



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 01:12 AM UTC

PDB ID : 5Z7D / pdb_00005z7d
Title : p204HINab-dsDNA complex structure
Authors : Jin, T.; Jiang, J.; Xiao, T.S.
Deposited on : 2018-01-28
Resolution : 4.50 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

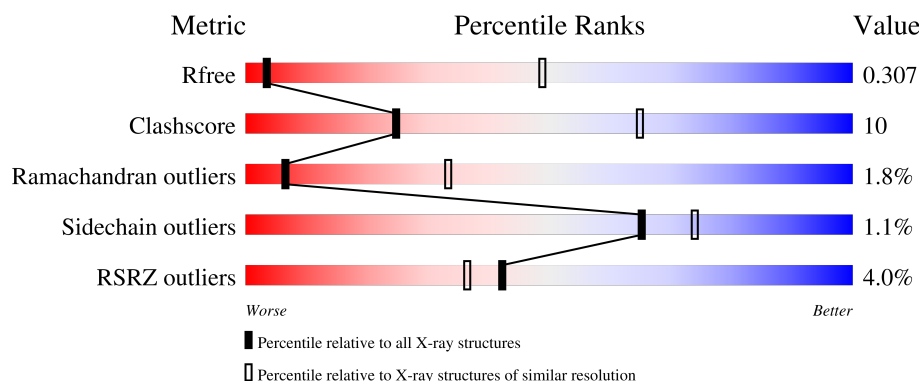
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.50 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.



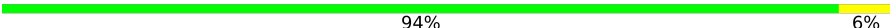
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1127 (5.10-3.90)
Clashscore	190562	1002 (5.06-3.94)
Ramachandran outliers	187476	1060 (5.10-3.90)
Sidechain outliers	187428	1043 (5.10-3.90)
RSRZ outliers	180081	1122 (5.10-3.90)

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 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	412	6% 79% 16% .
1	B	412	3% 71% 25% .
1	C	412	3% 68% 25% .
2	I	16	94% 6%
2	K	16	62% 38%

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Mol	Chain	Length	Quality of chain
3	J	16	 94%6%
3	L	16	 88%12%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10624 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 Interferon-activable protein 204.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	395	Total	C	N	O	S	0	0	0
			3087	1972	529	571	15			
1	B	397	Total	C	N	O	S	0	0	0
			3127	1993	534	584	16			
1	C	396	Total	C	N	O	S	0	0	0
			3098	1978	534	571	15			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	212	GLY	-	expression tag	UNP P0DOV2
A	213	SER	-	expression tag	UNP P0DOV2
A	214	VAL	-	expression tag	UNP P0DOV2
A	215	ASP	-	expression tag	UNP P0DOV2
A	620	ALA	-	expression tag	UNP P0DOV2
A	621	ALA	-	expression tag	UNP P0DOV2
A	622	ALA	-	expression tag	UNP P0DOV2
A	623	SER	-	expression tag	UNP P0DOV2
B	212	GLY	-	expression tag	UNP P0DOV2
B	213	SER	-	expression tag	UNP P0DOV2
B	214	VAL	-	expression tag	UNP P0DOV2
B	215	ASP	-	expression tag	UNP P0DOV2
B	620	ALA	-	expression tag	UNP P0DOV2
B	621	ALA	-	expression tag	UNP P0DOV2
B	622	ALA	-	expression tag	UNP P0DOV2
B	623	SER	-	expression tag	UNP P0DOV2
C	212	GLY	-	expression tag	UNP P0DOV2
C	213	SER	-	expression tag	UNP P0DOV2
C	214	VAL	-	expression tag	UNP P0DOV2
C	215	ASP	-	expression tag	UNP P0DOV2
C	620	ALA	-	expression tag	UNP P0DOV2
C	621	ALA	-	expression tag	UNP P0DOV2
C	622	ALA	-	expression tag	UNP P0DOV2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	623	SER	-	expression tag	UNP P0DOV2

- Molecule 2 is a DNA chain called DNA (5'-D(P*CP*CP*AP*TP*CP*AP*GP*AP*AP*AP*GP*AP*GP*AP*GP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	16	Total	C	N	O	P	0	0	0
			331	156	69	90	16			
2	K	16	Total	C	N	O	P	0	0	0
			331	156	69	90	16			

