



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 05:22 PM UTC

PDB ID : 1VR6 / pdb_00001vr6
Title : Crystal structure of Phospho-2-dehydro-3-deoxyheptonate aldolase (DAHP synthase) (TM0343) from *Thermotoga Maritima* at 1.92 Å resolution
Authors : Joint Center for Structural Genomics (JCSG)
Deposited on : 2005-02-14
Resolution : 1.92 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

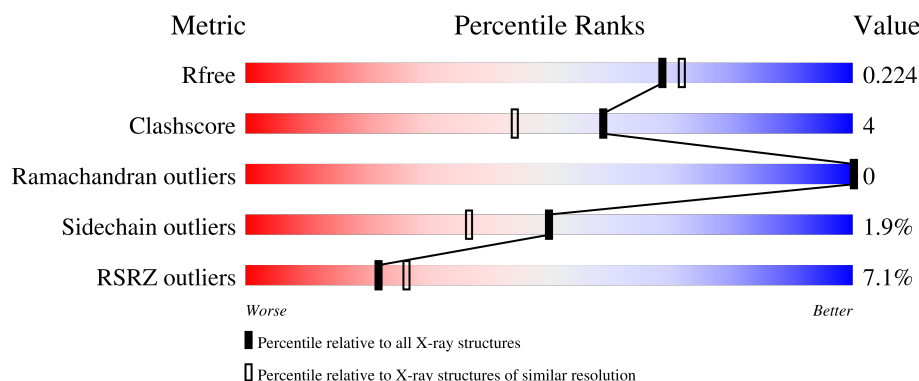
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.92 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	1188 (1.92-1.92)
Clashscore	190562	1209 (1.92-1.92)
Ramachandran outliers	187476	1195 (1.92-1.92)
Sidechain outliers	187428	1195 (1.92-1.92)
RSRZ outliers	180081	1188 (1.92-1.92)

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	350	5% 84% 14% .
1	B	350	7% 88% 8% ..
1	C	350	7% 85% 11% .
1	D	350	9% 89% 8% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11010 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 Phospho-2-dehydro-3-deoxyheptonate aldolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	343	Total	C	N	O	S	0	1	0
			2653	1686	461	496	10			
1	B	338	Total	C	N	O	S	0	3	0
			2611	1657	452	492	10			
1	C	339	Total	C	N	O	S	0	1	0
			2600	1653	447	490	10			
1	D	340	Total	C	N	O	S	0	1	0
			2531	1615	429	477	10			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	expression tag	UNP Q9WYH8
A	-10	GLY	-	expression tag	UNP Q9WYH8
A	-9	SER	-	expression tag	UNP Q9WYH8
A	-8	ASP	-	expression tag	UNP Q9WYH8
A	-7	LYS	-	expression tag	UNP Q9WYH8
A	-6	ILE	-	expression tag	UNP Q9WYH8
A	-5	HIS	-	expression tag	UNP Q9WYH8
A	-4	HIS	-	expression tag	UNP Q9WYH8
A	-3	HIS	-	expression tag	UNP Q9WYH8
A	-2	HIS	-	expression tag	UNP Q9WYH8
A	-1	HIS	-	expression tag	UNP Q9WYH8
A	0	HIS	-	expression tag	UNP Q9WYH8
B	-11	MET	-	expression tag	UNP Q9WYH8
B	-10	GLY	-	expression tag	UNP Q9WYH8
B	-9	SER	-	expression tag	UNP Q9WYH8
B	-8	ASP	-	expression tag	UNP Q9WYH8
B	-7	LYS	-	expression tag	UNP Q9WYH8
B	-6	ILE	-	expression tag	UNP Q9WYH8
B	-5	HIS	-	expression tag	UNP Q9WYH8
B	-4	HIS	-	expression tag	UNP Q9WYH8
B	-3	HIS	-	expression tag	UNP Q9WYH8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	HIS	-	expression tag	UNP Q9WYH8
B	-1	HIS	-	expression tag	UNP Q9WYH8
B	0	HIS	-	expression tag	UNP Q9WYH8
C	-11	MET	-	expression tag	UNP Q9WYH8
C	-10	GLY	-	expression tag	UNP Q9WYH8
C	-9	SER	-	expression tag	UNP Q9WYH8
C	-8	ASP	-	expression tag	UNP Q9WYH8
C	-7	LYS	-	expression tag	UNP Q9WYH8
C	-6	ILE	-	expression tag	UNP Q9WYH8
C	-5	HIS	-	expression tag	UNP Q9WYH8
C	-4	HIS	-	expression tag	UNP Q9WYH8
C	-3	HIS	-	expression tag	UNP Q9WYH8
C	-2	HIS	-	expression tag	UNP Q9WYH8
C	-1	HIS	-	expression tag	UNP Q9WYH8
C	0	HIS	-	expression tag	UNP Q9WYH8
D	-11	MET	-	expression tag	UNP Q9WYH8
D	-10	GLY	-	expression tag	UNP Q9WYH8
D	-9	SER	-	expression tag	UNP Q9WYH8
D	-8	ASP	-	expression tag	UNP Q9WYH8
D	-7	LYS	-	expression tag	UNP Q9WYH8
D	-6	ILE	-	expression tag	UNP Q9WYH8
D	-5	HIS	-	expression tag	UNP Q9WYH8
D	-4	HIS	-	expression tag	UNP Q9WYH8
D	-3	HIS	-	expression tag	UNP Q9WYH8
D	-2	HIS	-	expression tag	UNP Q9WYH8
D	-1	HIS	-	expression tag	UNP Q9WYH8
D	0	HIS	-	expression tag	UNP Q9WYH8

