



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:52 AM UTC

PDB ID : 9HIZ / pdb_00009hiz
Title : Complex of the Nanofitin Sac7d-C3(C24A) with a human IgG1 Fc fragment
Authors : Eichinger, A.; Skerra, A.
Deposited on : 2024-11-27
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

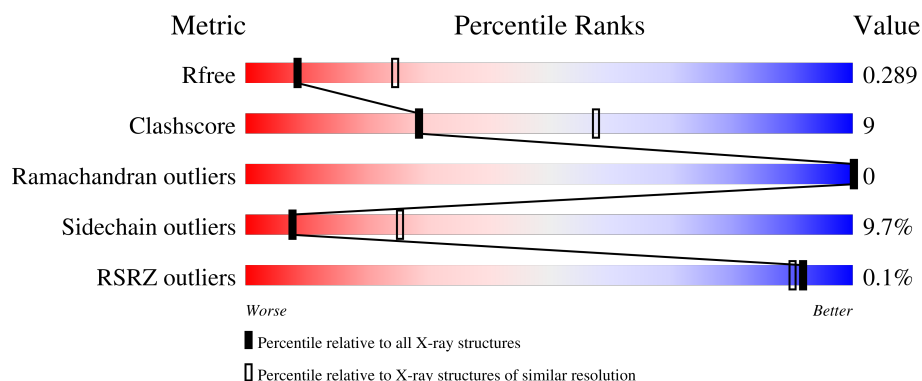
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION






The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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 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	217	
1	B	217	
1	C	217	
1	D	217	
2	R	69	

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Mol	Chain	Length	Quality of chain
2	S	69	 70% 23% 7%
2	T	69	 77% 20% 3%
2	U	69	 61% 30% 9%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8892 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 Immunoglobulin heavy constant gamma 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	209	Total	C	N	O	S	0	0	0
			1669	1061	281	321	6			
1	B	209	Total	C	N	O	S	0	0	0
			1669	1061	281	321	6			
1	C	209	Total	C	N	O	S	0	0	0
			1669	1061	281	321	6			
1	D	209	Total	C	N	O	S	0	0	0
			1669	1061	281	321	6			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	228	MET	-	initiating methionine	UNP P01857
A	229	LYS	-	expression tag	UNP P01857
A	230	HIS	-	expression tag	UNP P01857
A	231	HIS	-	expression tag	UNP P01857
A	232	HIS	-	expression tag	UNP P01857
A	233	HIS	-	expression tag	UNP P01857
A	234	HIS	-	expression tag	UNP P01857
A	235	HIS	-	expression tag	UNP P01857
B	228	MET	-	initiating methionine	UNP P01857
B	229	LYS	-	expression tag	UNP P01857
B	230	HIS	-	expression tag	UNP P01857
B	231	HIS	-	expression tag	UNP P01857
B	232	HIS	-	expression tag	UNP P01857
B	233	HIS	-	expression tag	UNP P01857
B	234	HIS	-	expression tag	UNP P01857
B	235	HIS	-	expression tag	UNP P01857
C	228	MET	-	initiating methionine	UNP P01857
C	229	LYS	-	expression tag	UNP P01857
C	230	HIS	-	expression tag	UNP P01857
C	231	HIS	-	expression tag	UNP P01857
C	232	HIS	-	expression tag	UNP P01857

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Chain	Residue	Modelled	Actual	Comment	Reference
C	233	HIS	-	expression tag	UNP P01857
C	234	HIS	-	expression tag	UNP P01857
C	235	HIS	-	expression tag	UNP P01857
D	228	MET	-	initiating methionine	UNP P01857
D	229	LYS	-	expression tag	UNP P01857
D	230	HIS	-	expression tag	UNP P01857
D	231	HIS	-	expression tag	UNP P01857
D	232	HIS	-	expression tag	UNP P01857
D	233	HIS	-	expression tag	UNP P01857
D	234	HIS	-	expression tag	UNP P01857
D	235	HIS	-	expression tag	UNP P01857

