



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 2, 2026 – 01:17 AM UTC

PDB ID : 8S05 / pdb_00008s05
Title : ArnAB complex an archaeal ortholog of the Sec23/24 core motif
Authors : Korf, L.; Steinchen, W.; Watad, M.; Bezold, F.; Vogt, M.S.; Selbach, L.;
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Deposited on : 2024-02-13
Resolution : 2.11 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

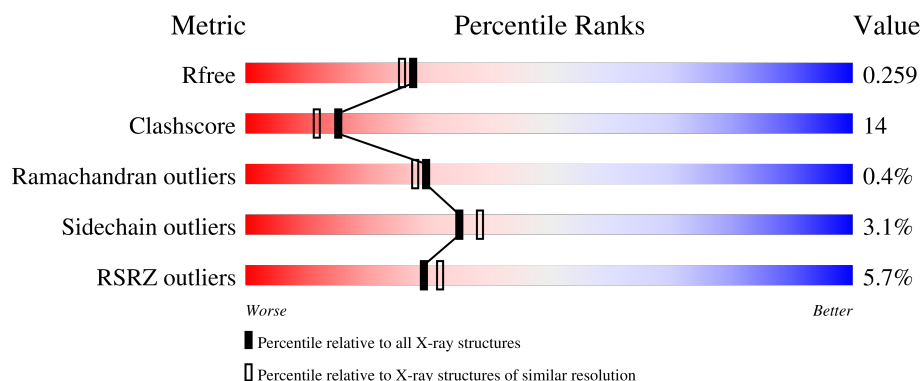
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.11 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	8290 (2.14-2.10)
Clashscore	190562	8817 (2.14-2.10)
Ramachandran outliers	187476	8738 (2.14-2.10)
Sidechain outliers	187428	8739 (2.14-2.10)
RSRZ outliers	180081	8294 (2.14-2.10)

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	387	3% 75% 21% ...
1	B	387	3% 76% 21% ..
2	C	223	3% 9% 88%
2	D	223	7% 5% 5% 88%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12981 atoms, of which 6517 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 Conserved protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	381	Total	C	H	N	O	S	0	0	0
			6105	1908	3088	518	583	8			
1	B	380	Total	C	H	N	O	S	0	0	0
			6071	1902	3064	515	582	8			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	MET	-	initiating methionine	UNP Q4J9H3
A	2A	ALA	-	expression tag	UNP Q4J9H3
A	2B	THR	-	expression tag	UNP Q4J9H3
A	382	HIS	-	expression tag	UNP Q4J9H3
A	383	HIS	-	expression tag	UNP Q4J9H3
A	384	HIS	-	expression tag	UNP Q4J9H3
A	385	HIS	-	expression tag	UNP Q4J9H3
A	386	HIS	-	expression tag	UNP Q4J9H3
B	2	MET	-	initiating methionine	UNP Q4J9H3
B	2A	ALA	-	expression tag	UNP Q4J9H3
B	2B	THR	-	expression tag	UNP Q4J9H3
B	382	HIS	-	expression tag	UNP Q4J9H3
B	383	HIS	-	expression tag	UNP Q4J9H3
B	384	HIS	-	expression tag	UNP Q4J9H3
B	385	HIS	-	expression tag	UNP Q4J9H3
B	386	HIS	-	expression tag	UNP Q4J9H3