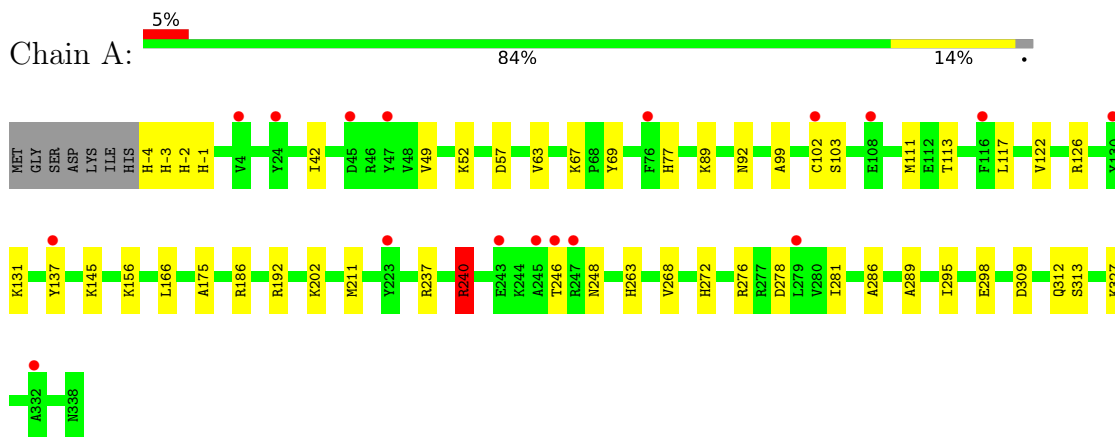
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	197	Total O 197 197	0	0
2	B	162	Total O 162 162	0	0
2	C	155	Total O 155 155	0	0
2	D	101	Total O 101 101	0	0