- Molecule 2 is a protein called DNA-binding protein 7d.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	R	69	Total	C	N	O	S	0	0	0
			554	345	98	110	1			
2	S	69	Total	C	N	O	S	0	0	0
			554	345	98	110	1			
2	T	69	Total	C	N	O	S	0	0	0
			554	345	98	110	1			
2	U	69	Total	C	N	O	S	0	0	0
			554	345	98	110	1			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	-2	ASP	-	expression tag	UNP P13123
R	-1	ALA	-	expression tag	UNP P13123
R	0	GLU	-	expression tag	UNP P13123
R	1	PHE	-	expression tag	UNP P13123
R	7	LEU	LYS	engineered mutation	UNP P13123
R	8	LEU	TYR	engineered mutation	UNP P13123
R	9	ASN	LYS	engineered mutation	UNP P13123
R	21	ARG	LYS	engineered mutation	UNP P13123
R	22	ASP	LYS	engineered mutation	UNP P13123
R	24	ALA	TRP	engineered mutation	UNP P13123
R	26	GLN	VAL	engineered mutation	UNP P13123
R	29	ASN	MET	engineered mutation	UNP P13123
R	31	LYS	SER	engineered mutation	UNP P13123
R	33	LEU	THR	engineered mutation	UNP P13123
R	35	ASN	ASP	engineered mutation	UNP P13123

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Chain	Residue	Modelled	Actual	Comment	Reference
R	40	TYR	THR	engineered mutation	UNP P13123
R	42	ALA	ARG	engineered mutation	UNP P13123
R	44	ASN	ALA	engineered mutation	UNP P13123
R	46	ASP	SER	engineered mutation	UNP P13123
S	-2	ASP	-	expression tag	UNP P13123
S	-1	ALA	-	expression tag	UNP P13123
S	0	GLU	-	expression tag	UNP P13123
S	1	PHE	-	expression tag	UNP P13123
S	7	LEU	LYS	engineered mutation	UNP P13123
S	8	LEU	TYR	engineered mutation	UNP P13123
S	9	ASN	LYS	engineered mutation	UNP P13123
S	21	ARG	LYS	engineered mutation	UNP P13123
S	22	ASP	LYS	engineered mutation	UNP P13123
S	24	ALA	TRP	engineered mutation	UNP P13123
S	26	GLN	VAL	engineered mutation	UNP P13123
S	29	ASN	MET	engineered mutation	UNP P13123
S	31	LYS	SER	engineered mutation	UNP P13123
S	33	LEU	THR	engineered mutation	UNP P13123
S	35	ASN	ASP	engineered mutation	UNP P13123
S	40	TYR	THR	engineered mutation	UNP P13123
S	42	ALA	ARG	engineered mutation	UNP P13123
S	44	ASN	ALA	engineered mutation	UNP P13123
S	46	ASP	SER	engineered mutation	UNP P13123
T	-2	ASP	-	expression tag	UNP P13123
T	-1	ALA	-	expression tag	UNP P13123
T	0	GLU	-	expression tag	UNP P13123
T	1	PHE	-	expression tag	UNP P13123
T	7	LEU	LYS	engineered mutation	UNP P13123
T	8	LEU	TYR	engineered mutation	UNP P13123
T	9	ASN	LYS	engineered mutation	UNP P13123
T	21	ARG	LYS	engineered mutation	UNP P13123
T	22	ASP	LYS	engineered mutation	UNP P13123
T	24	ALA	TRP	engineered mutation	UNP P13123
T	26	GLN	VAL	engineered mutation	UNP P13123
T	29	ASN	MET	engineered mutation	UNP P13123
T	31	LYS	SER	engineered mutation	UNP P13123
T	33	LEU	THR	engineered mutation	UNP P13123
T	35	ASN	ASP	engineered mutation	UNP P13123
T	40	TYR	THR	engineered mutation	UNP P13123
T	42	ALA	ARG	engineered mutation	UNP P13123
T	44	ASN	ALA	engineered mutation	UNP P13123
T	46	ASP	SER	engineered mutation	UNP P13123

