11	1:A:58:THR:CA	2.18	0.72
1:A:460:THR:HG23	1:A:462:THR:O	1.88	0.71
2:B:102:LYS:HA	2:B:191:ASN:HD21	1.54	0.71
1:A:436:ILE:O	1:A:436:ILE:HD12	1.90	0.71
1:A:46:LYS:HA	1:A:147:SER:HB2	1.73	0.70
1:A:522:GLU:HA	1:A:525:GLU:OE1	1.91	0.70
1:A:535:VAL:CG1	2:B:257:GLN:HB3	2.22	0.69
2:B:23:GLN:HE22	2:B:24:TRP:C	1.90	0.69
2:B:250:GLN:OE1	2:B:293:GLN:NE2	2.25	0.69
2:B:354:MET:CE	2:B:374:LYS:HD3	2.24	0.68
1:A:486:LEU:HA	1:A:493:MET:HE1	1.74	0.67
1:A:24:TRP:HE3	1:A:25:PRO:HD2	1.61	0.66
1:A:466:GLN:NE2	3:A:602:HOH:O	2.29	0.66
1:A:535:VAL:HG11	2:B:257:GLN:HB3	1.78	0.66
2:B:253:LEU:O	2:B:257:GLN:HG3	1.95	0.66
2:B:110:ILE:O	2:B:112:ASP:N	2.25	0.65
1:A:330:LEU:HD12	1:A:424:ILE:HG13	1.79	0.64
1:A:393:THR:OG1	1:A:424:ILE:HB	1.97	0.64
2:B:103:LYS:H	2:B:191:ASN:ND2	1.95	0.64
2:B:254:ASN:HA	2:B:257:GLN:HE21	1.63	0.63
1:A:134:LYS:HB3	1:A:137:ALA:HB2	1.80	0.62
1:A:436:ILE:HD13	1:A:439:ALA:HB3	1.82	0.62
2:B:327:LYS:HD3	2:B:424:ILE:HG21	1.82	0.61
2:B:179:ILE:HG13	2:B:188:ILE:HD13	1.80	0.61
2:B:30:LYS:O	2:B:34:LEU:HB2	2.00	0.61
1:A:127:THR:HG21	1:A:145:TRP:CB	2.30	0.60
2:B:23:GLN:NE2	2:B:23:GLN:C	2.54	0.60
1:A:516:ILE:HD12	1:A:516:ILE:H	1.66	0.60
1:A:517:TRP:CE3	1:A:520:VAL:HG11	2.36	0.60
1:A:522:GLU:O	1:A:525:GLU:CD	2.40	0.60
1:A:317:TYR:O	1:A:347:LYS:NZ	2.34	0.59
2:B:23:GLN:NE2	2:B:24:TRP:C	2.53	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:399:GLU:HA	2:B:402:LEU:HG	1.84	0.59
1:A:38:VAL:HG11	1:A:131:LEU:CD1	2.33	0.59
1:A:21:ILE:CD1	1:A:21:ILE:C	2.71	0.58
2:B:322:LYS:NZ	2:B:345:PRO:HD2	2.17	0.58
1:A:155:SER:HB2	1:A:159:TYR:CD1	2.38	0.58
2:B:205:ARG:NH2	2:B:217:GLU:OE2	2.37	0.58
1:A:319:ASP:H	1:A:342:GLN:HE22	1.50	0.58
2:B:354:MET:HE3	2:B:374:LYS:HD3	1.85	0.58
1:A:409:LYS:HG2	2:B:330:LEU:HD22	1.85	0.57
2:B:176:GLN:HG2	2:B:177:LEU:HD23	1.85	0.57
2:B:285:ASN:O	2:B:292:ARG:NH2	2.38	0.57
2:B:345:PRO:O	2:B:347:LYS:HG2	2.05	0.57
1:A:444:ILE:HD11	1:A:481:ALA:C	2.25	0.57
1:A:76:PHE:HD1	1:A:79:LEU:HD21	1.69	0.57
2:B:34:LEU:HD13	2:B:62:ALA:HB2	1.85	0.57
1:A:91:LEU:HD21	2:B:130:THR:HG21	1.86	0.57
1:A:95:HIS:HD2	1:A:97:ALA:H	1.52	0.57