- Molecule 2 is a protein called Conserved protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	27	Total	C	H	N	O	S	0	0	0
			397	129	189	34	41	4			
2	D	26	Total	C	H	N	O	S	0	0	0
			375	123	176	32	40	4			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	0	MET	-	initiating methionine	UNP Q4J9H4
C	1	TRP	-	expression tag	UNP Q4J9H4
C	2	SER	-	expression tag	UNP Q4J9H4
C	3	HIS	-	expression tag	UNP Q4J9H4
C	4	PRO	-	expression tag	UNP Q4J9H4
C	5	GLN	-	expression tag	UNP Q4J9H4
C	6	PHE	-	expression tag	UNP Q4J9H4
C	7	GLU	-	expression tag	UNP Q4J9H4
C	8	LYS	-	expression tag	UNP Q4J9H4
C	9	LEU	-	expression tag	UNP Q4J9H4
C	10	GLU	-	expression tag	UNP Q4J9H4
C	11	VAL	-	expression tag	UNP Q4J9H4
C	12	LEU	-	expression tag	UNP Q4J9H4
C	13	PHE	-	expression tag	UNP Q4J9H4
C	14	GLN	-	expression tag	UNP Q4J9H4
C	15	GLY	-	expression tag	UNP Q4J9H4
C	16	PRO	-	expression tag	UNP Q4J9H4
C	17	SER	-	expression tag	UNP Q4J9H4
D	0	MET	-	initiating methionine	UNP Q4J9H4
D	1	TRP	-	expression tag	UNP Q4J9H4
D	2	SER	-	expression tag	UNP Q4J9H4
D	3	HIS	-	expression tag	UNP Q4J9H4
D	4	PRO	-	expression tag	UNP Q4J9H4
D	5	GLN	-	expression tag	UNP Q4J9H4
D	6	PHE	-	expression tag	UNP Q4J9H4
D	7	GLU	-	expression tag	UNP Q4J9H4
D	8	LYS	-	expression tag	UNP Q4J9H4
D	9	LEU	-	expression tag	UNP Q4J9H4
D	10	GLU	-	expression tag	UNP Q4J9H4
D	11	VAL	-	expression tag	UNP Q4J9H4
D	12	LEU	-	expression tag	UNP Q4J9H4
D	13	PHE	-	expression tag	UNP Q4J9H4
D	14	GLN	-	expression tag	UNP Q4J9H4
D	15	GLY	-	expression tag	UNP Q4J9H4
D	16	PRO	-	expression tag	UNP Q4J9H4
D	17	SER	-	expression tag	UNP Q4J9H4

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Na 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Na	0	0
			1	1		

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total	Zn	0	0
			1	1		
4	D	1	Total	Zn	0	0
			1	1		

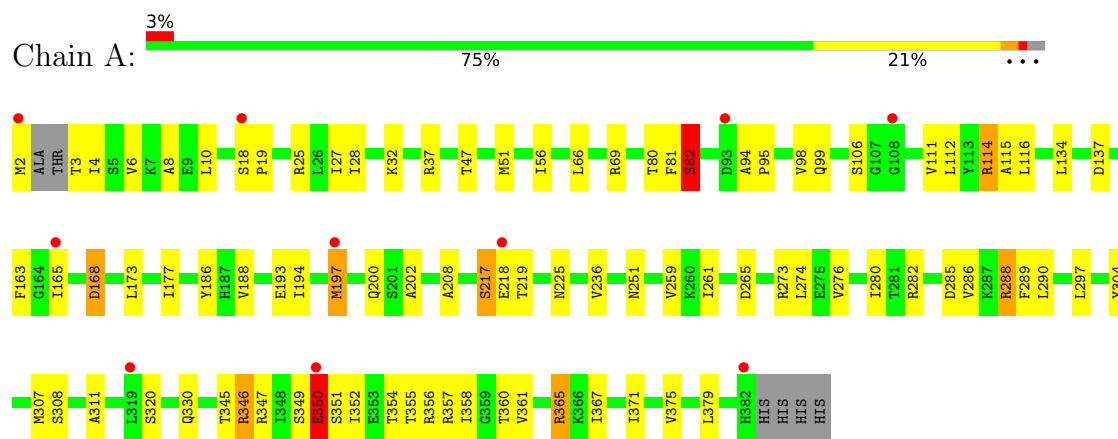
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	15	Total	O	0	0
			15	15		
5	B	13	Total	O	0	0
			13	13		
5	C	1	Total	O	0	0
			1	1		

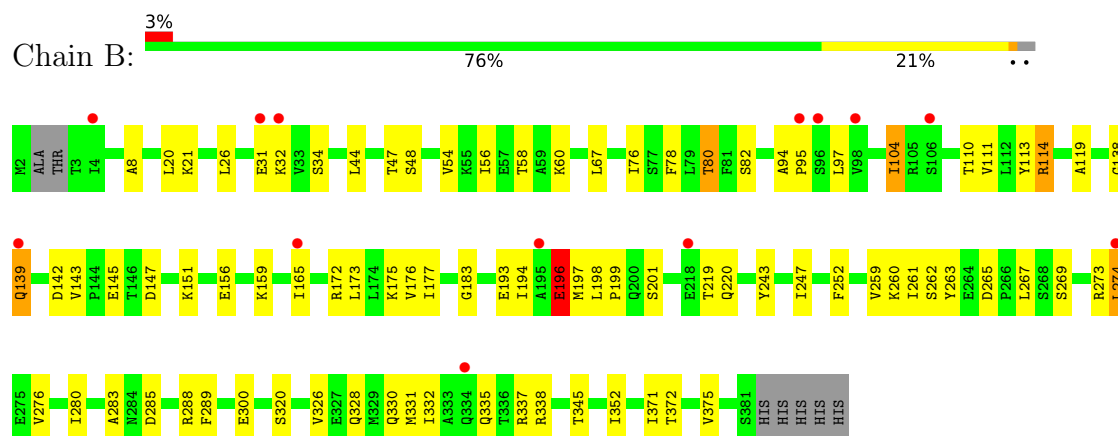
3 Residue-property plots [i](#)