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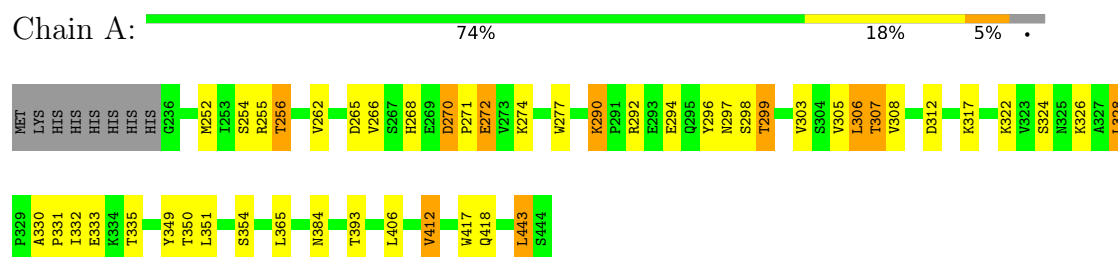
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Chain	Residue	Modelled	Actual	Comment	Reference
U	-2	ASP	-	expression tag	UNP P13123
U	-1	ALA	-	expression tag	UNP P13123
U	0	GLU	-	expression tag	UNP P13123
U	1	PHE	-	expression tag	UNP P13123
U	7	LEU	LYS	engineered mutation	UNP P13123
U	8	LEU	TYR	engineered mutation	UNP P13123
U	9	ASN	LYS	engineered mutation	UNP P13123
U	21	ARG	LYS	engineered mutation	UNP P13123
U	22	ASP	LYS	engineered mutation	UNP P13123
U	24	ALA	TRP	engineered mutation	UNP P13123
U	26	GLN	VAL	engineered mutation	UNP P13123
U	29	ASN	MET	engineered mutation	UNP P13123
U	31	LYS	SER	engineered mutation	UNP P13123
U	33	LEU	THR	engineered mutation	UNP P13123
U	35	ASN	ASP	engineered mutation	UNP P13123
U	40	TYR	THR	engineered mutation	UNP P13123
U	42	ALA	ARG	engineered mutation	UNP P13123
U	44	ASN	ALA	engineered mutation	UNP P13123
U	46	ASP	SER	engineered mutation	UNP P13123

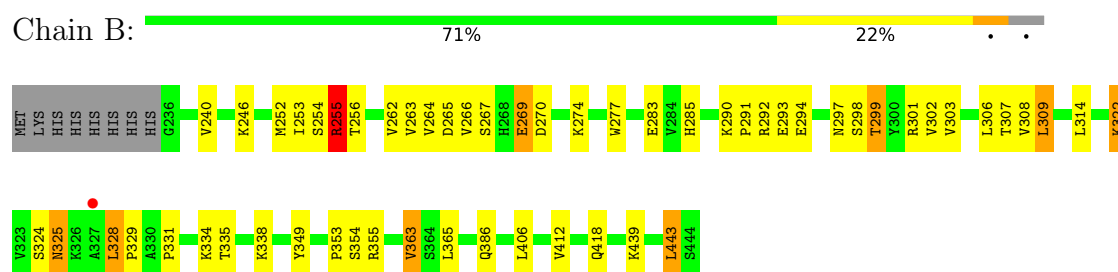
3 Residue-property plots [i](#)

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.

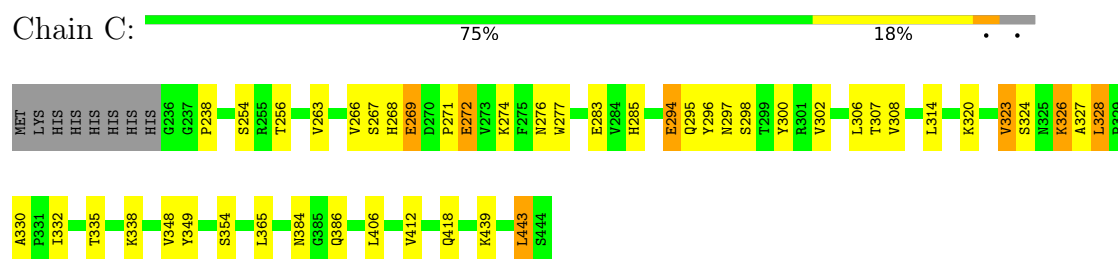
- Molecule 1: Immunoglobulin heavy constant gamma 1



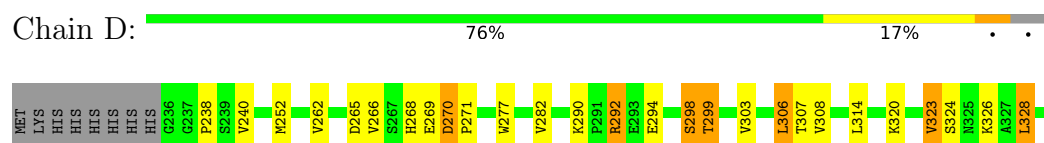
- Molecule 1: Immunoglobulin heavy constant gamma 1