1:A:448:ARG:CB	1:A:550:LEU:HD11	2.35	0.56
1:A:287:ASN:HB3	1:A:290:SER:HB3	1.86	0.56
1:A:391:ILE:HD12	1:A:415:VAL:HG11	1.87	0.56
1:A:130:THR:HG22	1:A:142:ARG:HG2	1.88	0.56
1:A:356:ARG:NH1	1:A:362:GLU:O	2.37	0.56
1:A:286:GLN:O	1:A:288:LEU:HD12	2.05	0.56
2:B:393:THR:HG22	2:B:394:SER:H	1.71	0.55
1:A:482:LEU:O	1:A:483:LEU:HB3	2.06	0.55
1:A:127:THR:CG2	1:A:145:TRP:HB2	2.32	0.55
2:B:96:PRO:HG2	2:B:99:LEU:HB2	1.89	0.55
2:B:153:ILE:HG23	2:B:154:LEU:HG	1.89	0.55
2:B:83:THR:OG1	2:B:84:GLU:N	2.38	0.55
1:A:546:GLU:H	1:A:546:GLU:CD	2.10	0.55
1:A:57:ASN:OD1	1:A:130:THR:HG23	2.07	0.54
1:A:95:HIS:CD2	1:A:97:ALA:H	2.24	0.54
2:B:401:ASN:O	2:B:405:SER:HB2	2.06	0.54
2:B:12:MET:HE1	2:B:83:THR:HG22	1.88	0.54
1:A:155:SER:O	1:A:159:TYR:HB2	2.06	0.54
1:A:237:THR:CG2	1:A:314:GLN:HB2	2.38	0.54
1:A:240:ILE:HG22	1:A:241:GLN:O	2.08	0.54
1:A:26:LEU:H	1:A:135:ASN:HD21	1.56	0.54
2:B:422:LEU:HD21	2:B:426:ARG:NH2	2.24	0.53
1:A:127:THR:HG21	1:A:145:TRP:N	2.16	0.53
1:A:435:PRO:HG3	1:A:531:PHE:CZ	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:PHE:CD1	1:A:79:LEU:HD21	2.43	0.53
2:B:108:LEU:HD11	2:B:216:PRO:HA	1.90	0.53
2:B:338:TYR:CZ	2:B:352:GLY:HA3	2.43	0.53
1:A:253:LEU:HD11	1:A:282:MET:HB3	1.89	0.53
1:A:431:ILE:HD12	1:A:431:ILE:N	2.24	0.53
1:A:393:THR:HG22	1:A:394:SER:O	2.09	0.53
1:A:444:ILE:HD11	1:A:481:ALA:O	2.09	0.53
1:A:156:PRO:HG3	1:A:183:MET:SD	2.49	0.53
2:B:156:PRO:HG3	2:B:183:MET:O	2.09	0.53
2:B:239:THR:OG1	2:B:241:GLN:NE2	2.42	0.53
1:A:357:GLN:N	1:A:362:GLU:OE1	2.38	0.53
1:A:373:TYR:OH	1:A:411:PRO:HD2	2.09	0.52
1:A:33:ALA:O	1:A:37:ILE:HD13	2.09	0.52
1:A:113:ALA:HA	1:A:159:TYR:OH	2.11	0.51
2:B:354:MET:HE1	2:B:374:LYS:HD3	1.92	0.51
1:A:100:GLN:OE1	3:A:601:HOH:O	2.19	0.51
1:A:392:PRO:HA	1:A:418:ILE:O	2.10	0.51
1:A:125:PRO:C	1:A:127:THR:H	2.13	0.51
1:A:164:ASP:O	1:A:168:GLN:HB2	2.11	0.51
1:A:281:MET:HE2	1:A:294:TRP:HA	1.93	0.51
2:B:242:GLN:HG3	2:B:310:GLU:OE2	2.11	0.51
1:A:406:PRO:HB2	2:B:330:LEU:HD23	1.93	0.51
2:B:149:PRO:HG2	2:B:152:TRP:HB2	1.92	0.51
1:A:61:PHE:CE1	1:A:288:LEU:HD13	2.45	0.51
1:A:64:LYS:HZ1	1:A:68:GLY:H	1.59	0.51
1:A:252:THR:HG22	1:A:291:THR:HG22	1.93	0.50
