



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2024 – 05:32 AM EST

PDB ID : 4J4J
Title : Crystal structure of the APOBEC3F Vif binding domain
Authors : Siu, K.K.; Sultana, A.; Lee, J.E.
Deposited on : 2013-02-06
Resolution : 3.10 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 : 4.02b-467
Xtrriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

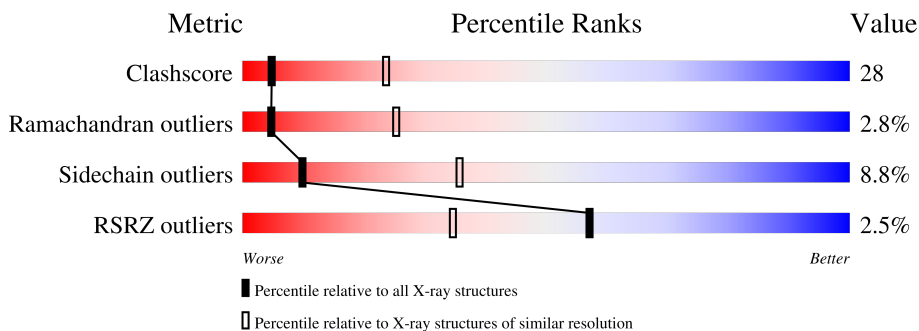
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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))
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	209	 3% 50% 31% 6% 12%
1	B	209	 3% 44% 38% 5% 12%

2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 5753 atoms, of which 2747 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 DNA dC->dU-editing enzyme APOBEC-3F.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	183	2871	973	1370	242	276	10	0	0	0
1	B	183	2880	971	1377	243	279	10	0	0	0