- Molecule 1: Immunoglobulin heavy constant gamma 1

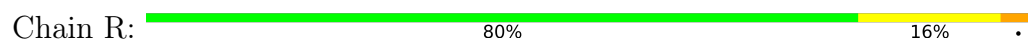


- Molecule 1: Immunoglobulin heavy constant gamma 1

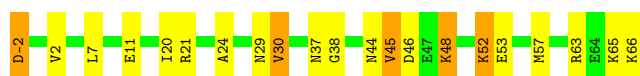




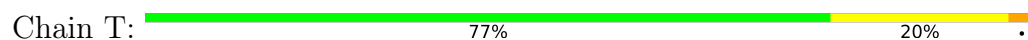
- Molecule 2: DNA-binding protein 7d



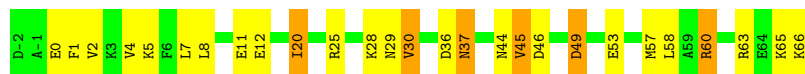
- Molecule 2: DNA-binding protein 7d



- Molecule 2: DNA-binding protein 7d



- Molecule 2: DNA-binding protein 7d



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	68.27Å 136.84Å 69.76Å 90.00° 90.12° 90.00°	Depositor
Resolution (Å)	69.76 – 2.90 69.76 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.0 (69.76-2.90) 96.5 (69.76-2.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.227 , 0.279 (Not available) , 0.289	Depositor DCC
R_{free} test set	1379 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	72.1	Xtriage
Anisotropy	0.508	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 68.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.011 for l,k,-h 0.427 for h,-k,-l 0.022 for l,-k,h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8892	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.23% 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	0.55	0/1715	1.02	4/2335 (0.2%)
1	B	0.55	0/1715	1.05	3/2335 (0.1%)
1	C	0.55	0/1715	1.02	4/2335 (0.2%)
1	D	0.55	0/1715	1.01	1/2335 (0.0%)
2	R	0.51	0/559	1.04	0/742
2	S	0.54	0/559	1.13	1/742 (0.1%)
2	T	0.54	0/559	1.14	1/742 (0.1%)
2	U	0.52	0/559	1.12	0/742
All	All	0.55	0/9096	1.05	14/12308 (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	B	0	2
1	D	0	1
2	R	0	1
2	S	0	1
2	T	0	1
2	U	0	1
All	All	0	7

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	256	THR	CA-CB-OG1	-6.95	99.18	109.60
1	C	256	THR	CA-CB-OG1	-6.92	99.22	109.60
1	A	256	THR	CA-CB-OG1	-6.70	99.56	109.60
2	S	-2	ASP	CA-CB-CG	6.47	119.07	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	270	ASP	CA-CB-CG	5.93	118.53	112.60
1	B	363	VAL	N-CA-CB	-5.93	102.48	112.44
1	C	271	PRO	N-CA-CB	-5.59	97.38	103.25
1	A	270	ASP	CA-CB-CG	5.43	118.03	112.60
1	B	307	THR	CA-CB-OG1	-5.32	101.62	109.60
1	A	307	THR	CA-CB-OG1	-5.27	101.69	109.60
1	C	272	GLU	CB-CG-CD	5.27	121.56	112.60
1	C	307	THR	CA-CB-OG1	-5.22	101.76	109.60
2	T	30	VAL	N-CA-CB	-5.20	104.92	111.41
1	A	393	THR	CA-CB-OG1	-5.17	101.85	109.60

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	255	ARG	Sidechain
1	B	292	ARG	Sidechain
1	D	292	ARG	Sidechain
2	R	25	ARG	Sidechain
2	S	21	ARG	Sidechain
2	T	21	ARG	Sidechain
2	U	25	ARG	Sidechain

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	1669	0	1638	34	0
1	B	1669	0	1638	36	0
1	C	1669	0	1638	28	0
1	D	1669	0	1638	29	0
2	R	554	0	560	5	0
2	S	554	0	560	14	0
2	T	554	0	560	7	0
2	U	554	0	560	13	0
All	All	8892	0	8792	156	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 9.