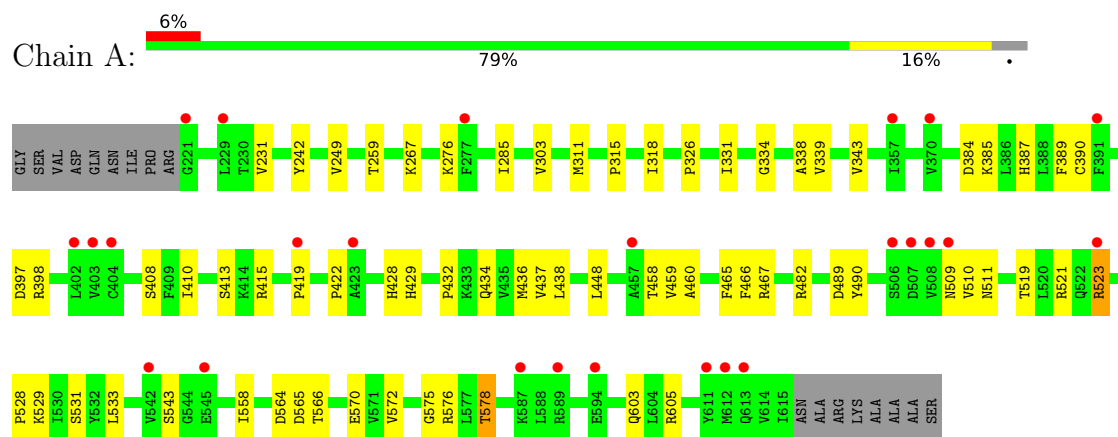
- Molecule 3 is a DNA chain called DNA (5'-D(P*CP*CP*AP*TP*CP*AP*GP*AP*AP*AP*GP*AP*GP*AP*GP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	J	16	Total	C	N	O	P	0	0	0
			325	156	51	102	16			
3	L	16	Total	C	N	O	P	0	0	0
			325	156	51	102	16			

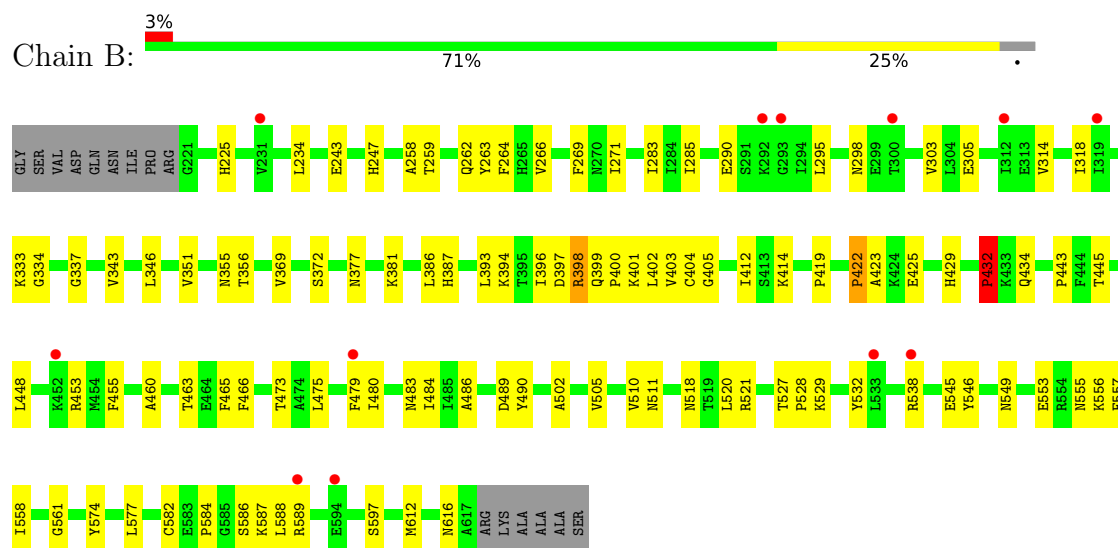
3 Residue-property plots [i](#)

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.