There are 106 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-53	MET	-	expression tag	UNP Q8IUX4
A	-52	ALA	-	expression tag	UNP Q8IUX4
A	-51	HIS	-	expression tag	UNP Q8IUX4
A	-50	HIS	-	expression tag	UNP Q8IUX4
A	-49	HIS	-	expression tag	UNP Q8IUX4
A	-48	HIS	-	expression tag	UNP Q8IUX4
A	-47	HIS	-	expression tag	UNP Q8IUX4
A	-46	HIS	-	expression tag	UNP Q8IUX4
A	-45	VAL	-	expression tag	UNP Q8IUX4
A	-44	ASP	-	expression tag	UNP Q8IUX4
A	-43	ASP	-	expression tag	UNP Q8IUX4
A	-42	ASP	-	expression tag	UNP Q8IUX4
A	-41	ASP	-	expression tag	UNP Q8IUX4
A	-40	LYS	-	expression tag	UNP Q8IUX4
A	-39	MET	-	expression tag	UNP Q8IUX4
A	-38	LEU	-	expression tag	UNP Q8IUX4
A	-37	VAL	-	expression tag	UNP Q8IUX4
A	-36	PRO	-	expression tag	UNP Q8IUX4
A	-35	ARG	-	expression tag	UNP Q8IUX4
A	-34	GLY	-	expression tag	UNP Q8IUX4
A	-33	SER	-	expression tag	UNP Q8IUX4
A	-32	GLU	-	expression tag	UNP Q8IUX4
A	-31	ASN	-	expression tag	UNP Q8IUX4
A	-30	LEU	-	expression tag	UNP Q8IUX4
A	-29	TYR	-	expression tag	UNP Q8IUX4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-28	PHE	-	expression tag	UNP Q8IUX4
A	-27	GLN	-	expression tag	UNP Q8IUX4
A	-26	GLY	-	expression tag	UNP Q8IUX4
A	-25	SER	-	expression tag	UNP Q8IUX4
A	-24	ALA	-	expression tag	UNP Q8IUX4
A	-23	MET	-	expression tag	UNP Q8IUX4
A	-22	ASP	-	expression tag	UNP Q8IUX4
A	-21	PRO	-	expression tag	UNP Q8IUX4
A	-20	PRO	-	expression tag	UNP Q8IUX4
A	-19	THR	-	expression tag	UNP Q8IUX4
A	-18	PHE	-	expression tag	UNP Q8IUX4
A	-17	THR	-	expression tag	UNP Q8IUX4
A	-16	PHE	-	expression tag	UNP Q8IUX4
A	-15	ASN	-	expression tag	UNP Q8IUX4
A	-14	PHE	-	expression tag	UNP Q8IUX4
A	-13	ASN	-	expression tag	UNP Q8IUX4
A	-12	ASN	-	expression tag	UNP Q8IUX4
A	-11	GLU	-	expression tag	UNP Q8IUX4
A	-10	PRO	-	expression tag	UNP Q8IUX4
A	-9	TRP	-	expression tag	UNP Q8IUX4
A	-8	VAL	-	expression tag	UNP Q8IUX4
A	-7	ARG	-	expression tag	UNP Q8IUX4
A	-6	GLY	-	expression tag	UNP Q8IUX4
A	-5	ARG	-	expression tag	UNP Q8IUX4
A	-4	HIS	-	expression tag	UNP Q8IUX4
A	-3	GLU	-	expression tag	UNP Q8IUX4
A	-2	THR	-	expression tag	UNP Q8IUX4
A	-1	TYR	-	expression tag	UNP Q8IUX4
B	-53	MET	-	expression tag	UNP Q8IUX4
B	-52	ALA	-	expression tag	UNP Q8IUX4
B	-51	HIS	-	expression tag	UNP Q8IUX4
B	-50	HIS	-	expression tag	UNP Q8IUX4
B	-49	HIS	-	expression tag	UNP Q8IUX4
B	-48	HIS	-	expression tag	UNP Q8IUX4
B	-47	HIS	-	expression tag	UNP Q8IUX4
B	-46	HIS	-	expression tag	UNP Q8IUX4
B	-45	VAL	-	expression tag	UNP Q8IUX4
B	-44	ASP	-	expression tag	UNP Q8IUX4
B	-43	ASP	-	expression tag	UNP Q8IUX4
B	-42	ASP	-	expression tag	UNP Q8IUX4
B	-41	ASP	-	expression tag	UNP Q8IUX4
B	-40	LYS	-	expression tag	UNP Q8IUX4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-39	MET	-	expression tag	UNP Q8IUX4
B	-38	LEU	-	expression tag	UNP Q8IUX4
B	-37	VAL	-	expression tag	UNP Q8IUX4
B	-36	PRO	-	expression tag	UNP Q8IUX4
B	-35	ARG	-	expression tag	UNP Q8IUX4
B	-34	GLY	-	expression tag	UNP Q8IUX4
B	-33	SER	-	expression tag	UNP Q8IUX4
B	-32	GLU	-	expression tag	UNP Q8IUX4
B	-31	ASN	-	expression tag	UNP Q8IUX4
B	-30	LEU	-	expression tag	UNP Q8IUX4
B	-29	TYR	-	expression tag	UNP Q8IUX4
B	-28	PHE	-	expression tag	UNP Q8IUX4
B	-27	GLN	-	expression tag	UNP Q8IUX4
B	-26	GLY	-	expression tag	UNP Q8IUX4
B	-25	SER	-	expression tag	UNP Q8IUX4
B	-24	ALA	-	expression tag	UNP Q8IUX4
B	-23	MET	-	expression tag	UNP Q8IUX4
B	-22	ASP	-	expression tag	UNP Q8IUX4
B	-21	PRO	-	expression tag	UNP Q8IUX4
B	-20	PRO	-	expression tag	UNP Q8IUX4
B	-19	THR	-	expression tag	UNP Q8IUX4
B	-18	PHE	-	expression tag	UNP Q8IUX4
B	-17	THR	-	expression tag	UNP Q8IUX4
B	-16	PHE	-	expression tag	UNP Q8IUX4
B	-15	ASN	-	expression tag	UNP Q8IUX4
B	-14	PHE	-	expression tag	UNP Q8IUX4
B	-13	ASN	-	expression tag	UNP Q8IUX4
B	-12	ASN	-	expression tag	UNP Q8IUX4
B	-11	GLU	-	expression tag	UNP Q8IUX4
B	-10	PRO	-	expression tag	UNP Q8IUX4
B	-9	TRP	-	expression tag	UNP Q8IUX4
B	-8	VAL	-	expression tag	UNP Q8IUX4
B	-7	ARG	-	expression tag	UNP Q8IUX4
B	-6	GLY	-	expression tag	UNP Q8IUX4
B	-5	ARG	-	expression tag	UNP Q8IUX4
B	-4	HIS	-	expression tag	UNP Q8IUX4
B	-3	GLU	-	expression tag	UNP Q8IUX4
B	-2	THR	-	expression tag	UNP Q8IUX4
B	-1	TYR	-	expression tag	UNP Q8IUX4