All (156) 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:S:38:GLY:HA3	1:C:384:ASN:HD21	1.29	0.92
2:U:60:ARG:HD2	2:U:63:ARG:HH22	1.48	0.78
1:A:350:THR:C	1:A:351:LEU:HD12	2.12	0.74
2:S:38:GLY:HA3	1:C:384:ASN:ND2	2.04	0.73
1:A:277:TRP:CE3	1:A:306:LEU:HD12	2.25	0.71
1:D:290:LYS:HB2	1:D:303:VAL:HG23	1.71	0.71
1:D:277:TRP:CE3	1:D:306:LEU:HD12	2.26	0.70
1:D:240:VAL:HG21	1:D:323:VAL:HG11	1.72	0.70
1:B:252:MET:HB2	1:B:255:ARG:HG3	1.73	0.69
2:R:30:VAL:HG22	2:R:45:VAL:HG12	1.78	0.66
2:S:30:VAL:HG22	2:S:45:VAL:HG12	1.78	0.65
1:B:290:LYS:HG2	1:B:291:PRO:HD2	1.76	0.65
1:A:272:GLU:HA	1:A:292:ARG:NH2	2.11	0.65
2:U:30:VAL:HG22	2:U:45:VAL:HG12	1.80	0.64
2:T:12:GLU:N	2:T:12:GLU:OE1	2.30	0.63
2:U:46:ASP:HB3	2:U:49:ASP:OD1	1.98	0.63
1:D:323:VAL:HG13	1:D:332:ILE:HB	1.81	0.63
1:C:323:VAL:HG13	1:C:332:ILE:HB	1.81	0.62
1:D:420:GLY:HA2	1:D:443:LEU:HG	1.81	0.62
1:A:328:LEU:HD22	1:A:332:ILE:HG13	1.81	0.62
2:R:20:ILE:HB	2:R:57:MET:HE1	1.83	0.60
1:A:418:GLN:HA	1:A:443:LEU:HD13	1.84	0.60
2:U:20:ILE:HB	2:U:57:MET:HE1	1.84	0.59
1:A:322:LYS:HE2	1:A:333:GLU:OE2	2.03	0.59
1:D:306:LEU:HD23	1:D:307:THR:O	2.02	0.59
1:B:353:PRO:CG	1:B:363:VAL:CG1	2.82	0.58
1:D:262:VAL:HG22	1:D:303:VAL:HG12	1.85	0.58
2:T:52:LYS:HE2	2:T:53:GLU:HB2	1.85	0.58
2:U:12:GLU:O	2:U:12:GLU:HG3	2.04	0.58
1:A:406:LEU:C	1:A:406:LEU:HD12	2.29	0.58
1:D:306:LEU:CD2	1:D:307:THR:O	2.52	0.58
1:B:262:VAL:HG22	1:B:303:VAL:HG12	1.86	0.57
2:T:52:LYS:HE2	2:T:53:GLU:CB	2.33	0.57
1:D:406:LEU:C	1:D:406:LEU:HD12	2.30	0.57
1:D:238:PRO:HG2	1:D:328:LEU:HD23	1.87	0.57
1:A:306:LEU:CD2	1:A:307:THR:O	2.53	0.57
1:B:406:LEU:HD12	1:B:406:LEU:C	2.30	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:GLU:HA	1:A:292:ARG:HH21	1.69	0.57
1:A:351:LEU:HD12	1:A:351:LEU:N	2.20	0.57
1:A:306:LEU:HD23	1:A:307:THR:O	2.04	0.56
1:C:406:LEU:C	1:C:406:LEU:HD12	2.30	0.56
1:B:353:PRO:HB3	1:B:363:VAL:HG13	1.89	0.55
2:S:37:ASN:O	1:C:384:ASN:ND2	2.40	0.55
2:S:20:ILE:HB	2:S:57:MET:HE1	1.89	0.54
2:T:20:ILE:HB	2:T:57:MET:HE1	1.89	0.54
1:B:328:LEU:HD23	1:B:329:PRO:HD2	1.90	0.54
2:U:12:GLU:O	2:U:12:GLU:CG	2.55	0.54
1:B:263:VAL:HG22	1:B:302:VAL:O	2.08	0.54
1:D:443:LEU:O	1:D:444:SER:CB	2.56	0.54
1:C:274:LYS:HE3	1:C:276:ASN:HD21	1.73	0.54
1:C:294:GLU:OE1	1:C:300:TYR:HE2	1.91	0.53
1:C:320:LYS:HB2	1:C:335:THR:HG22	1.90	0.52
1:B:264:VAL:HG21	1:B:301:ARG:NH2	2.24	0.52
1:A:418:GLN:O	1:A:443:LEU:HD22	2.09	0.51