2:B:324:LEU:HG	2:B:387:PRO:HB3	1.92	0.50
1:A:38:VAL:HG11	1:A:131:LEU:HD11	1.94	0.50
1:A:486:LEU:HA	1:A:493:MET:CE	2.42	0.50
2:B:254:ASN:HA	2:B:257:GLN:NE2	2.26	0.50
2:B:402:LEU:HD12	2:B:403:ILE:N	2.26	0.50
2:B:330:LEU:HD12	2:B:335:GLN:O	2.12	0.50
1:A:31:ILE:O	1:A:35:THR:OG1	2.26	0.50
1:A:58:THR:HG21	1:A:76:PHE:CE1	2.47	0.50
1:A:27:THR:HB	1:A:30:LYS:HG3	1.93	0.49
1:A:486:LEU:O	1:A:527:LYS:NZ	2.35	0.49
1:A:21:ILE:CD1	1:A:59:PRO:HD3	2.42	0.49
1:A:64:LYS:NZ	1:A:68:GLY:H	2.10	0.49
2:B:35:THR:HG22	2:B:131:LEU:HD21	1.94	0.49
1:A:460:THR:HG21	1:A:464:LYS:HB2	1.94	0.49
1:A:237:THR:HG23	1:A:314:GLN:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:480:GLN:O	1:A:484:LEU:HD13	2.12	0.49
2:B:280:ASN:HA	2:B:283:ARG:HG3	1.95	0.49
1:A:328:LEU:HD12	1:A:391:ILE:HG23	1.95	0.49
1:A:521:LEU:HA	1:A:524:LEU:HD12	1.95	0.49
1:A:500:GLN:HA	1:A:503:ILE:HG22	1.95	0.49
2:B:190:SER:OG	2:B:192:LEU:HG	2.13	0.49
2:B:83:THR:HG21	2:B:123:TYR:OH	2.13	0.48
2:B:5:ILE:HG22	2:B:118:PRO:HD2	1.95	0.48
1:A:245:LEU:HD21	1:A:263:ILE:HD11	1.94	0.48
1:A:155:SER:O	1:A:159:TYR:N	2.41	0.48
2:B:170:PHE:HA	2:B:173:GLN:HE21	1.79	0.48
1:A:390:GLU:HA	1:A:416:GLU:O	2.14	0.48
2:B:79:LEU:O	2:B:83:THR:HG23	2.14	0.47
1:A:244:GLN:O	1:A:244:GLN:HG3	2.14	0.47
1:A:168:GLN:HA	1:A:171:ILE:HD12	1.96	0.47
1:A:468:MET:CB	1:A:470:LEU:HD23	2.44	0.47
2:B:152:TRP:HE3	2:B:155:SER:HG	1.62	0.47
1:A:550:LEU:C	1:A:550:LEU:HD12	2.35	0.47
2:B:151:GLY:N	2:B:184:ASP:OD2	2.46	0.47
2:B:257:GLN:HE22	2:B:288:LEU:HD22	1.80	0.47
1:A:114:TYR:O	1:A:149:PRO:HD2	2.15	0.47
2:B:222:GLU:HG3	2:B:381:ILE:HG21	1.96	0.47
2:B:190:SER:HB3	2:B:197:HIS:ND1	2.30	0.47
2:B:305:ALA:O	2:B:309:ILE:HG13	2.15	0.47
1:A:96:PRO:HD3	1:A:231:TYR:CE2	2.50	0.46
1:A:254:ASN:HB2	1:A:288:LEU:HB3	1.97	0.46
1:A:356:ARG:HG3	1:A:367:ILE:HD11	1.97	0.46
2:B:399:GLU:HA	2:B:402:LEU:CG	2.45	0.46
2:B:222:GLU:N	2:B:222:GLU:OE1	2.40	0.46
1:A:252:THR:HA	1:A:291:THR:HA	1.98	0.46
2:B:198:LYS:O	2:B:201:VAL:HG12	2.16	0.46
2:B:222:GLU:CD	2:B:222:GLU:H	2.17	0.45
1:A:517:TRP:O	1:A:520:VAL:HG12	2.17	0.45
1:A:430:MET:CE	1:A:531:PHE:HA	2.46	0.45