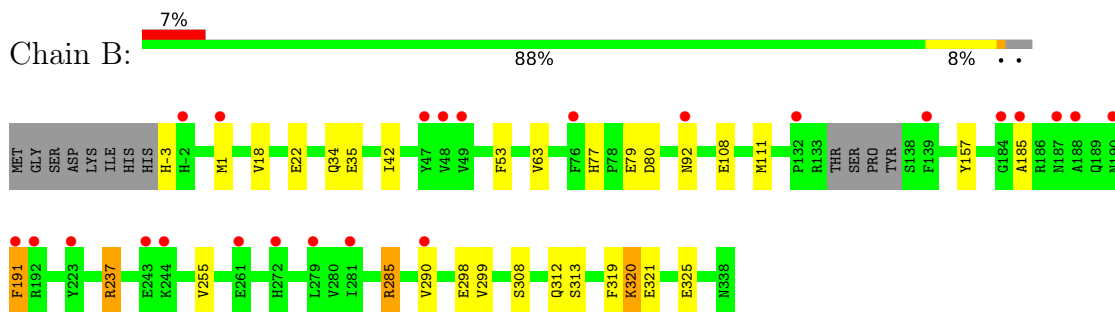
3 Residue-property plots [i](#)

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.

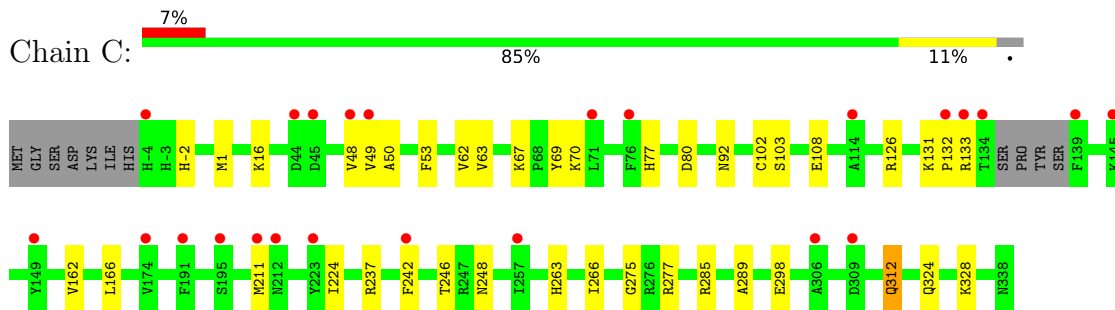
- Molecule 1: Phospho-2-dehydro-3-deoxyheptonate aldolase



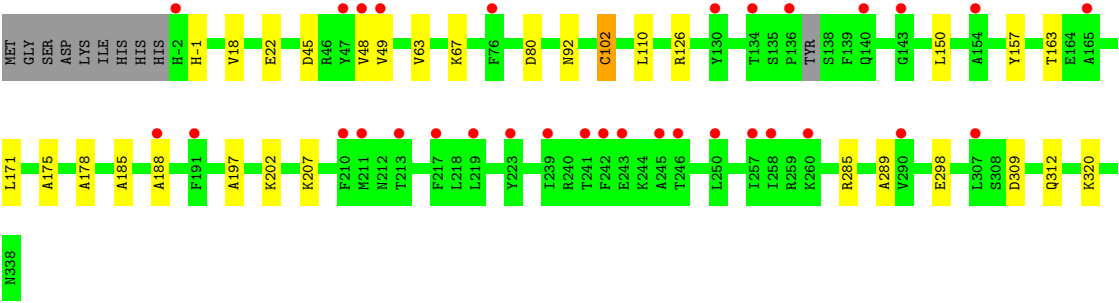
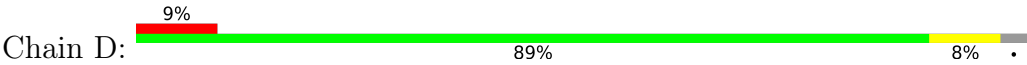
- Molecule 1: Phospho-2-dehydro-3-deoxyheptonate aldolase