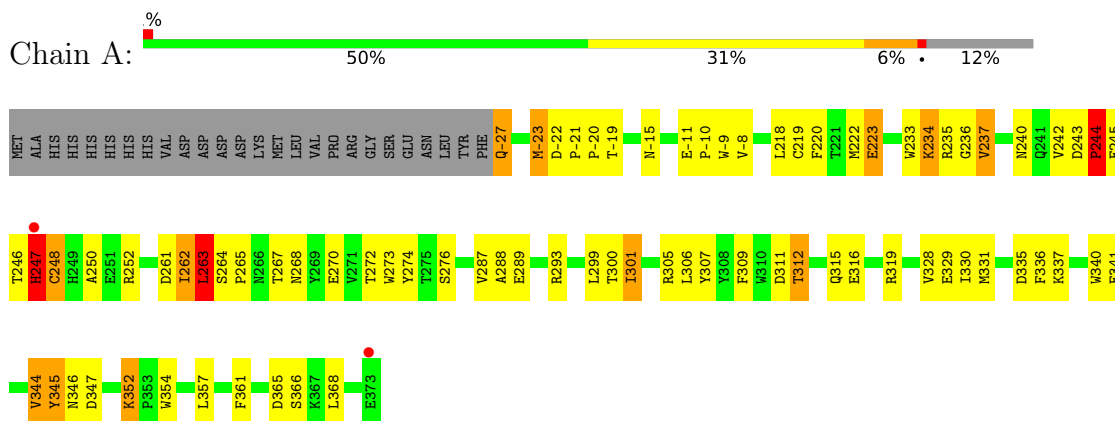
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

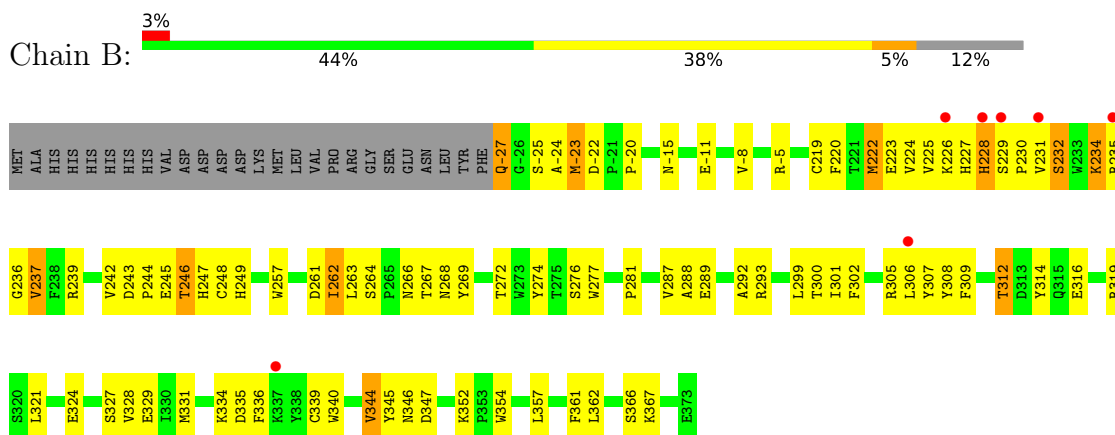
3 Residue-property plots

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: DNA dC->dU-editing enzyme APOBEC-3F



- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3F



4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	164.05Å 164.05Å 135.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.49 – 3.10 43.49 – 3.00	Depositor EDS
% Data completeness (in resolution range)	96.7 (43.49-3.10) 96.0 (43.49-3.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 3.01Å)	Xtrriage
Refinement program	PHENIX 1.8_1069	Depositor
R, R_{free}	0.236 , 0.277 0.252 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	121.8	Xtrriage
Anisotropy	0.253	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 88.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.36$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5753	wwPDB-VP
Average B, all atoms (Å ²)	99.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.10% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section:
ZN

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	0.57	0/1556	0.72	0/2125
1	B	0.57	0/1556	0.75	0/2122
All	All	0.57	0/3112	0.73	0/4247

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	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	244	PRO	Peptide
1	A	247	HIS	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	1501	1370	1351	84	0
1	B	1503	1377	1362	89	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
All	All	3006	2747	2713	159	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 28.