2:B:194:LYS:HB2	2:B:194:LYS:HE2	1.74	0.45
1:A:124:ALA:N	1:A:125:PRO:HD2	2.31	0.45
2:B:4:LYS:HB3	2:B:4:LYS:HE3	1.65	0.45
1:A:241:GLN:HG3	1:A:242:GLN:N	2.32	0.45
1:A:494:ASN:HD22	1:A:531:PHE:HB3	1.82	0.45
2:B:152:TRP:CZ2	2:B:154:LEU:HD12	2.52	0.45
1:A:110:ILE:HD13	1:A:163:LEU:HD21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:460:THR:CG2	1:A:464:LYS:HB2	2.46	0.45
1:A:393:THR:O	1:A:417:TYR:HB3	2.17	0.45
2:B:190:SER:C	2:B:191:ASN:HD22	2.20	0.45
2:B:276:LYS:O	2:B:279:THR:HB	2.16	0.44
1:A:363:ASN:HD21	1:A:365:CYS:HB2	1.83	0.44
1:A:490:SER:OG	1:A:491:GLU:N	2.51	0.44
2:B:93:LEU:HD11	2:B:179:ILE:HG22	1.99	0.44
1:A:127:THR:HG22	1:A:127:THR:O	2.16	0.44
1:A:533:ASP:OD1	1:A:534:TRP:N	2.40	0.44
2:B:348:ILE:HG21	2:B:351:TYR:CE2	2.52	0.44
2:B:142:ARG:HH11	2:B:142:ARG:HG2	1.83	0.44
1:A:227:THR:HG23	1:A:241:GLN:NE2	2.33	0.44
1:A:369:LEU:HD21	1:A:410:ALA:HB1	2.00	0.44
1:A:319:ASP:HB2	1:A:347:LYS:HZ1	1.82	0.43
1:A:404:ASN:O	1:A:406:PRO:HD3	2.18	0.43
1:A:444:ILE:HA	1:A:547:VAL:HG11	1.99	0.43
1:A:449:LYS:HD3	1:A:454:ALA:HB2	2.00	0.43
2:B:37:ILE:HD13	2:B:40:ARG:HH21	1.82	0.43
1:A:61:PHE:HE1	1:A:288:LEU:HD13	1.83	0.43
1:A:402:LEU:HA	1:A:402:LEU:HD13	1.87	0.43
1:A:533:ASP:OD2	2:B:258:LYS:NZ	2.50	0.43
1:A:491:GLU:HA	1:A:527:LYS:HD3	2.00	0.43
1:A:517:TRP:CE3	1:A:520:VAL:CG1	3.01	0.43
2:B:167:ILE:HD12	2:B:167:ILE:HA	1.88	0.43
1:A:35:THR:HG23	1:A:131:LEU:HD21	2.01	0.43
2:B:307:LYS:HD2	2:B:307:LYS:HA	1.75	0.43
2:B:395:ARG:HA	2:B:417:TYR:CZ	2.54	0.42
1:A:483:LEU:CD1	1:A:519:GLU:HG3	2.49	0.42
2:B:188:ILE:CD1	2:B:204:LEU:HD23	2.50	0.42
2:B:23:GLN:CD	2:B:24:TRP:N	2.72	0.42
2:B:5:ILE:HG13	2:B:6:PRO:HD2	2.01	0.42
1:A:40:ARG:O	1:A:44:GLU:HG2	2.19	0.42
2:B:34:LEU:HD11	2:B:72:MET:HG3	2.01	0.42
2:B:249:GLU:O	2:B:251:PRO:HD3	2.18	0.42
1:A:430:MET:SD	1:A:532:ILE:HG22	2.60	0.42
2:B:327:LYS:O	2:B:338:TYR:HA	2.20	0.42
1:A:483:LEU:H	1:A:486:LEU:CD1	2.32	0.42
2:B:128:ALA:HA	2:B:143:PHE:O	2.20	0.42
2:B:296:LYS:HD3	2:B:296:LYS:HA	1.56	0.42
1:A:409:LYS:NZ	2:B:392:PRO:O	2.53	0.42
1:A:131:LEU:HD23	1:A:132:PRO:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:TYR:CZ	1:A:352:GLY:HA3	2.55	0.42