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.

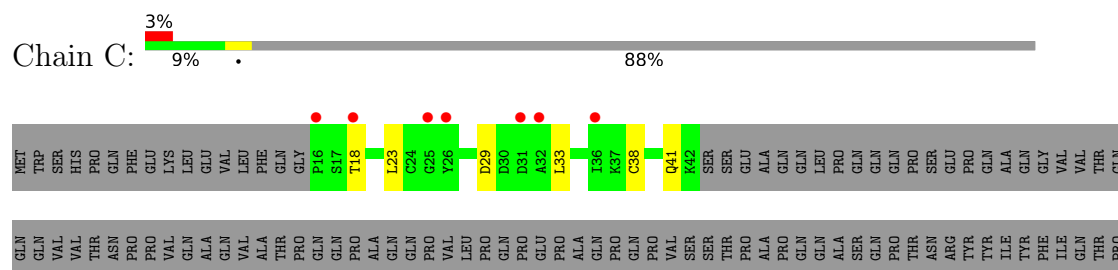
• Molecule 1: Conserved protein



• Molecule 1: Conserved protein



• Molecule 2: Conserved protein



THR	TYR	VAL	TYR	ASP	GLY	LYS	GLN	PHE	THR	PRO	PRO	ILE	LYS	GLY	LYS	GLN	LYS	ILE	GLU	PRO	ASN	SER	SER	ILE	ILE	LYS	LEU	GLY	ASN	GLN	THR	THR	ILE	VAL	ARG	ILE	LYS	LEU	GLU
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- Molecule 2: Conserved protein



GLN	GLY	VAL	VAL	THR	GLN	GLN	VAL	VAL	THR	ASN	PRO	VAL	GLN	ALA	GLN	GLN	GLN	PRO	PRO	ALA	GLN	GLN	GLY	PRO	ALA	GLN	GLN	VAL	LEU	PRO	PRO	GLN	GLN	GLN	PRO	PRO	VAL	VAL	VAL	VAL	THR	THR	PRO	ASN	ARG	TYR	TYR	TYR
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TYR	PHE	ILE	GLN	THR	PRO	ASN	GLU	ASN	ASN	VAL	VAL	ASN	LYS	LYS	VAL	LEU	LEU	ASN	PHE	ASP	ASP	LEU	PHE	PRO	SER	SER	VAL	SER	PRO	GLU	GLU	ASN	ASN	ILE	ILE	ILE	VAL	VAL	PRO	PRO	ASP	SER	SER	GLU	VAL	SER	SER	ARG	ARG	LYS	HIS	ALA	ALA	VAL	ILE	ILE	TYR	TYR	LEU	LEU	ASN	ASN	SER	SER	GLU	GLU	LEU	LEU	TYR	ILE	ILE	GLU	GLU	ASP
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LEU ASN SER THR ASN GLY TYR VAL TYR ASP GLY GLN PHE THR PRO ILE LYS GLY LYS GLN LYS ILE GLU PRO ASN SER ILE ILE LYS LEU GLY ASN GLN THR ILE VAL ARG ILE LEU LYS GLU

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	50.10Å 147.40Å 62.64Å 90.00° 107.16° 90.00°	Depositor
Resolution (Å)	47.87 – 2.11 47.87 – 2.11	Depositor EDS
% Data completeness (in resolution range)	55.0 (47.87-2.11) 55.1 (47.87-2.11)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 2.10Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.208 , 0.264 0.205 , 0.259	Depositor DCC
R_{free} test set	1365 reflections (4.08%)	wwPDB-VP
Wilson B-factor (Å ²)	37.1	Xtriage
Anisotropy	0.223	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 46.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12981	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.92% 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, NA