All (159) 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:A:237:VAL:HG12	1:A:237:VAL:O	1.81	0.80
1:B:281:PRO:HD3	1:B:314:TYR:CE1	2.19	0.76
1:B:231:VAL:O	1:B:232:SER:CB	2.34	0.75
1:B:272:THR:HG22	1:B:300:THR:OG1	1.87	0.75
1:A:272:THR:HG22	1:A:300:THR:HB	1.68	0.73
1:B:-27:GLN:HG3	1:B:235:ARG:O	1.88	0.72
1:A:345:TYR:CD2	1:B:345:TYR:CB	2.74	0.71
1:B:231:VAL:O	1:B:232:SER:OG	2.11	0.69
1:A:-23:MET:O	1:A:344:VAL:HG12	1.93	0.68
1:B:262:ILE:HG22	1:B:263:LEU:H	1.59	0.66
1:A:345:TYR:CB	1:B:345:TYR:CD2	2.80	0.65
1:A:-11:GLU:O	1:A:-8:VAL:HG13	1.96	0.64
1:A:264:SER:OG	1:A:265:PRO:HD2	1.97	0.64
1:A:223:GLU:HB2	1:A:233:TRP:CD1	2.33	0.63
1:A:330:ILE:HD13	1:A:365:ASP:HA	1.81	0.63
1:A:345:TYR:HB3	1:B:345:TYR:CD2	2.34	0.63
1:A:328:VAL:O	1:A:329:GLU:HG3	1.99	0.63
1:A:220:PHE:CE2	1:A:236:GLY:CA	2.82	0.62
1:B:231:VAL:O	1:B:231:VAL:HG13	2.00	0.61
1:A:237:VAL:O	1:A:237:VAL:CG1	2.48	0.61
1:B:225:VAL:O	1:B:225:VAL:HG23	2.00	0.61
1:A:345:TYR:CD2	1:B:345:TYR:HD2	2.20	0.60
1:A:261:ASP:O	1:A:262:ILE:HG12	2.02	0.60
1:A:330:ILE:HD12	1:A:368:LEU:HD22	1.82	0.60
1:A:345:TYR:CD2	1:B:345:TYR:HB2	2.36	0.60
1:B:300:THR:HB	1:B:327:SER:HB3	1.83	0.60
1:A:273:TRP:CE3	1:A:301:ILE:HD13	2.38	0.59
1:A:272:THR:CG2	1:A:300:THR:HB	2.34	0.58
1:A:270:GLU:HA	1:A:270:GLU:OE1	2.02	0.58
1:B:292:ALA:HB2	1:B:324:GLU:OE1	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:GLU:O	1:A:245:GLU:HG3	2.03	0.57
1:B:-22:ASP:HB3	1:B:-20:PRO:HG2	1.86	0.57
1:A:345:TYR:CD2	1:B:345:TYR:HB3	2.40	0.57
1:A:345:TYR:CD2	1:B:345:TYR:CD2	2.93	0.57
1:B:220:PHE:CE2	1:B:236:GLY:CA	2.87	0.57
1:B:261:ASP:O	1:B:262:ILE:HG12	2.04	0.57
1:B:267:THR:HG22	1:B:268:ASN:N	2.19	0.57
1:A:299:LEU:HD21	1:A:301:ILE:HD11	1.87	0.57
1:A:316:GLU:HA	1:A:319:ARG:HG3	1.86	0.56
1:A:240:ASN:OD1	1:A:250:ALA:N	2.38	0.56
1:A:247:HIS:CB	1:A:252:ARG:CD	2.83	0.56
1:A:262:ILE:O	1:A:263:LEU:C	2.44	0.56
1:A:267:THR:HG22	1:A:268:ASN:N	2.21	0.56
1:A:219:CYS:HB2	1:A:274:TYR:HB2	1.87	0.55
1:B:-15:ASN:O	1:B:276:SER:HB2	2.06	0.55
1:A:299:LEU:HG	1:A:300:THR:N	2.21	0.55
1:A:345:TYR:HD2	1:B:345:TYR:HD2	1.54	0.55
1:B:288:ALA:HB2	1:B:321:LEU:HD23	1.87	0.55
1:A:220:PHE:O	1:A:235:ARG:HB2	2.06	0.55
1:A:-15:ASN:O	1:A:305:ARG:NH2	2.40	0.54
1:B:-11:GLU:O	1:B:-8:VAL:HG13	2.07	0.54
1:A:-22:ASP:OD1	1:B:239:ARG:NH2	2.33	0.54
1:A:-22:ASP:N	1:B:-22:ASP:OD2	2.36	0.54
1:B:289:GLU:OE1	1:B:293:ARG:HD2	2.06	0.54