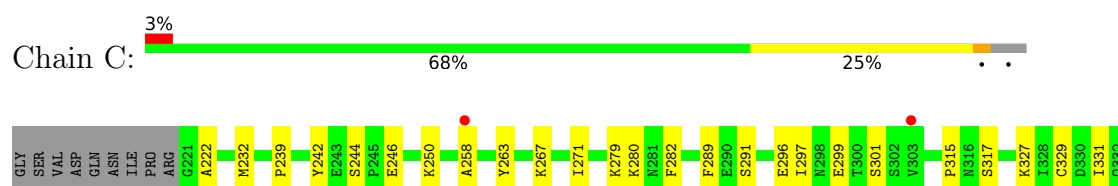
• Molecule 1: Interferon-activable protein 204

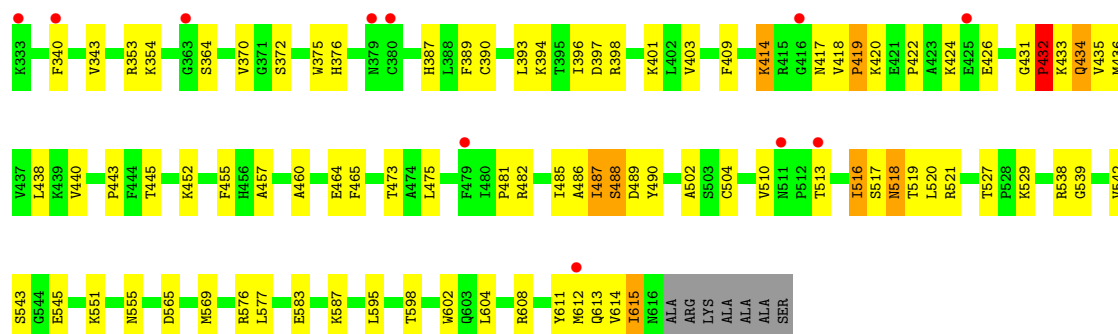


• Molecule 1: Interferon-activable protein 204



• Molecule 1: Interferon-activable protein 204





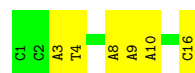
- Molecule 2: DNA (5'-D(P*CP*CP*AP*TP*CP*AP*GP*AP*AP*AP*GP*AP*GP*AP*GP*C)-3')

Chain I: 94% 6%



- Molecule 2: DNA (5'-D(P*CP*CP*AP*TP*CP*AP*GP*AP*AP*AP*GP*AP*GP*AP*GP*C)-3')

Chain K: 62% 38%



- Molecule 3: DNA (5'-D(P*CP*CP*AP*TP*CP*AP*GP*AP*AP*AP*GP*AP*GP*AP*GP*C)-3')

Chain J: 94% 6%



- Molecule 3: DNA (5'-D(P*CP*CP*AP*TP*CP*AP*GP*AP*AP*AP*GP*AP*GP*AP*GP*C)-3')

Chain L: 88% 12%



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	101.39Å 101.39Å 783.61Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.26 – 4.50 47.26 – 4.50	Depositor EDS
% Data completeness (in resolution range)	91.9 (47.26-4.50) 91.8 (47.26-4.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 4.45Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.260 , 0.297 0.261 , 0.307	Depositor DCC
R_{free} test set	709 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	112.1	Xtriage
Anisotropy	0.226	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 130.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	10624	wwPDB-VP
Average B, all atoms (Å ²)	162.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% 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 [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	0.24	0/3154	0.58	0/4266
1	B	0.21	0/3193	0.39	1/4317 (0.0%)
1	C	0.24	0/3164	0.43	3/4277 (0.1%)
2	I	0.19	0/373	0.35	0/573
2	K	0.18	0/373	0.34	0/573
3	J	0.19	0/361	0.40	0/555
3	L	0.18	0/361	0.40	0/555
All	All	0.22	0/10979	0.46	4/15116 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	C	487	ILE	CA-C-N	6.30	133.58	121.54
1	C	487	ILE	C-N-CA	6.30	133.58	121.54
1	B	432	PRO	N-CA-CB	-5.62	97.35	103.25
1	C	432	PRO	N-CA-CB	-5.16	97.83	103.25

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	3087	0	3037	43	0
1	B	3127	0	3100	76	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3098	0	3063	72	0
2	I	331	0	178	3	0
2	K	331	0	178	5	0
3	J	325	0	184	4	0
3	L	325	0	184	6	0
All	All	10624	0	9924	194	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 10.