2:B:176:GLN:HG3	2:B:192:LEU:HD21	2.01	0.42
2:B:188:ILE:HD11	2:B:204:LEU:HD23	2.01	0.42
1:A:221:GLN:HE21	1:A:221:GLN:HB2	1.63	0.41
2:B:334:HIS:CD2	2:B:356:ARG:HD2	2.55	0.41
2:B:339:GLN:HG2	2:B:428:LEU:HD11	2.01	0.41
2:B:347:LYS:HE3	2:B:347:LYS:HB3	1.92	0.41
2:B:107:VAL:HG13	2:B:218:ASP:HB3	2.02	0.41
1:A:492:GLU:C	1:A:493:MET:HG2	2.40	0.41
1:A:499:SER:HB3	1:A:502:VAL:HG22	2.01	0.41
1:A:283:ARG:H	1:A:292:ARG:NH1	2.18	0.41
1:A:478:GLU:HG2	1:A:499:SER:HB2	2.01	0.41
1:A:271:PRO:HG3	1:A:351:TYR:HB3	2.02	0.41
1:A:341:TYR:HB2	1:A:347:LYS:O	2.21	0.41
2:B:78:GLU:O	2:B:82:LEU:HD13	2.21	0.41
1:A:155:SER:N	1:A:156:PRO:CD	2.84	0.41
1:A:279:THR:HA	1:A:282:MET:HG3	2.01	0.41
2:B:152:TRP:HB3	2:B:155:SER:OG	2.21	0.41
2:B:292:ARG:HA	2:B:292:ARG:HD3	1.91	0.41
2:B:376:ARG:HG3	2:B:386:GLU:HG3	2.01	0.41
2:B:333:PRO:HB2	2:B:334:HIS:ND1	2.36	0.41
1:A:328:LEU:O	1:A:392:PRO:HD3	2.21	0.41
2:B:160:GLN:NE2	2:B:181:GLN:HB3	2.36	0.41
1:A:436:ILE:HG21	1:A:529:ALA:HB1	2.02	0.40
2:B:123:TYR:HH	2:B:152:TRP:HE1	1.66	0.40
2:B:124:ALA:N	2:B:125:PRO:HD2	2.36	0.40
2:B:293:GLN:HA	2:B:293:GLN:NE2	2.36	0.40
1:A:347:LYS:HB3	1:A:347:LYS:HE3	1.88	0.40
1:A:396:GLU:HG2	1:A:396:GLU:H	1.73	0.40
1:A:495:ILE:O	1:A:532:ILE:HA	2.21	0.40
1:A:300:LEU:HA	1:A:300:LEU:HD23	1.79	0.40
1:A:326:ALA:HB1	1:A:375:ILE:HD13	2.03	0.40
2:B:204:LEU:HD12	2:B:207:LEU:HB3	2.03	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	526/532 (99%)	475 (90%)	49 (9%)	2 (0%)	34	64
2	B	399/428 (93%)	372 (93%)	24 (6%)	3 (1%)	19	49
All	All	925/960 (96%)	847 (92%)	73 (8%)	5 (0%)	29	60

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	345	PRO
2	B	344	ASP
2	B	111	GLY
2	B	343	LYS
1	A	411	PRO

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	432/467 (92%)	418 (97%)	14 (3%)	39	70
2	B	349/384 (91%)	342 (98%)	7 (2%)	55	80
All	All	781/851 (92%)	760 (97%)	21 (3%)	44	74

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	ASN

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Mol	Chain	Res	Type
1	A	77	ARG
1	A	141	ARG
1	A	152	TRP
1	A	159	TYR
1	A	200	LYS