- Molecule 1: Phospho-2-dehydro-3-deoxyheptonate aldolase



- Molecule 1: Phospho-2-dehydro-3-deoxyheptonate aldolase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.15Å 74.23Å 249.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.76 – 1.92 47.76 – 1.93	Depositor EDS
% Data completeness (in resolution range)	98.5 (47.76-1.92) 98.5 (47.76-1.93)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.99 (at 1.92Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.171 , 0.215 0.179 , 0.224	Depositor DCC
R_{free} test set	5111 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	36.2	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 52.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.016 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11010	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.37% 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

5.1 Standard geometry

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	1.03	4/2704 (0.1%)	0.97	3/3649 (0.1%)
1	B	0.94	1/2666 (0.0%)	0.94	2/3598 (0.1%)
1	C	0.93	2/2649 (0.1%)	0.93	2/3578 (0.1%)
1	D	0.85	1/2578 (0.0%)	0.91	1/3494 (0.0%)
All	All	0.94	8/10597 (0.1%)	0.94	8/14319 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	157	TYR	C-O	9.20	1.36	1.24
1	A	240	ARG	CD-NE	-6.29	1.37	1.46
1	A	137	TYR	CA-CB	5.42	1.62	1.53
1	C	266	ILE	CA-CB	5.36	1.61	1.54
1	B	255	VAL	CA-CB	5.25	1.60	1.54
1	C	242	PHE	CA-C	5.14	1.59	1.52
1	A	281	ILE	CA-C	5.12	1.58	1.52
1	A	286	ALA	CA-CB	-5.04	1.45	1.53

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	285	ARG	NE-CZ-NH2	-7.40	112.54	119.20
1	A	92	ASN	N-CA-C	6.94	120.91	110.64
1	A	240	ARG	NE-CZ-NH2	-6.22	113.60	119.20
1	C	224	ILE	N-CA-C	-6.17	104.73	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	285	ARG	NE-CZ-NH1	6.13	127.63	121.50
1	A	-3	HIS	N-CA-C	-5.47	99.60	108.41
1	D	309	ASP	N-CA-C	5.03	118.53	111.74
1	C	133	ARG	N-CA-C	5.02	117.01	110.53

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	-4	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	2653	0	2684	39	0
1	B	2611	0	2625	20	0
1	C	2600	0	2603	26	0
1	D	2531	0	2479	16	0
2	A	197	0	0	7	0
2	B	162	0	0	2	0
2	C	155	0	0	4	0
2	D	101	0	0	3	0
All	All	11010	0	10391	92	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 4.