1:B:261:ASP:O	1:B:262:ILE:CG1	2.56	0.53
1:B:-8:VAL:HB	1:B:-5:ARG:NH1	2.24	0.53
1:B:242:VAL:CG2	1:B:307:TYR:CZ	2.91	0.53
1:B:262:ILE:HG22	1:B:263:LEU:N	2.24	0.52
1:B:361:PHE:C	1:B:361:PHE:CD2	2.82	0.52
1:B:-25:SER:O	1:B:237:VAL:HG21	2.09	0.52
1:B:227:HIS:O	1:B:228:HIS:HB2	2.10	0.52
1:B:-5:ARG:HB3	1:B:277:TRP:HE1	1.75	0.52
1:B:231:VAL:O	1:B:232:SER:HB3	2.09	0.52
1:A:289:GLU:OE2	1:A:289:GLU:HA	2.10	0.51
1:A:247:HIS:CB	1:A:252:ARG:HD2	2.41	0.51
1:B:263:LEU:HA	1:B:269:TYR:OH	2.10	0.51
1:A:361:PHE:CD2	1:A:361:PHE:C	2.85	0.50
1:A:220:PHE:CE2	1:A:236:GLY:N	2.80	0.50
1:A:218:LEU:C	1:A:218:LEU:HD23	2.32	0.50
1:A:-10:PRO:HB2	1:A:-9:TRP:CE3	2.47	0.50
1:B:328:VAL:C	1:B:329:GLU:HG3	2.32	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:PHE:CE2	1:B:236:GLY:C	2.85	0.50
1:B:-8:VAL:HG21	1:B:305:ARG:NH1	2.27	0.49
1:A:330:ILE:HD11	1:A:368:LEU:HB2	1.94	0.49
1:B:301:ILE:N	1:B:327:SER:O	2.40	0.49
1:A:-15:ASN:O	1:A:276:SER:HB2	2.12	0.49
1:A:315:GLN:O	1:A:319:ARG:HG2	2.11	0.49
1:B:308:TYR:HD2	1:B:314:TYR:CE2	2.31	0.49
1:B:354:TRP:CE2	1:B:357:LEU:HD12	2.47	0.49
1:B:331:MET:HG3	1:B:335:ASP:HB2	1.95	0.49
1:A:345:TYR:HD2	1:B:345:TYR:CD2	2.32	0.48
1:B:-25:SER:O	1:B:237:VAL:CG2	2.62	0.48
1:B:300:THR:CB	1:B:327:SER:HB3	2.43	0.48
1:A:306:LEU:HD11	1:A:368:LEU:HD13	1.96	0.48
1:A:337:LYS:NZ	1:A:341:GLU:OE2	2.47	0.48
1:A:340:TRP:O	1:A:344:VAL:HG23	2.13	0.47
1:A:330:ILE:CD1	1:A:368:LEU:HD22	2.44	0.47
1:A:243:ASP:OD1	1:A:243:ASP:C	2.52	0.47
1:B:-5:ARG:HG2	1:B:305:ARG:NH1	2.29	0.47
1:B:246:THR:HA	1:B:247:HIS:CB	2.43	0.47
1:B:264:SER:N	1:B:269:TYR:OH	2.47	0.47
1:A:-23:MET:O	1:A:344:VAL:CG1	2.62	0.47
1:B:234:LYS:HD2	1:B:234:LYS:HA	1.51	0.46
1:A:262:ILE:HG22	1:A:263:LEU:N	2.31	0.46
1:B:340:TRP:HA	1:B:344:VAL:HG21	1.97	0.46
1:B:220:PHE:CE2	1:B:236:GLY:HA3	2.50	0.46
1:B:346:ASN:O	1:B:347:ASP:HB2	2.16	0.46
1:B:328:VAL:O	1:B:329:GLU:HG3	2.16	0.46
1:A:345:TYR:CE2	1:B:345:TYR:HB2	2.52	0.45
1:B:289:GLU:OE2	1:B:289:GLU:HA	2.15	0.45
1:B:302:PHE:CE2	1:B:329:GLU:OE1	2.70	0.45
1:B:281:PRO:HD3	1:B:314:TYR:CD1	2.50	0.45
1:B:245:GLU:O	1:B:246:THR:C	2.54	0.45
1:B:336:PHE:CD1	1:B:354:TRP:HH2	2.34	0.45
1:A:247:HIS:CB	1:A:252:ARG:HD3	2.46	0.45
1:A:273:TRP:HE3	1:A:301:ILE:HD13	1.79	0.45
1:A:264:SER:OG	1:A:265:PRO:CD	2.64	0.45
1:A:345:TYR:CB	1:B:345:TYR:HD2	2.30	0.44
1:A:346:ASN:O	1:A:347:ASP:HB2	2.16	0.44