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	0.43	4/3062 (0.1%)	0.62	7/4142 (0.2%)
1	B	0.32	1/3050 (0.0%)	0.55	6/4124 (0.1%)
2	C	0.21	0/212	0.55	0/284
2	D	0.43	0/203	1.19	3/273 (1.1%)
All	All	0.38	5/6527 (0.1%)	0.61	16/8823 (0.2%)

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
1	B	0	1
2	D	0	1
All	All	0	5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	274	LEU	CG-CD2	10.20	1.86	1.52
1	A	350	GLU	CB-CG	10.11	1.82	1.52
1	A	350	GLU	CG-CD	8.85	1.74	1.52
1	A	197	MET	CG-SD	6.20	1.96	1.80
1	A	350	GLU	CD-OE2	5.02	1.34	1.25

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	197	MET	CG-SD-CE	10.80	124.67	100.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	138	GLY	CA-C-N	9.96	135.07	120.83
1	B	138	GLY	C-N-CA	9.96	135.07	120.83
2	D	29	ASP	N-CA-C	-9.65	96.20	110.48
1	A	197	MET	CB-CG-SD	-8.58	86.97	112.70
1	A	197	MET	CB-CA-C	-8.18	94.66	110.11
1	B	139	GLN	CA-CB-CG	7.33	128.76	114.10
1	B	196	GLU	CA-CB-CG	6.77	127.63	114.10
1	A	82	SER	CA-C-N	-6.73	110.73	120.29
1	A	82	SER	C-N-CA	-6.73	110.73	120.29
1	B	274	LEU	CB-CG-CD1	6.70	130.80	110.70
2	D	30	ASP	N-CA-C	6.46	120.64	113.21
1	B	274	LEU	CA-CB-CG	-5.68	96.43	116.30
1	A	365	ARG	CB-CG-CD	5.39	123.70	111.30
1	A	365	ARG	CA-CB-CG	5.24	124.58	114.10
2	D	29	ASP	N-CA-CB	5.03	117.94	110.29

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	114	ARG	Sidechain
1	A	346	ARG	Sidechain
1	A	349	SER	Peptide
1	B	114	ARG	Sidechain
2	D	29	ASP	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	3017	3088	3094	75	0
1	B	3007	3064	3086	81	0
2	C	208	189	190	7	0
2	D	199	176	176	17	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	1	0	0	0	0
5	A	15	0	0	0	0
5	B	13	0	0	0	0
5	C	1	0	0	0	0
All	All	6464	6517	6546	176	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 14.