All (92) 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:D:102:CYS:SG	1:D:298:GLU:OE2	2.05	1.14
1:A:298[B]:GLU:CD	1:A:313:SER:OG	2.17	0.88
1:C:102:CYS:SG	1:C:298:GLU:OE2	2.32	0.86
1:A:102:CYS:SG	1:A:298[A]:GLU:OE1	2.43	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298[B]:GLU:OE2	1:A:313:SER:OG	2.03	0.76
1:A:276:ARG:HD2	1:A:278:ASP:OD1	1.85	0.75
1:A:240:ARG:HD3	2:A:404:HOH:O	1.83	0.75
1:A:126:ARG:NH1	1:A:298[A]:GLU:HG2	2.07	0.70
1:C:324:GLN:O	1:C:328:LYS:HG3	1.93	0.67
1:A:-2:HIS:CE1	1:A:42:ILE:HD11	2.32	0.64
1:B:1:MET:HE1	1:B:53:PHE:CD2	2.33	0.64
1:B:79:GLU:H	1:B:79:GLU:CD	2.06	0.63
2:B:424:HOH:O	1:C:67:LYS:HE2	1.99	0.62
1:A:175:ALA:O	1:A:202:LYS:NZ	2.33	0.61
1:B:63:VAL:HG21	1:C:63:VAL:HG11	1.82	0.61
1:A:63:VAL:HG11	1:D:63:VAL:HG21	1.84	0.60
1:C:1:MET:HE1	1:C:53:PHE:CD2	2.36	0.60
1:A:-1:HIS:O	1:A:42:ILE:HD12	2.01	0.60
1:C:275:GLY:HA2	1:C:312:GLN:HG2	1.84	0.59
1:B:34:GLN:HG2	1:C:-2:HIS:CE1	2.39	0.58
1:A:111:MET:HE1	1:A:156:LYS:HD3	1.86	0.57
1:A:240:ARG:CD	2:A:404:HOH:O	2.46	0.56
1:C:103:SER:HB3	1:C:131:LYS:HE3	1.88	0.56
1:A:240:ARG:HB3	1:C:211:MET:HE1	1.87	0.56
1:A:289:ALA:O	1:B:285:ARG:HD2	2.05	0.56
1:A:192:ARG:NH1	1:C:166:LEU:HD23	2.21	0.56
1:B:111:MET:CE	1:B:157:TYR:HE2	2.20	0.54
1:D:80:ASP:OD2	1:D:92:ASN:CB	2.55	0.54
1:B:321:GLU:OE2	1:B:325:GLU:OE2	2.26	0.53
1:D:207:LYS:NZ	2:D:350:HOH:O	2.41	0.53
1:B:80:ASP:OD2	1:B:92:ASN:HB2	2.09	0.52
1:D:175:ALA:O	1:D:202:LYS:NZ	2.42	0.52
1:C:126:ARG:NH1	2:C:474:HOH:O	2.41	0.52
1:A:102:CYS:CB	1:A:298[A]:GLU:OE1	2.57	0.52
1:A:67:LYS:NZ	2:A:372:HOH:O	2.27	0.51
1:A:-2:HIS:NE2	1:A:42:ILE:HD11	2.24	0.51
1:A:166:LEU:HG	1:A:186:ARG:NH2	2.25	0.51
1:A:309:ASP:OD1	2:A:531:HOH:O	2.20	0.51
1:B:111:MET:HE3	1:B:157:TYR:HE2	1.75	0.51
1:C:69:TYR:O	1:C:70:LYS:HD3	2.12	0.50
1:B:185:ALA:HB2	1:B:237:ARG:HD2	1.94	0.50
1:B:191:PHE:CD1	1:B:191:PHE:C	2.90	0.49
1:A:246:THR:HB	1:A:248:ASN:O	2.13	0.49
1:C:67:LYS:NZ	2:C:350:HOH:O	2.46	0.48
1:A:103:SER:OG	1:A:131:LYS:HE3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:VAL:O	1:B:22:GLU:HG2	2.13	0.48
1:B:237:ARG:HG3	2:B:342:HOH:O	2.13	0.48
1:C:50:ALA:HB1	1:C:62:VAL:HG11	1.96	0.48
1:D:126:ARG:NH1	2:D:350:HOH:O	2.47	0.48
1:A:89:LYS:NZ	2:A:535:HOH:O	2.47	0.48
1:B:80:ASP:OD2	1:B:92:ASN:CB	2.61	0.48