1:B:219:CYS:HB2	1:B:274:TYR:HB2	1.98	0.44
1:B:224:VAL:O	1:B:230:PRO:HA	2.18	0.44
1:B:223:GLU:OE1	1:B:230:PRO:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:VAL:O	1:B:288:ALA:C	2.56	0.44
1:A:289:GLU:OE1	1:A:293:ARG:NH2	2.42	0.44
1:A:340:TRP:HA	1:A:344:VAL:HG21	1.99	0.44
1:A:243:ASP:OD1	1:A:244:PRO:N	2.51	0.44
1:A:-21:PRO:N	1:A:-20:PRO:HD2	2.33	0.43
1:A:242:VAL:CG2	1:A:307:TYR:CZ	3.01	0.43
1:B:247:HIS:C	1:B:249:HIS:H	2.21	0.43
1:A:331:MET:HE2	1:A:336:PHE:CD1	2.53	0.43
1:B:299:LEU:HG	1:B:300:THR:N	2.33	0.43
1:A:246:THR:O	1:A:248:CYS:N	2.51	0.43
1:B:226:LYS:O	1:B:227:HIS:CD2	2.71	0.43
1:A:311:ASP:O	1:A:312:THR:C	2.57	0.43
1:B:242:VAL:HG21	1:B:307:TYR:CZ	2.54	0.43
1:A:220:PHE:CE2	1:A:236:GLY:C	2.92	0.43
1:A:352:LYS:HE3	1:A:352:LYS:HB3	1.72	0.43
1:B:316:GLU:HA	1:B:319:ARG:HG3	2.01	0.43
1:A:262:ILE:O	1:A:264:SER:N	2.52	0.42
1:B:339:CYS:O	1:B:344:VAL:HG23	2.19	0.42
1:B:226:LYS:HE3	1:B:266:ASN:O	2.19	0.42
1:B:261:ASP:C	1:B:262:ILE:CG1	2.88	0.42
1:B:261:ASP:C	1:B:262:ILE:HG13	2.38	0.42
1:A:245:GLU:O	1:A:246:THR:C	2.56	0.42
1:B:302:PHE:CZ	1:B:329:GLU:OE1	2.72	0.42
1:A:287:VAL:O	1:A:288:ALA:C	2.57	0.42
1:B:361:PHE:HD2	1:B:362:LEU:N	2.18	0.42
1:A:-27:GLN:HG3	1:A:235:ARG:O	2.19	0.42
1:A:331:MET:HG3	1:A:335:ASP:HB2	2.01	0.42
1:B:300:THR:HG22	1:B:327:SER:CB	2.50	0.42
1:B:269:TYR:CD2	1:B:269:TYR:N	2.88	0.42
1:B:257:TRP:CH2	1:B:262:ILE:HD12	2.55	0.41
1:A:306:LEU:HD11	1:A:368:LEU:CD1	2.51	0.41
1:A:306:LEU:HB3	1:A:309:PHE:HB3	2.02	0.41
1:A:234:LYS:HA	1:A:234:LYS:HD3	1.81	0.41
1:B:222:MET:HE3	1:B:222:MET:HB3	1.81	0.41
1:B:306:LEU:HD23	1:B:306:LEU:HA	1.81	0.41
1:A:220:PHE:HA	1:A:272:THR:O	2.21	0.41
1:A:345:TYR:CE2	1:B:345:TYR:CB	3.03	0.41
1:B:-24:ALA:HB3	1:B:345:TYR:CE1	2.56	0.41
1:A:223:GLU:O	1:A:223:GLU:HG2	2.20	0.41
1:A:331:MET:HE2	1:A:336:PHE:CE1	2.56	0.41
1:A:354:TRP:CE2	1:A:357:LEU:HD12	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:306:LEU:HB3	1:B:309:PHE:HB3	2.03	0.40
1:B:-23:MET:O	1:B:344:VAL:HG12	2.21	0.40
1:A:-22:ASP:OD2	1:A:-19:THR:HB	2.21	0.40
1:A:246:THR:HG22	1:A:247:HIS:CB	2.52	0.40
1:B:-5:ARG:HG2	1:B:305:ARG:HH12	1.87	0.40
1:B:226:LYS:C	1:B:228:HIS:N	2.74	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	181/209 (87%)	150 (83%)	26 (14%)	5 (3%)	5	25
1	B	181/209 (87%)	150 (83%)	26 (14%)	5 (3%)	5	25
All	All	362/418 (87%)	300 (83%)	52 (14%)	10 (3%)	5	25