2:T:65:LYS:O	2:T:66:LYS:OXT	2.28	0.51
1:A:354:SER:CB	1:B:349:TYR:HB3	2.40	0.51
1:D:268:HIS:NE2	1:D:298:SER:O	2.43	0.51
1:C:294:GLU:HB3	1:C:300:TYR:CE2	2.45	0.51
1:C:418:GLN:HA	1:C:443:LEU:HD12	1.93	0.51
1:C:328:LEU:CD1	1:C:332:ILE:HD11	2.41	0.51
1:D:418:GLN:HA	1:D:443:LEU:HD23	1.92	0.51
1:A:365:LEU:HD13	1:A:412:VAL:CG1	2.41	0.50
1:A:252:MET:HB2	1:A:255:ARG:HG3	1.94	0.50
1:B:264:VAL:HB	1:B:301:ARG:NH1	2.26	0.49
1:D:328:LEU:CD1	1:D:331:PRO:HA	2.42	0.49
2:U:29:ASN:OD1	2:U:44:ASN:ND2	2.45	0.49
1:A:349:TYR:HB3	1:B:354:SER:CB	2.42	0.49
1:A:290:LYS:HE2	1:A:305:VAL:HG21	1.93	0.49
1:A:328:LEU:HD13	1:A:331:PRO:HA	1.94	0.49
2:U:65:LYS:O	2:U:66:LYS:OXT	2.29	0.49
1:A:265:ASP:HA	1:A:299:THR:OG1	2.12	0.49
2:R:29:ASN:OD1	2:R:44:ASN:ND2	2.46	0.49
1:C:268:HIS:HB3	1:C:300:TYR:HE1	1.78	0.49
1:B:418:GLN:HA	1:B:443:LEU:HD12	1.95	0.48
2:R:65:LYS:O	2:R:66:LYS:OXT	2.31	0.48
1:C:263:VAL:HG12	1:C:302:VAL:O	2.14	0.48
2:S:65:LYS:O	2:S:66:LYS:OXT	2.32	0.48
1:C:386:GLN:HE21	1:C:386:GLN:HA	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:29:ASN:OD1	2:S:44:ASN:ND2	2.48	0.47
2:S:52:LYS:HE3	2:S:53:GLU:CB	2.43	0.47
1:D:265:ASP:HA	1:D:299:THR:OG1	2.15	0.47
1:B:277:TRP:CE3	1:B:306:LEU:HD22	2.49	0.47
1:B:290:LYS:HG2	1:B:291:PRO:CD	2.44	0.47
1:A:268:HIS:NE2	1:A:298:SER:HB3	2.30	0.47
2:S:52:LYS:N	2:S:52:LYS:HD3	2.30	0.47
1:C:328:LEU:HD12	1:C:330:ALA:O	2.15	0.47
1:C:443:LEU:O	1:C:443:LEU:CD2	2.62	0.47
1:C:314:LEU:O	1:C:338:LYS:HE2	2.15	0.47
1:B:443:LEU:CD2	1:B:443:LEU:O	2.63	0.47
1:C:349:TYR:HB3	1:D:354:SER:CB	2.44	0.47
2:T:29:ASN:OD1	2:T:44:ASN:ND2	2.48	0.46
1:C:277:TRP:CE3	1:C:306:LEU:HD22	2.50	0.46
1:B:283:GLU:HG2	1:B:285:HIS:CE1	2.51	0.46
1:A:256:THR:HG23	1:A:256:THR:O	2.15	0.46
1:B:325:ASN:ND2	1:B:328:LEU:O	2.48	0.46
2:S:46:ASP:OD2	2:S:48:LYS:CE	2.63	0.46
1:B:265:ASP:HA	1:B:299:THR:OG1	2.15	0.46
2:R:36:ASP:O	2:R:37:ASN:CG	2.59	0.46
2:U:36:ASP:O	2:U:37:ASN:CG	2.59	0.46
1:D:443:LEU:O	1:D:444:SER:HB2	2.15	0.45
1:A:262:VAL:HG22	1:A:303:VAL:HG22	1.98	0.45
1:A:297:ASN:OD1	1:A:299:THR:HG22	2.16	0.45
1:A:351:LEU:N	1:A:351:LEU:CD1	2.78	0.45
1:C:283:GLU:HG2	1:C:285:HIS:CE1	2.52	0.45
1:B:322:LYS:HD2	1:B:331:PRO:HB3	1.99	0.45
2:T:1:PHE:O	2:T:2:VAL:C	2.60	0.45
2:S:46:ASP:OD2	2:S:48:LYS:HG2	2.16	0.44
1:C:267:SER:HB2	1:C:269:GLU:HG2	1.98	0.44
1:B:314:LEU:O	1:B:338:LYS:HE2	2.18	0.44
2:S:46:ASP:OD2	2:S:48:LYS:HE2	2.17	0.44
1:C:238:PRO:HD2	1:C:328:LEU:HD23	1.98	0.44