1:B:34:GLN:HG3	1:B:35:GLU:HG3	1.95	0.47
1:D:48:VAL:HG22	1:D:49:VAL:N	2.30	0.47
1:A:272:HIS:NE2	1:A:298[A]:GLU:OE2	2.48	0.47
1:A:111:MET:CE	1:A:156:LYS:HD3	2.44	0.46
1:D:163:THR:HG22	1:D:178:ALA:HB2	1.98	0.46
1:C:16:LYS:NZ	2:C:417:HOH:O	2.49	0.46
1:C:285:ARG:HD2	1:D:289:ALA:O	2.16	0.45
1:D:110:LEU:HD21	1:D:150:LEU:HA	1.99	0.45
1:C:289:ALA:O	1:D:285:ARG:HD2	2.17	0.45
1:C:80:ASP:OD2	1:C:92:ASN:CB	2.64	0.45
1:C:211:MET:HB3	1:C:211:MET:HE2	1.54	0.44
1:D:185:ALA:O	1:D:188:ALA:HB2	2.17	0.44
1:B:77:HIS:CE1	1:B:79:GLU:HG2	2.53	0.44
1:A:268:VAL:O	1:A:295:ILE:HA	2.18	0.44
1:B:299:VAL:HG21	1:B:319:PHE:CD1	2.53	0.44
1:A:113:THR:O	1:A:117:LEU:HG	2.17	0.43
1:D:126:ARG:NH1	2:D:368:HOH:O	2.50	0.43
1:C:77:HIS:HB3	1:C:263:HIS:CD2	2.54	0.43
1:D:171:LEU:HD21	1:D:197:ALA:HA	2.00	0.43
1:C:246:THR:HB	1:C:248:ASN:O	2.18	0.43
1:C:108:GLU:HG2	2:C:435:HOH:O	2.19	0.43
1:D:18:VAL:O	1:D:22:GLU:HG3	2.19	0.42
1:A:67:LYS:HE2	1:A:69:TYR:CE1	2.55	0.42
1:A:327:LYS:NZ	2:A:508:HOH:O	2.38	0.42
1:A:117:LEU:HB3	1:A:122:VAL:HB	2.01	0.42
1:A:126:ARG:HH12	1:A:298[A]:GLU:HG2	1.82	0.42
1:A:272:HIS:NE2	1:A:298[A]:GLU:CD	2.77	0.42
1:B:298:GLU:CD	1:B:313[A]:SER:OG	2.63	0.42
1:A:77:HIS:HB3	1:A:263:HIS:CD2	2.55	0.42
1:A:49:VAL:O	1:A:52:LYS:HB2	2.20	0.41
1:C:102:CYS:CB	1:C:298:GLU:OE2	2.68	0.41
1:D:-1:HIS:NE2	1:D:45:ASP:O	2.45	0.41
1:A:57:ASP:OD1	1:C:277:ARG:NH1	2.54	0.41
1:B:320:LYS:NZ	1:B:320:LYS:CB	2.84	0.41
1:B:320:LYS:NZ	1:B:320:LYS:HB2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298[B]:GLU:CG	1:A:313:SER:OG	2.69	0.41
1:A:186:ARG:HG2	2:A:394:HOH:O	2.20	0.40
1:C:48:VAL:HG22	1:C:49:VAL:N	2.36	0.40
1:A:99:ALA:C	1:A:126:ARG:HG2	2.46	0.40
1:C:131:LYS:HA	1:C:132:PRO:HD3	1.97	0.40
1:A:52:LYS:N	1:A:52:LYS:HD2	2.37	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	342/350 (98%)	335 (98%)	7 (2%)	0	100	100
1	B	337/350 (96%)	332 (98%)	5 (2%)	0	100	100
1	C	336/350 (96%)	331 (98%)	5 (2%)	0	100	100
1	D	337/350 (96%)	330 (98%)	7 (2%)	0	100	100
All	All	1352/1400 (97%)	1328 (98%)	24 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	284/297 (96%)	279 (98%)	5 (2%)	51	39
1	B	279/297 (94%)	270 (97%)	9 (3%)	34	18
1	C	276/297 (93%)	273 (99%)	3 (1%)	65	60
1	D	257/297 (86%)	253 (98%)	4 (2%)	55	44
All	All	1096/1188 (92%)	1075 (98%)	21 (2%)	50	37