1	A	218	ASP
1	A	221	GLN
1	A	244	GLN
1	A	282	MET
1	A	283	ARG
1	A	465	TRP
1	A	480	GLN
1	A	527	LYS
2	B	4	LYS
2	B	23	GLN
2	B	133	ARG
2	B	185	ASP
2	B	194	LYS
2	B	210	TRP
2	B	388	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	HIS
1	A	241	GLN
1	A	342	GLN
2	B	23	GLN
2	B	174	ASN
2	B	191	ASN
2	B	241	GLN
2	B	250	GLN
2	B	257	GLN
2	B	293	GLN
2	B	335	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)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	222:GLU	C	223:GLU	N	1.78

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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(Å²)	Q<0.9
1	A	530/532 (99%)	0.74	50 (9%)	8	7	33, 99, 165, 224	0
2	B	405/428 (94%)	0.47	20 (4%)	29	29	45, 88, 146, 179	0
All	All	935/960 (97%)	0.63	70 (7%)	14	12	33, 93, 159, 224	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	434	ALA	5.7
1	A	70	TRP	5.5
1	A	38	VAL	5.2
1	A	146	CYS	4.9
1	A	145	TRP	4.7
1	A	403	ILE	4.5
1	A	140	GLY	4.3
2	B	216	PRO	4.1
1	A	402	LEU	4.1
2	B	5	ILE	4.0
1	A	60	VAL	3.9
1	A	153	ILE	3.8
1	A	433	ASP	3.8
1	A	151	GLY	3.7
1	A	245	LEU	3.7
1	A	34	LEU	3.6
1	A	129	PHE	3.6
1	A	31	ILE	3.6
1	A	61	PHE	3.5
1	A	37	ILE	3.3
2	B	222	GLU	3.2
2	B	61	PHE	3.2
1	A	369	LEU	3.2
2	B	223	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
2	B	34	LEU	3.1
1	A	249	GLU	3.1
1	A	130	THR	2.9
2	B	369	LEU	2.8
1	A	430	MET	2.8
1	A	137	ALA	2.8
2	B	245	LEU	2.7
1	A	224	PRO	2.7
1	A	272	ASP	2.7
1	A	328	LEU	2.6
1	A	115	PHE	2.6
1	A	479	ILE	2.6
2	B	73	LEU	2.6
2	B	85	LYS	2.5
1	A	35	THR	2.5
1	A	336	ILE	2.5
2	B	99	LEU	2.5
1	A	114	TYR	2.5
2	B	114	TYR	2.5
1	A	495	ILE	2.4
1	A	63	ILE	2.4
1	A	532	ILE	2.4
1	A	69	LYS	2.3
2	B	108	LEU	2.3
2	B	247	ILE	2.3
1	A	158	ILE	2.3
1	A	431	ILE	2.3
1	A	135	ASN	2.3
1	A	29	GLU	2.3
1	A	159	TYR	2.3
1	A	298	ALA	2.2
1	A	345	PRO	2.2
2	B	170	PHE	2.2
2	B	309	ILE	2.2
1	A	82	LEU	2.1
1	A	263	ILE	2.1
1	A	397	ALA	2.1
1	A	213	PHE	2.1
1	A	428	LEU	2.1
2	B	59	PRO	2.1
1	A	398	TRP	2.0
1	A	472	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	154	LEU	2.0
2	B	101	ILE	2.0
1	A	309	ILE	2.0
2	B	256	LEU	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.