All (194) 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:C:434:GLN:HA	1:C:485:ILE:O	1.68	0.93
1:C:434:GLN:HA	1:C:486:ALA:HA	1.55	0.89
3:L:16:DG:H4'	3:L:1:DG:H5'	1.58	0.86
1:B:258:ALA:HA	1:B:263:TYR:HA	1.66	0.77
1:B:434:GLN:OE1	1:B:510:VAL:HG12	1.85	0.77
1:A:529:LYS:HB3	1:A:566:THR:HG21	1.69	0.73
1:C:577:LEU:HB3	1:C:612:MET:HE2	1.74	0.70
1:C:615:ILE:H	1:C:615:ILE:HD12	1.57	0.69
1:A:384:ASP:HA	1:A:415:ARG:HA	1.73	0.69
1:C:353:ARG:HG3	1:C:354:LYS:HG3	1.74	0.69
1:C:587:LYS:HB3	1:C:615:ILE:HD11	1.75	0.69
1:B:577:LEU:HB3	1:B:612:MET:HE2	1.73	0.69
1:B:465:PHE:HB3	1:B:520:LEU:HD11	1.74	0.68
1:C:434:GLN:CA	1:C:485:ILE:O	2.42	0.68
1:B:414:LYS:NZ	3:L:2:DC:OP1	2.23	0.67
1:C:279:LYS:HE3	1:C:280:LYS:HE2	1.77	0.67
1:C:517:SER:O	1:C:519:THR:N	2.27	0.66
1:A:267:LYS:NZ	1:A:390:CYS:SG	2.67	0.66
1:C:487:ILE:HA	1:C:504:CYS:O	1.96	0.66
1:B:443:PRO:HA	1:B:455:PHE:HB3	1.77	0.65
1:B:445:THR:HG21	1:C:538:ARG:NH2	2.12	0.64
1:A:315:PRO:HD2	1:A:318:ILE:HD12	1.80	0.64
1:A:570:GLU:O	1:A:603:GLN:HA	1.97	0.63
1:B:528:PRO:HB3	1:B:532:TYR:HD2	1.64	0.62
1:A:558:ILE:HD11	1:A:578:THR:HG23	1.81	0.62
1:A:519:THR:O	1:A:523:ARG:HB2	1.99	0.62
1:A:448:LEU:HD21	1:A:576:ARG:HD3	1.83	0.61
1:B:397:ASP:O	1:B:398:ARG:CB	2.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:289:PHE:HB2	1:C:296:GLU:HB2	1.82	0.61
1:A:326:PRO:HG2	1:A:331:ILE:HD11	1.83	0.60
1:C:267:LYS:NZ	1:C:390:CYS:SG	2.67	0.60
1:C:434:GLN:CA	1:C:486:ALA:HA	2.27	0.60
1:C:297:ILE:HG23	1:C:301:SER:HB2	1.83	0.59
1:B:369:VAL:HG22	1:B:402:LEU:HB2	1.85	0.58
1:B:386:LEU:HD23	1:B:412:ILE:HG23	1.86	0.58
1:B:397:ASP:C	1:B:398:ARG:HG2	2.29	0.57
1:C:475:LEU:HD11	1:C:502:ALA:HA	1.86	0.57
1:B:269:PHE:HB2	1:B:298:ASN:HA	1.87	0.57
1:C:340:PHE:HE2	1:C:393:LEU:HB2	1.68	0.57
1:B:266:VAL:HG22	1:B:295:LEU:HB2	1.85	0.56
1:B:538:ARG:CZ	1:B:597:SER:HB3	2.36	0.56
1:C:518:ASN:O	1:C:521:ARG:HB2	2.06	0.56
1:A:389:PHE:O	1:A:408:SER:HA	2.05	0.56
2:I:1:DC:H5"	2:K:16:DC:C6	2.40	0.56
1:B:355:ASN:HB3	1:B:372:SER:HB3	1.87	0.56
1:C:370:VAL:HB	1:C:403:VAL:HG12	1.88	0.56
1:B:285:ILE:HG22	1:B:303:VAL:HG22	1.86	0.56
1:C:569:MET:HE1	1:C:604:LEU:HG	1.87	0.56
1:A:334:GLY:HA2	1:B:334:GLY:HA2	1.88	0.55