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

Mol	Chain	Res	Type
1	A	145	LYS
1	A	211	MET
1	A	237	ARG
1	A	240	ARG
1	A	312	GLN
1	B	-3	HIS
1	B	42	ILE
1	B	108	GLU
1	B	191	PHE
1	B	237	ARG
1	B	290	VAL
1	B	308	SER
1	B	312	GLN
1	B	320	LYS
1	C	162	VAL
1	C	237	ARG
1	C	312	GLN
1	D	67	LYS
1	D	102	CYS
1	D	312	GLN
1	D	320	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	-1	HIS
1	B	182	GLN
1	B	312	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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	343/350 (98%)	0.76	17 (4%) 34 38	27, 44, 55, 76	1 (0%)
1	B	338/350 (96%)	0.88	24 (7%) 22 26	28, 45, 61, 77	3 (0%)
1	C	339/350 (96%)	0.91	24 (7%) 22 26	26, 45, 55, 71	1 (0%)
1	D	340/350 (97%)	1.06	32 (9%) 14 17	27, 45, 61, 82	1 (0%)
All	All	1360/1400 (97%)	0.90	97 (7%) 22 26	26, 45, 58, 82	6 (0%)

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	48	VAL	5.1
1	C	48	VAL	4.9
1	D	47	TYR	4.9
1	C	134	THR	4.3
1	D	242	PHE	4.2
1	B	185	ALA	4.1
1	D	49	VAL	4.0
1	B	49	VAL	4.0
1	C	49	VAL	3.9
1	B	76	PHE	3.8
1	B	191	PHE	3.7
1	B	139	PHE	3.4
1	B	223	TYR	3.4
1	C	139	PHE	3.4
1	D	76	PHE	3.3
1	D	191	PHE	3.3
1	D	257	ILE	3.3
1	D	136	PRO	3.2
1	B	188	ALA	3.1
1	D	211	MET	3.1
1	B	92	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	154	ALA	3.0
1	C	223	TYR	3.0
1	C	133	ARG	2.9
1	C	191	PHE	2.9
1	D	188	ALA	2.9
1	D	-2	HIS	2.8
1	D	219	LEU	2.8
1	D	165	ALA	2.8
1	C	309	ASP	2.8
1	A	245	ALA	2.7
1	D	245	ALA	2.7
1	D	217	PHE	2.7
1	B	244	LYS	2.7
1	A	332	ALA	2.7
1	B	132	PRO	2.7
1	C	132	PRO	2.7
1	C	211	MET	2.6
1	D	260	LYS	2.6
1	B	47	TYR	2.6
1	C	76	PHE	2.5
1	D	134	THR	2.5
1	B	192	ARG	2.5
1	A	243	GLU	2.5
1	D	213	THR	2.5
1	C	71	LEU	2.5
1	D	250	LEU	2.5
1	D	239	ILE	2.5
1	A	4	VAL	2.5
1	B	190	ASN	2.4
1	D	258	ILE	2.4
1	C	174	VAL	2.4
1	C	145	LYS	2.4
1	A	223	TYR	2.4
1	D	246	THR	2.4
1	C	-4	HIS	2.4
1	A	246	THR	2.3
1	D	243	GLU	2.3
1	B	281	ILE	2.3
1	B	290	VAL	2.3
1	A	24	TYR	2.3
1	A	130	TYR	2.3
1	D	210	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	307	LEU	2.3
1	B	1	MET	2.3
1	C	45	ASP	2.3
1	B	243	GLU	2.2
1	C	114	ALA	2.2
1	D	130	TYR	2.2
1	D	241	THR	2.2
1	B	279	LEU	2.2
1	A	76	PHE	2.2
1	D	290	VAL	2.2
1	A	47	TYR	2.2
1	C	257	ILE	2.2
1	B	48	VAL	2.2
1	A	45	ASP	2.2
1	B	-2	HIS	2.1
1	B	184	GLY	2.1
1	A	279	LEU	2.1
1	C	149	TYR	2.1
1	D	223	TYR	2.1
1	C	44	ASP	2.1
1	D	143	GLY	2.1
1	A	137	TYR	2.1
1	A	247	ARG	2.1
1	A	108	GLU	2.1
1	B	187	ASN	2.1
1	A	102	CYS	2.1
1	A	116	PHE	2.0
1	B	261	GLU	2.0
1	B	272	HIS	2.0
1	C	212	ASN	2.0
1	C	306	ALA	2.0
1	C	195	SER	2.0
1	C	242	PHE	2.0
1	D	140	GLN	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 [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.