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	262	ILE
1	A	263	LEU
1	B	232	SER
1	B	262	ILE
1	A	247	HIS
1	B	228	HIS
1	A	244	PRO
1	A	345	TYR
1	B	244	PRO
1	B	312	THR

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	159/192 (83%)	146 (92%)	13 (8%)	11	38
1	B	161/192 (84%)	146 (91%)	15 (9%)	9	32
All	All	320/384 (83%)	292 (91%)	28 (9%)	10	36

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-27	GLN
1	A	-23	MET
1	A	222	MET
1	A	223	GLU
1	A	234	LYS
1	A	237	VAL
1	A	248	CYS
1	A	263	LEU
1	A	301	ILE
1	A	312	THR
1	A	344	VAL
1	A	352	LYS
1	A	366	SER
1	B	-27	GLN
1	B	-23	MET
1	B	222	MET
1	B	229	SER
1	B	234	LYS
1	B	237	VAL
1	B	243	ASP
1	B	246	THR
1	B	248	CYS
1	B	312	THR
1	B	334	LYS
1	B	344	VAL
1	B	352	LYS
1	B	366	SER

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Mol	Chain	Res	Type
1	B	367	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	227	HIS
1	B	294	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

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(Å ²)	Q<0.9
1	A	183/209 (87%)	0.16	2 (1%) 80 64	74, 99, 138, 206	0
1	B	183/209 (87%)	0.28	7 (3%) 40 20	73, 103, 146, 219	0
All	All	366/418 (87%)	0.22	9 (2%) 57 34	73, 101, 146, 219	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	247	HIS	6.3
1	A	373	GLU	4.3
1	B	231	VAL	4.2
1	B	229	SER	3.7
1	B	228	HIS	2.9
1	B	337	LYS	2.6
1	B	226	LYS	2.5
1	B	235	ARG	2.4
1	B	306	LEU	2.1

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 monosaccharides 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(Å ²)	Q<0.9
2	ZN	A	401	1/1	0.99	0.24	78,78,78,78	0
2	ZN	B	401	1/1	0.99	0.25	73,73,73,73	0

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.