1:B:397:ASP:O	1:B:398:ARG:CG	2.55	0.55
1:C:576:ARG:NH2	1:C:608:ARG:O	2.38	0.55
1:C:239:PRO:HB3	1:C:271:ILE:HD11	1.88	0.55
1:A:429:HIS:ND1	1:A:490:TYR:CE2	2.75	0.54
1:C:372:SER:HA	1:C:376:HIS:HB2	1.87	0.54
1:B:582:CYS:SG	1:B:588:LEU:HG	2.47	0.54
1:C:327:LYS:HD2	1:C:364:SER:HB3	1.89	0.54
1:B:343:VAL:HG22	1:B:387:HIS:CG	2.43	0.53
1:C:396:ILE:HB	1:C:401:LYS:HD2	1.90	0.53
1:C:440:VAL:HG23	1:C:457:ALA:HB2	1.90	0.53
1:B:225:HIS:NE2	1:B:290:GLU:OE1	2.42	0.52
1:B:397:ASP:O	1:B:398:ARG:HB2	2.09	0.52
1:C:587:LYS:CB	1:C:615:ILE:HD11	2.38	0.52
1:A:509:ASN:C	1:A:511:ASN:H	2.18	0.52
1:C:222:ALA:HB2	1:C:291:SER:HB2	1.92	0.52
1:C:250:LYS:NZ	1:C:299:GLU:OE2	2.33	0.52
1:B:480:ILE:O	1:B:483:ASN:HB2	2.09	0.52
1:B:445:THR:HG21	1:C:538:ARG:HH22	1.75	0.51
1:B:475:LEU:HD11	1:B:502:ALA:HA	1.91	0.51
1:B:394:LYS:HD3	1:B:403:VAL:HG11	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:429:HIS:CB	1:B:490:TYR:CE1	2.93	0.51
1:A:509:ASN:O	1:A:511:ASN:N	2.44	0.51
1:B:393:LEU:HD11	1:B:400:PRO:HB3	1.92	0.51
1:B:545:GLU:OE2	1:B:589:ARG:NE	2.44	0.51
1:C:615:ILE:HD12	1:C:615:ILE:N	2.22	0.51
1:B:283:ILE:HG22	1:B:305:GLU:HA	1.92	0.51
1:A:419:PRO:HD2	1:A:523:ARG:HE	1.76	0.51
1:C:239:PRO:HG3	1:C:271:ILE:HD11	1.93	0.51
1:C:551:LYS:NZ	1:C:583:GLU:OE2	2.34	0.51
1:B:484:ILE:H	1:B:484:ILE:HD12	1.77	0.50
1:A:231:VAL:HG12	1:A:259:THR:HG22	1.93	0.50
1:B:453:ARG:HB2	1:B:473:THR:HG23	1.94	0.50
2:K:3:DA:H2''	2:K:4:DT:C6	2.46	0.50
1:A:429:HIS:O	1:A:489:ASP:HA	2.12	0.49
1:C:516:ILE:HG23	1:C:520:LEU:HD23	1.94	0.49
1:B:422:PRO:HB3	1:B:466:PHE:HA	1.94	0.49
1:B:243:GLU:HG2	1:B:247:HIS:HA	1.94	0.49
1:C:436:MET:HE3	1:C:482:ARG:HA	1.94	0.49
1:B:414:LYS:HB3	3:L:1:DG:H4'	1.94	0.49
1:A:436:MET:HE3	1:A:482:ARG:HA	1.94	0.48
1:C:615:ILE:CD1	1:C:615:ILE:C	2.87	0.48
1:B:397:ASP:O	1:B:399:GLN:NE2	2.46	0.48
1:B:314:VAL:HG13	1:B:318:ILE:HD12	1.95	0.48
1:B:448:LEU:HG	1:C:598:THR:O	2.13	0.48
1:C:424:LYS:NZ	1:C:490:TYR:OH	2.29	0.48
1:A:438:LEU:HD11	1:A:460:ALA:HB2	1.96	0.48
1:A:460:ALA:HA	1:A:465:PHE:HA	1.95	0.48
1:B:529:LYS:HD3	1:B:529:LYS:HA	1.68	0.48
1:B:234:LEU:HD11	1:B:258:ALA:HB2	1.96	0.48
2:I:1:DC:H5''	2:K:16:DC:C5	2.49	0.48