1:C:348:VAL:HG12	1:C:439:LYS:HG3	2.00	0.44
1:A:417:TRP:O	1:A:443:LEU:HB2	2.17	0.44
1:B:353:PRO:HG2	1:B:363:VAL:CG1	2.47	0.43
1:C:365:LEU:HD13	1:C:412:VAL:HG22	1.98	0.43
1:D:314:LEU:O	1:D:338:LYS:HE2	2.17	0.43
1:D:320:LYS:HB2	1:D:335:THR:HG22	2.01	0.43
1:B:309:LEU:N	1:B:309:LEU:CD1	2.82	0.43
1:D:240:VAL:CG2	1:D:323:VAL:HG11	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:365:LEU:HD13	1:D:412:VAL:HG22	1.99	0.43
1:D:252:MET:HE3	2:U:65:LYS:HB3	1.99	0.43
1:D:271:PRO:O	1:D:292:ARG:NH1	2.51	0.43
1:D:348:VAL:HG12	1:D:439:LYS:HG3	2.00	0.43
1:B:365:LEU:HD13	1:B:412:VAL:HG22	2.00	0.43
1:B:267:SER:HB2	1:B:269:GLU:OE1	2.19	0.43
1:B:240:VAL:O	1:B:334:LYS:HE3	2.19	0.42
1:B:353:PRO:CB	1:B:363:VAL:HG13	2.48	0.42
2:U:2:VAL:HG21	2:U:53:GLU:HG2	2.00	0.42
1:C:296:TYR:CD1	1:C:297:ASN:N	2.87	0.42
1:A:312:ASP:OD1	1:A:317:LYS:HE2	2.20	0.42
1:B:386:GLN:HA	1:B:386:GLN:HE21	1.83	0.42
1:B:443:LEU:O	1:B:443:LEU:HD23	2.20	0.42
1:C:354:SER:CB	1:D:349:TYR:HB3	2.49	0.42
2:U:0:GLU:O	2:U:1:PHE:C	2.63	0.42
1:C:326:LYS:HD3	1:C:327:ALA:N	2.34	0.42
1:B:386:GLN:HA	1:B:386:GLN:NE2	2.34	0.42
1:D:282:VAL:O	1:D:282:VAL:HG23	2.19	0.41
2:U:2:VAL:HG21	2:U:53:GLU:CG	2.50	0.41
1:A:328:LEU:CD1	1:A:331:PRO:HA	2.49	0.41
1:B:355:ARG:HD2	1:B:355:ARG:C	2.45	0.41
1:A:271:PRO:HD2	1:A:272:GLU:CD	2.46	0.41
1:A:306:LEU:CD2	1:A:306:LEU:C	2.94	0.41
1:B:353:PRO:CG	1:B:363:VAL:HG13	2.51	0.41
1:A:365:LEU:HD13	1:A:412:VAL:HG13	2.02	0.41
1:A:328:LEU:HD13	1:A:330:ALA:O	2.21	0.41
1:B:290:LYS:HB3	1:B:303:VAL:HG23	2.02	0.41
1:C:386:GLN:HA	1:C:386:GLN:NE2	2.35	0.41
1:B:365:LEU:HD12	1:B:365:LEU:N	2.35	0.40
1:A:384:ASN:CG	1:A:384:ASN:O	2.64	0.40
1:D:306:LEU:CD2	1:D:306:LEU:C	2.95	0.40
1:D:369:VAL:O	1:D:405:PHE:HA	2.21	0.40
1:A:354:SER:HB2	1:B:349:TYR:HB3	2.03	0.40
1:B:253:ILE:HG23	2:S:24:ALA:HB3	2.02	0.40
2:S:48:LYS:HB3	2:S:48:LYS:NZ	2.37	0.40
1:A:322:LYS:CE	1:A:333:GLU:OE2	2.69	0.40
1:D:365:LEU:HD12	1:D:365:LEU:N	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	127/217 (58%)	121 (95%)	6 (5%)	0	100	100
1	B	207/217 (95%)	194 (94%)	13 (6%)	0	100	100
1	C	207/217 (95%)	191 (92%)	16 (8%)	0	100	100
1	D	207/217 (95%)	193 (93%)	14 (7%)	0	100	100
2	R	67/69 (97%)	61 (91%)	6 (9%)	0	100	100
2	S	67/69 (97%)	64 (96%)	3 (4%)	0	100	100
2	T	67/69 (97%)	61 (91%)	6 (9%)	0	100	100
2	U	67/69 (97%)	61 (91%)	6 (9%)	0	100	100
All	All	1016/1144 (89%)	946 (93%)	70 (7%)	0	100	100