All (176) 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:350:GLU:CB	1:A:350:GLU:CG	1.82	1.54
1:B:274:LEU:CD2	1:B:274:LEU:CG	1.86	1.54
2:D:27:GLU:OE1	2:D:28:ASN:N	2.01	0.93
1:B:326:VAL:HG21	1:B:352:ILE:HD12	1.51	0.91
1:A:2:MET:HE3	1:A:265:ASP:OD2	1.76	0.86
1:B:263:TYR:HE1	1:B:274:LEU:CD1	1.92	0.83
1:A:186:TYR:HB3	1:A:197:MET:HE2	1.60	0.82
1:A:218:GLU:N	1:A:218:GLU:OE1	2.15	0.79
1:B:78:PHE:HB2	1:B:97:LEU:HD11	1.64	0.78
1:A:311:ALA:HB2	1:A:375:VAL:HG21	1.66	0.77
1:B:274:LEU:CD2	1:B:274:LEU:CB	2.63	0.75
1:A:163:PHE:HE2	1:A:197:MET:HG2	1.52	0.74
1:B:111:VAL:HG13	1:B:111:VAL:O	1.86	0.74
1:A:25:ARG:HH11	1:A:27:ILE:HD11	1.53	0.73
1:B:111:VAL:HG21	1:B:114:ARG:HE	1.53	0.72
1:B:337:ARG:HA	1:B:337:ARG:HE	1.52	0.72
2:C:33:LEU:HD23	2:C:33:LEU:O	1.92	0.70
2:D:17:SER:O	2:D:18:THR:HG23	1.92	0.70
1:B:47:THR:HG1	1:B:82:SER:HG	1.37	0.70
1:B:243:TYR:OH	1:B:300:GLU:OE1	2.10	0.69
1:A:355:THR:OG1	1:A:367:ILE:HD13	1.93	0.69
1:B:263:TYR:CE1	1:B:274:LEU:CD1	2.76	0.69
1:B:8:ALA:HB3	1:B:276:VAL:HG11	1.74	0.68
1:B:219:THR:HG21	1:B:247:ILE:O	1.94	0.67
1:B:261:ILE:HB	1:B:274:LEU:HB2	1.76	0.67
1:A:188:VAL:HG11	1:A:194:ILE:HG13	1.76	0.66
1:B:263:TYR:HE1	1:B:274:LEU:HD13	1.60	0.65
1:B:172:ARG:O	1:B:176:VAL:HG23	1.97	0.65
1:A:346:ARG:O	1:A:350:GLU:HB2	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:33:LEU:HD21	2:C:41:GLN:HE21	1.62	0.64
1:B:283:ALA:HA	1:B:288:ARG:HD2	1.77	0.64
1:A:6:VAL:HG21	1:A:261:ILE:HD12	1.79	0.64
2:D:29:ASP:C	2:D:29:ASP:OD1	2.40	0.64
1:B:110:THR:OG1	1:B:139:GLN:O	2.09	0.63
1:B:328:GLN:O	1:B:332:ILE:HD13	1.98	0.63
1:A:4:ILE:HD11	1:A:236:VAL:HG11	1.81	0.63
1:B:165:ILE:HD12	1:B:194:ILE:HD11	1.79	0.62
1:A:285:ASP:OD1	1:A:286:VAL:N	2.32	0.62
1:A:347:ARG:C	1:A:350:GLU:HB2	2.25	0.62
1:B:26:LEU:HD21	1:B:259:VAL:HG21	1.81	0.62
1:B:261:ILE:O	1:B:274:LEU:HB2	2.00	0.61
1:A:188:VAL:HG13	1:A:193:GLU:HB2	1.83	0.60
1:B:337:ARG:HA	1:B:337:ARG:NE	2.17	0.60
1:B:326:VAL:HG21	1:B:352:ILE:CD1	2.29	0.60
1:A:273:ARG:C	1:A:274:LEU:HD12	2.27	0.60
2:D:24:CYS:HB2	2:D:37:LYS:NZ	2.16	0.59
1:B:145:GLU:OE1	1:B:145:GLU:N	2.35	0.59
1:B:67:LEU:HD22	1:B:76:ILE:HD13	1.85	0.59
1:A:289:PHE:CD2	1:A:290:LEU:HD12	2.38	0.58
1:A:51:MET:HE2	1:A:137:ASP:HB3	1.85	0.58
1:A:347:ARG:O	1:A:350:GLU:HB2	2.04	0.58
2:C:18:THR:HG23	2:C:29:ASP:HA	1.86	0.57
1:B:331:MET:O	1:B:335:GLN:HG3	2.04	0.57
1:B:34:SER:OG	1:B:267:LEU:HD13	2.05	0.56
1:A:2:MET:HG3	1:A:3:THR:HG23	1.86	0.56
2:D:18:THR:HG22	2:D:29:ASP:HA	1.86	0.56
1:A:4:ILE:HD12	1:A:28:ILE:HG22	1.88	0.56
1:B:252:PHE:HD2	1:B:280:ILE:HD11	1.71	0.55
1:A:10:LEU:HD23	1:A:280:ILE:HD11	1.88	0.54
1:A:346:ARG:HG2	1:A:350:GLU:HG2	1.89	0.54