1:B:397:ASP:C	1:B:398:ARG:CG	2.85	0.47
1:C:460:ALA:HA	1:C:465:PHE:HA	1.94	0.47
1:A:565:ASP:OD1	1:A:565:ASP:N	2.47	0.47
1:B:396:ILE:HD12	1:B:401:LYS:HD2	1.97	0.47
1:B:557:PHE:CE2	1:B:574:TYR:HB2	2.50	0.47
1:C:343:VAL:HG22	1:C:387:HIS:CG	2.49	0.47
1:C:595:LEU:HD11	1:C:602:TRP:HE3	1.79	0.47
1:B:586:SER:HB3	1:B:616:ASN:HB3	1.96	0.47
1:C:527:THR:HG23	1:C:545:GLU:H	1.80	0.47
1:A:242:TYR:O	1:A:249:VAL:HA	2.15	0.47
1:A:572:VAL:HB	1:A:605:ARG:HG2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:423:ALA:HB3	1:B:466:PHE:HE1	1.81	0.46
1:C:542:VAL:HG12	1:C:543:SER:H	1.79	0.46
1:B:518:ASN:HA	1:B:521:ARG:HD2	1.97	0.46
1:C:443:PRO:HA	1:C:455:PHE:HB3	1.97	0.46
1:C:611:TYR:OH	1:C:613:GLN:OE1	2.33	0.46
1:C:232:MET:HB2	1:C:282:PHE:CE2	2.51	0.46
1:A:343:VAL:HG22	1:A:387:HIS:CG	2.52	0.45
1:B:434:GLN:NE2	1:B:511:ASN:HB3	2.31	0.44
1:B:453:ARG:CB	1:B:473:THR:HG23	2.47	0.44
1:C:397:ASP:O	1:C:398:ARG:HB2	2.17	0.44
1:B:527:THR:HG21	1:B:545:GLU:O	2.17	0.44
1:C:375:TRP:CZ2	1:C:409:PHE:HA	2.52	0.44
1:C:431:GLY:O	1:C:488:SER:HA	2.18	0.44
1:C:329:CYS:HB3	1:C:364:SER:O	2.17	0.44
1:C:542:VAL:HG12	1:C:543:SER:N	2.33	0.44
1:A:276:LYS:NZ	1:A:303:VAL:O	2.43	0.43
1:B:404:CYS:SG	1:B:405:GLY:N	2.91	0.43
1:A:338:ALA:HB1	1:B:333:LYS:HD3	2.00	0.43
1:B:486:ALA:HB2	1:B:510:VAL:HG21	1.99	0.43
1:B:528:PRO:HB3	1:B:532:TYR:CD2	2.48	0.43
1:C:244:SER:C	1:C:246:GLU:H	2.26	0.43
1:C:329:CYS:SG	1:C:364:SER:HB2	2.58	0.43
1:C:529:LYS:HD3	1:C:529:LYS:HA	1.69	0.43
1:B:271:ILE:HD12	1:B:271:ILE:HA	1.88	0.43
1:B:546:TYR:O	1:B:587:LYS:HG3	2.18	0.43
1:A:467:ARG:NH2	1:A:543:SER:HB2	2.34	0.43
1:B:549:ASN:ND2	1:B:561:GLY:O	2.51	0.43
1:A:285:ILE:HG22	1:A:303:VAL:HG22	2.01	0.43
1:A:438:LEU:HB2	1:A:458:THR:O	2.18	0.43
1:B:269:PHE:HD2	1:B:298:ASN:HB3	1.83	0.43
1:C:232:MET:HE2	1:C:232:MET:HB3	1.94	0.43
1:B:549:ASN:HA	1:B:584:PRO:HB3	1.99	0.43
2:K:9:DA:H2"	2:K:10:DA:C8	2.54	0.43
1:A:564:ASP:OD1	1:A:566:THR:OG1	2.30	0.43
1:B:479:PHE:HE1	1:B:505:VAL:HG21	1.84	0.43
1:B:553:GLU:HG2	1:B:558:ILE:HG23	1.99	0.43
1:A:531:SER:CB	1:A:566:THR:HB	2.49	0.43
1:C:414:LYS:HA	1:C:414:LYS:HD2	1.60	0.43
1:C:455:PHE:HE1	1:C:473:THR:HA	1.84	0.43
1:C:595:LEU:HA	1:C:604:LEU:HD23	2.01	0.43