There are no Ramachandran outliers to report.

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	194/202 (96%)	177 (91%)	17 (9%)	9	29
1	B	194/202 (96%)	173 (89%)	21 (11%)	6	21
1	C	194/202 (96%)	181 (93%)	13 (7%)	15	43
1	D	194/202 (96%)	180 (93%)	14 (7%)	13	39
2	R	58/58 (100%)	52 (90%)	6 (10%)	7	23
2	S	58/58 (100%)	49 (84%)	9 (16%)	2	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	T	58/58 (100%)	53 (91%)	5 (9%)	10	30
2	U	58/58 (100%)	45 (78%)	13 (22%)	1	3
All	All	1008/1040 (97%)	910 (90%)	98 (10%)	8	25

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	254	SER
1	A	266	VAL
1	A	270	ASP
1	A	272	GLU
1	A	274	LYS
1	A	290	LYS
1	A	294	GLU
1	A	296	TYR
1	A	299	THR
1	A	306	LEU
1	A	308	VAL
1	A	324	SER
1	A	326	LYS
1	A	328	LEU
1	A	335	THR
1	A	412	VAL
1	A	443	LEU
1	B	246	LYS
1	B	254	SER
1	B	255	ARG
1	B	266	VAL
1	B	269	GLU
1	B	270	ASP
1	B	274	LYS
1	B	293	GLU
1	B	294	GLU
1	B	297	ASN
1	B	298	SER
1	B	299	THR
1	B	308	VAL
1	B	309	LEU
1	B	322	LYS
1	B	324	SER
1	B	325	ASN

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Mol	Chain	Res	Type
1	B	328	LEU
1	B	335	THR
1	B	439	LYS
1	B	443	LEU
2	R	2	VAL
2	R	7	LEU
2	R	30	VAL
2	R	37	ASN
2	R	45	VAL
2	R	58	LEU
2	S	-2	ASP
2	S	2	VAL
2	S	7	LEU
2	S	11	GLU
2	S	30	VAL
2	S	45	VAL
2	S	48	LYS
2	S	52	LYS
2	S	63	ARG
1	C	254	SER
1	C	266	VAL
1	C	269	GLU
1	C	272	GLU
1	C	294	GLU
1	C	295	GLN
1	C	298	SER
1	C	308	VAL
1	C	323	VAL
1	C	324	SER
1	C	326	LYS
1	C	328	LEU
1	C	443	LEU
1	D	266	VAL
1	D	269	GLU
1	D	270	ASP
1	D	294	GLU
1	D	298	SER
1	D	299	THR
1	D	306	LEU
1	D	308	VAL
1	D	323	VAL
1	D	324	SER

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Mol	Chain	Res	Type
1	D	326	LYS
1	D	328	LEU
1	D	415	SER
1	D	443	LEU
2	T	2	VAL
2	T	7	LEU
2	T	11	GLU
2	T	45	VAL
2	T	52	LYS
2	U	4	VAL
2	U	5	LYS
2	U	7	LEU
2	U	8	LEU
2	U	11	GLU
2	U	20	ILE
2	U	28	LYS
2	U	30	VAL
2	U	37	ASN
2	U	45	VAL
2	U	49	ASP
2	U	58	LEU
2	U	60	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	347	GLN
1	A	418	GLN
1	B	276	ASN
1	B	285	HIS
1	B	325	ASN
1	B	342	GLN
1	B	347	GLN
1	B	386	GLN
2	R	9	ASN
2	R	29	ASN
2	R	37	ASN
2	R	44	ASN
2	S	9	ASN
2	S	44	ASN
1	C	276	ASN
1	C	285	HIS

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Mol	Chain	Res	Type
1	C	325	ASN
1	C	384	ASN
1	C	386	GLN
1	D	285	HIS
1	D	347	GLN
1	D	418	GLN
1	D	433	HIS
2	T	9	ASN
2	T	37	ASN
2	T	44	ASN
2	U	29	ASN
2	U	37	ASN
2	U	44	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 [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	209/217 (96%)	-0.58	0 100 100	53, 83, 142, 160	0
1	B	209/217 (96%)	-0.63	1 (0%) 87 83	48, 75, 164, 193	0
1	C	209/217 (96%)	-0.65	0 100 100	46, 71, 157, 200	0
1	D	209/217 (96%)	-0.83	0 100 100	45, 78, 136, 164	0
2	R	69/69 (100%)	-0.78	0 100 100	74, 97, 130, 153	0
2	S	69/69 (100%)	-0.93	0 100 100	53, 71, 113, 128	0
2	T	69/69 (100%)	-1.05	0 100 100	53, 71, 106, 144	0
2	U	69/69 (100%)	-0.77	0 100 100	76, 100, 136, 150	0
All	All	1112/1144 (97%)	-0.72	1 (0%) 92 90	45, 80, 148, 200	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	327	ALA	2.5

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.