1:B:219:THR:HG22	1:B:220:GLN:N	2.22	0.54
1:A:347:ARG:O	1:A:350:GLU:CB	2.55	0.54
1:A:352:ILE:O	1:A:356:ARG:HG3	2.08	0.53
1:B:60:LYS:HD2	1:B:104:ILE:HB	1.91	0.53
1:A:37:ARG:HG2	1:A:37:ARG:HH11	1.74	0.53
1:A:4:ILE:HG23	1:A:28:ILE:HG23	1.89	0.53
1:B:21:LYS:HB2	2:D:34:PHE:CD2	2.44	0.53
1:B:198:LEU:O	1:B:201:SER:OG	2.27	0.53
2:D:23:LEU:N	2:D:23:LEU:HD12	2.24	0.53
1:A:354:THR:O	1:A:358:ILE:HD13	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:371:ILE:O	1:A:375:VAL:HG23	2.09	0.52
1:A:163:PHE:CE2	1:A:197:MET:HG2	2.40	0.52
1:B:273:ARG:C	1:B:274:LEU:HG	2.33	0.52
1:B:20:LEU:HD21	1:B:289:PHE:CE1	2.44	0.52
1:A:2:MET:N	1:A:32:LYS:O	2.43	0.52
1:A:297:LEU:HD12	1:A:297:LEU:O	2.10	0.51
1:A:285:ASP:HB3	1:A:288:ARG:NE	2.26	0.51
1:B:47:THR:HG22	1:B:56:ILE:HD11	1.91	0.51
1:B:338:ARG:HH11	1:B:338:ARG:HG3	1.76	0.51
1:A:361:VAL:O	1:A:365:ARG:HB2	2.10	0.51
1:B:172:ARG:HH11	1:B:172:ARG:HG3	1.75	0.51
1:B:114:ARG:HD3	1:B:142:ASP:OD2	2.09	0.51
1:B:26:LEU:HD23	1:B:261:ILE:HD11	1.93	0.50
1:B:274:LEU:HD23	1:B:274:LEU:HA	1.93	0.50
2:D:19:TRP:O	2:D:27:GLU:OE1	2.30	0.50
1:A:307:MET:HG3	1:A:375:VAL:HG22	1.93	0.50
1:A:173:LEU:O	1:A:177:ILE:HG12	2.10	0.50
1:A:19:PRO:HG2	2:C:41:GLN:OE1	2.12	0.50
1:A:47:THR:HG22	1:A:56:ILE:HD11	1.93	0.50
1:B:219:THR:HG21	1:B:247:ILE:HB	1.94	0.50
1:A:346:ARG:O	1:A:350:GLU:CB	2.60	0.49
1:A:217:SER:OG	1:A:219:THR:O	2.25	0.49
1:B:338:ARG:HG3	1:B:338:ARG:NH1	2.26	0.49
2:C:23:LEU:HD12	2:C:23:LEU:N	2.28	0.49
1:A:4:ILE:HD12	1:A:28:ILE:CG2	2.43	0.48
1:B:159:LYS:HG2	1:B:183:GLY:HA2	1.95	0.48
1:A:285:ASP:HB3	1:A:288:ARG:HB3	1.96	0.48
1:A:304:TYR:HB3	1:A:379:LEU:HD21	1.96	0.48
2:D:28:ASN:HD21	2:D:35:CYS:HA	1.79	0.48
1:B:113:TYR:HB3	1:B:142:ASP:OD2	2.14	0.48
1:B:47:THR:CG2	1:B:80:THR:HG23	2.44	0.47
1:A:358:ILE:HD12	1:A:358:ILE:N	2.30	0.47
1:B:219:THR:CG2	1:B:247:ILE:HB	2.45	0.47
1:B:371:ILE:O	1:B:375:VAL:HG23	2.15	0.47
1:B:172:ARG:HG3	1:B:172:ARG:NH1	2.30	0.47
2:D:24:CYS:HB2	2:D:37:LYS:HZ3	1.78	0.47
1:A:330:GLN:HG3	1:A:345:THR:HG22	1.95	0.47
1:A:347:ARG:HA	1:A:350:GLU:HG3	1.95	0.47
1:B:111:VAL:O	1:B:111:VAL:CG1	2.57	0.47
1:B:54:VAL:O	1:B:58:THR:OG1	2.28	0.47
2:C:33:LEU:HD23	2:C:33:LEU:C	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:ASP:OD1	1:B:143:VAL:N	2.46	0.47
1:B:261:ILE:HB	1:B:274:LEU:CB	2.44	0.47
1:A:289:PHE:HD2	1:A:290:LEU:HD12	1.80	0.47
1:A:94:ALA:N	1:A:95:PRO:HD2	2.30	0.46
1:B:198:LEU:HB3	1:B:199:PRO:HD3	1.97	0.46
1:A:111:VAL:HG22	1:A:111:VAL:O	2.15	0.46
1:B:48:SER:CB	1:B:110:THR:HG23	2.44	0.46
1:B:196:GLU:OE1	1:B:196:GLU:C	2.59	0.46
1:B:48:SER:HB3	1:B:110:THR:HG23	1.97	0.46
1:A:188:VAL:HG11	1:A:194:ILE:CG1	2.44	0.46