1:B:346:LEU:HD23	1:B:381:LYS:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:258:ALA:HA	1:C:263:TYR:HA	2.01	0.42
1:B:414:LYS:CB	3:L:1:DG:H4'	2.49	0.42
1:C:242:TYR:CE1	1:C:250:LYS:HB2	2.54	0.42
1:B:259:THR:OG1	1:B:262:GLN:O	2.34	0.42
1:C:565:ASP:OD1	1:C:565:ASP:N	2.49	0.42
1:A:531:SER:HB3	1:A:566:THR:HB	2.01	0.42
1:B:429:HIS:O	1:B:489:ASP:HA	2.19	0.42
1:B:555:ASN:O	1:B:556:LYS:HG2	2.19	0.42
1:C:445:THR:HA	1:C:452:LYS:O	2.19	0.42
1:C:595:LEU:HD11	1:C:602:TRP:CE3	2.55	0.42
1:A:385:LYS:HB2	1:A:413:SER:HB2	2.02	0.42
1:A:437:VAL:HA	1:A:459:VAL:HG12	2.02	0.42
1:C:422:PRO:HG2	1:C:464:GLU:HB3	2.02	0.42
1:A:311:MET:HE3	1:A:311:MET:HB2	1.79	0.42
1:A:528:PRO:HB2	1:A:533:LEU:HD21	2.02	0.41
1:B:460:ALA:HB1	1:B:520:LEU:HD21	2.02	0.41
1:C:489:ASP:HB2	1:C:504:CYS:SG	2.60	0.41
1:A:436:MET:HE1	1:A:521:ARG:HH22	1.86	0.41
1:B:351:VAL:HA	1:B:356:THR:HG23	2.02	0.41
1:B:381:LYS:HD2	1:B:463:THR:HG22	2.01	0.41
1:C:315:PRO:C	1:C:317:SER:H	2.29	0.41
1:B:589:ARG:O	1:B:612:MET:HA	2.20	0.41
2:I:1:DC:H42	3:J:16:DG:H1	1.69	0.41
1:A:397:ASP:O	1:A:398:ARG:HB2	2.20	0.41
1:B:486:ALA:O	1:B:505:VAL:HA	2.21	0.41
1:A:387:HIS:O	1:A:410:ILE:HA	2.21	0.41
1:A:422:PRO:HB3	1:A:466:PHE:CD2	2.56	0.41
1:C:438:LEU:O	1:C:481:PRO:HB3	2.21	0.41
3:J:16:DG:H1'	3:L:1:DG:C8	2.56	0.41
1:B:434:GLN:HE22	1:B:511:ASN:HB3	1.86	0.41
1:C:327:LYS:O	1:C:331:ILE:HG13	2.21	0.41
1:A:339:VAL:O	1:B:333:LYS:NZ	2.50	0.40
1:A:575:GLY:O	1:A:578:THR:HB	2.21	0.40
3:J:16:DG:H1'	3:L:1:DG:N7	2.36	0.40
2:K:8:DA:H2''	2:K:9:DA:C8	2.57	0.40
1:B:337:GLY:N	1:B:393:LEU:O	2.43	0.40
1:B:453:ARG:HB3	1:B:473:THR:CG2	2.51	0.40
1:C:394:LYS:HD3	1:C:396:ILE:HD11	2.02	0.40
1:C:419:PRO:HB2	1:C:420:LYS:H	1.68	0.40
1:B:264:PHE:HB3	1:B:295:LEU:HG	2.02	0.40
1:C:389:PHE:HB2	1:C:409:PHE:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:448:LEU:CD2	1:A:576:ARG:HD3	2.50	0.40
1:C:239:PRO:CB	1:C:271:ILE:HD11	2.51	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	393/412 (95%)	369 (94%)	21 (5%)	3 (1%)	16	53
1	B	395/412 (96%)	346 (88%)	44 (11%)	5 (1%)	9	41
1	C	394/412 (96%)	331 (84%)	50 (13%)	13 (3%)	3	21
All	All	1182/1236 (96%)	1046 (88%)	115 (10%)	21 (2%)	6	33