1:A:112:LEU:HD11	1:A:134:LEU:HD11	1.98	0.46
1:B:263:TYR:CE1	1:B:274:LEU:HD13	2.46	0.46
2:D:24:CYS:SG	2:D:37:LYS:HB3	2.56	0.46
1:B:111:VAL:HG21	1:B:114:ARG:NE	2.28	0.45
1:A:4:ILE:HG12	1:A:208:ALA:HB2	1.98	0.45
1:A:354:THR:O	1:A:357:ARG:HB2	2.17	0.45
1:B:193:GLU:HB3	1:B:197:MET:SD	2.57	0.45
2:C:33:LEU:CD2	2:C:41:GLN:HG3	2.47	0.45
1:B:31:GLU:C	1:B:32:LYS:N	2.75	0.45
1:B:94:ALA:N	1:B:95:PRO:CD	2.81	0.44
1:B:173:LEU:O	1:B:177:ILE:HG12	2.17	0.44
1:B:47:THR:HG21	1:B:80:THR:HG23	2.00	0.44
1:B:111:VAL:CG2	1:B:114:ARG:HE	2.28	0.43
1:B:260:LYS:HA	1:B:274:LEU:O	2.18	0.43
2:D:27:GLU:OE1	2:D:27:GLU:C	2.60	0.43
1:A:98:VAL:HG23	1:A:99:GLN:N	2.32	0.43
1:B:21:LYS:CB	2:D:34:PHE:CD2	3.01	0.43
2:D:28:ASN:HD21	2:D:36:ILE:H	1.66	0.43
2:D:22:ASN:N	2:D:22:ASN:OD1	2.52	0.43
1:A:47:THR:CG2	1:A:80:THR:HG23	2.49	0.43
1:A:330:GLN:N	1:A:345:THR:HG21	2.34	0.43
1:A:273:ARG:O	1:A:274:LEU:HD12	2.18	0.43
1:B:252:PHE:CD2	1:B:280:ILE:HD11	2.53	0.42
1:B:56:ILE:O	1:B:60:LYS:HG3	2.19	0.42
1:B:330:GLN:HA	1:B:345:THR:HG21	2.00	0.42
1:B:175:LYS:HD3	1:B:372:THR:HG23	2.02	0.42
1:A:8:ALA:HB3	1:A:276:VAL:HG11	2.00	0.42
1:B:44:LEU:HD11	1:B:119:ALA:HB2	2.00	0.42
1:B:21:LYS:HB2	2:D:34:PHE:CE2	2.54	0.42
1:B:260:LYS:HB2	1:B:260:LYS:HE2	1.79	0.42
1:A:81:PHE:CB	1:A:115:ALA:HB2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:28:ASN:ND2	2:D:35:CYS:HA	2.35	0.42
1:A:225:ASN:OD1	1:A:225:ASN:N	2.53	0.42
1:B:265:ASP:OD1	1:B:265:ASP:C	2.62	0.42
1:A:51:MET:HE2	1:A:137:ASP:CB	2.47	0.41
1:A:168:ASP:OD1	1:A:168:ASP:N	2.52	0.41
1:A:286:VAL:HG12	1:A:290:LEU:HD13	2.02	0.41
1:B:285:ASP:OD1	1:B:288:ARG:HG2	2.20	0.41
1:A:4:ILE:HD11	1:A:236:VAL:CG1	2.49	0.41
1:A:66:LEU:HD12	1:A:202:ALA:HB2	2.02	0.41
1:A:111:VAL:HG22	1:A:114:ARG:HB2	2.02	0.41
1:A:358:ILE:O	1:A:360:THR:HG23	2.20	0.41
1:B:78:PHE:HB3	1:B:97:LEU:HD21	2.02	0.41
1:A:98:VAL:CG2	1:A:99:GLN:N	2.83	0.41
1:B:274:LEU:CD2	1:B:274:LEU:HA	2.50	0.41
1:A:165:ILE:CD1	1:A:188:VAL:HB	2.50	0.41
1:B:220:GLN:OE1	1:B:220:GLN:HA	2.21	0.41
1:A:111:VAL:CG2	1:A:114:ARG:HG3	2.52	0.40
1:A:346:ARG:O	1:A:350:GLU:HG2	2.21	0.40
1:A:69:ARG:HE	1:A:69:ARG:HB3	1.76	0.40
1:B:283:ALA:CA	1:B:288:ARG:HD2	2.47	0.40
1:A:251:ASN:HB3	1:A:282:ARG:HD2	2.03	0.40
1:A:307:MET:CG	1:A:375:VAL:HG22	2.51	0.40
1:A:347:ARG:HA	1:A:350:GLU:CG	2.51	0.40
1:B:147:ASP:O	1:B:151:LYS:HG3	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	379/387 (98%)	370 (98%)	7 (2%)	2 (0%)	24 22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	376/387 (97%)	369 (98%)	7 (2%)	0	100	100
2	C	25/223 (11%)	24 (96%)	1 (4%)	0	100	100
2	D	24/223 (11%)	21 (88%)	2 (8%)	1 (4%)	2	0
All	All	804/1220 (66%)	784 (98%)	17 (2%)	3 (0%)	30	28

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	82	SER
1	A	350	GLU
2	D	18	THR

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	338/343 (98%)	326 (96%)	12 (4%)	31	33
1	B	337/343 (98%)	330 (98%)	7 (2%)	47	54
2	C	23/203 (11%)	22 (96%)	1 (4%)	26	26
2	D	22/203 (11%)	20 (91%)	2 (9%)	9	6
All	All	720/1092 (66%)	698 (97%)	22 (3%)	35	38

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	SER
1	A	82	SER
1	A	106	SER
1	A	116	LEU
1	A	168	ASP
1	A	200	GLN
1	A	217	SER
1	A	259	VAL

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Mol	Chain	Res	Type
1	A	288	ARG
1	A	308	SER
1	A	320	SER
1	A	351	SER
1	B	80	THR
1	B	104	ILE
1	B	156	GLU
1	B	196	GLU
1	B	262	SER
1	B	269	SER
1	B	320	SER
2	C	38	CYS
2	D	18	THR
2	D	29	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	ASN
1	A	84	ASN
1	A	200	GLN
1	A	315	ASN
1	B	61	GLN
1	B	100	GLN
1	B	251	ASN
1	B	284	ASN
2	D	28	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](#)

Of 4 ligands modelled in this entry, 4 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 [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	31:GLU	C	32:LYS	N	2.75

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	381/387 (98%)	0.29	10 (2%) 57 60	22, 47, 77, 103	0
1	B	380/387 (98%)	0.31	13 (3%) 48 51	23, 49, 78, 119	0
2	C	27/223 (12%)	1.46	7 (25%) 1 2	59, 81, 102, 113	0
2	D	26/223 (11%)	2.46	16 (61%) 0 0	78, 114, 143, 162	0
All	All	814/1220 (66%)	0.41	46 (5%) 29 32	22, 49, 88, 162	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	33	LEU	4.8
1	B	334	GLN	4.4
2	D	26	TYR	4.3
1	B	274	LEU	4.2
1	B	96	SER	3.9
2	D	19	TRP	3.9
2	D	16	PRO	3.9
2	C	25	GLY	3.8
1	B	139	GLN	3.6
2	C	16	PRO	3.4
2	D	23	LEU	3.4
1	B	32	LYS	3.4
1	B	195	ALA	3.1
2	D	29	ASP	3.1
2	D	25	GLY	3.0
2	C	18	THR	3.0
1	B	98	VAL	2.9
1	A	382	HIS	2.9
1	A	108	GLY	2.7
2	C	32	ALA	2.7
2	C	36	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	4	ILE	2.6
2	D	39	GLY	2.6
1	A	218	GLU	2.6
2	D	18	THR	2.6
2	D	20	LYS	2.6
1	B	165	ILE	2.5
1	A	2	MET	2.5
2	C	26	TYR	2.4
2	D	38	CYS	2.4
1	A	197	MET	2.4
2	D	32	ALA	2.4
1	B	31	GLU	2.4
1	A	18	SER	2.4
1	A	350	GLU	2.3
2	D	41	GLN	2.3
1	A	165	ILE	2.3
1	B	218	GLU	2.2
2	D	27	GLU	2.2
2	D	40	ALA	2.2
1	A	93	ASP	2.2
1	B	95	PRO	2.1
1	A	319	LEU	2.1
2	C	31	ASP	2.1
1	B	106	SER	2.0
2	D	21	CYS	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 ⓘ

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($\text{\AA}^2$)	Q<0.9
3	NA	A	401	1/1	0.92	0.05	43,43,43,43	0
3	NA	B	401	1/1	0.94	0.10	43,43,43,43	0
4	ZN	D	301	1/1	0.97	0.05	86,86,86,86	0
4	ZN	C	301	1/1	0.99	0.05	63,63,63,63	0

6.5 Other polymers [i](#)

There are no such residues in this entry.