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	510	VAL
1	C	434	GLN
1	C	510	VAL
1	C	518	ASN
1	C	555	ASN
1	A	434	GLN
1	B	419	PRO
1	A	428	HIS
1	B	422	PRO
1	B	432	PRO
1	C	419	PRO
1	B	377	ASN
1	C	426	GLU
1	C	488	SER
1	C	513	THR

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Mol	Chain	Res	Type
1	B	398	ARG
1	C	432	PRO
1	C	433	LYS
1	C	516	ILE
1	C	539	GLY
1	C	435	VAL

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	334/366 (91%)	331 (99%)	3 (1%)	70	76
1	B	345/366 (94%)	343 (99%)	2 (1%)	78	80
1	C	336/366 (92%)	330 (98%)	6 (2%)	51	67
All	All	1015/1098 (92%)	1004 (99%)	11 (1%)	65	74

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	432	PRO
1	A	523	ARG
1	A	578	THR
1	B	425	GLU
1	B	432	PRO
1	C	414	LYS
1	C	417	ASN
1	C	418	VAL
1	C	432	PRO
1	C	614	VAL
1	C	615	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	321	ASN
1	B	494	ASN
1	B	549	ASN
1	B	555	ASN
1	C	251	ASN
1	C	265	HIS
1	C	494	ASN

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 oligosaccharides 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](#)

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	395/412 (95%)	0.59	25 (6%)	26 27	79, 162, 203, 265	2 (0%)
1	B	397/412 (96%)	0.41	12 (3%)	52 41	78, 131, 238, 280	0
1	C	396/412 (96%)	0.30	13 (3%)	49 40	60, 159, 252, 277	1 (0%)
2	I	16/16 (100%)	0.92	0	100 100	178, 190, 232, 233	0
2	K	16/16 (100%)	0.66	0	100 100	196, 219, 249, 256	0
3	J	16/16 (100%)	0.76	0	100 100	163, 201, 230, 231	0
3	L	16/16 (100%)	0.51	0	100 100	188, 203, 222, 246	1 (6%)
All	All	1252/1300 (96%)	0.45	50 (3%)	42 36	60, 156, 241, 280	4 (0%)

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	507	ASP	6.8
1	A	370	VAL	4.8
1	A	509	ASN	4.6
1	A	589	ARG	4.0
1	A	612	MET	3.7
1	A	403	VAL	3.5
1	B	319	ILE	3.5
1	A	542	VAL	3.3
1	A	419	PRO	3.3
1	A	277	PHE	3.3
1	B	589	ARG	3.2
1	C	363	GLY	3.2
1	B	538	ARG	3.1
1	A	404	CYS	3.1
1	A	402	LEU	3.1
1	B	594	GLU	3.0
1	B	533	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	513	THR	2.8
1	C	379	ASN	2.8
1	C	380	CYS	2.7
1	A	545	GLU	2.7
1	C	340	PHE	2.7
1	A	594	GLU	2.7
1	B	231	VAL	2.7
1	B	293	GLY	2.6
1	C	612	MET	2.6
1	B	479	PHE	2.6
1	A	611	TYR	2.6
1	B	452	LYS	2.5
1	C	333	LYS	2.5
1	A	613	GLN	2.5
1	C	258	ALA	2.4
1	A	508	VAL	2.4
1	B	312	ILE	2.4
1	A	523	ARG	2.4
1	A	221	GLY	2.3
1	A	391	PHE	2.3
1	C	416	GLY	2.3
1	A	423	ALA	2.3
1	A	229	LEU	2.3
1	A	357	ILE	2.3
1	B	300	THR	2.2
1	C	425	GLU	2.2
1	A	506	SER	2.2
1	C	479	PHE	2.1
1	A	457	ALA	2.1
1	C	511	ASN	2.0
1	C	303	VAL	2.0
1	A	587	LYS	2.0
1	B	292	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no oligosaccharides 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.