



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 14, 2023 – 02:01 PM EDT

PDB ID : 1VR6
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 : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.35.1
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) : 2.35.1

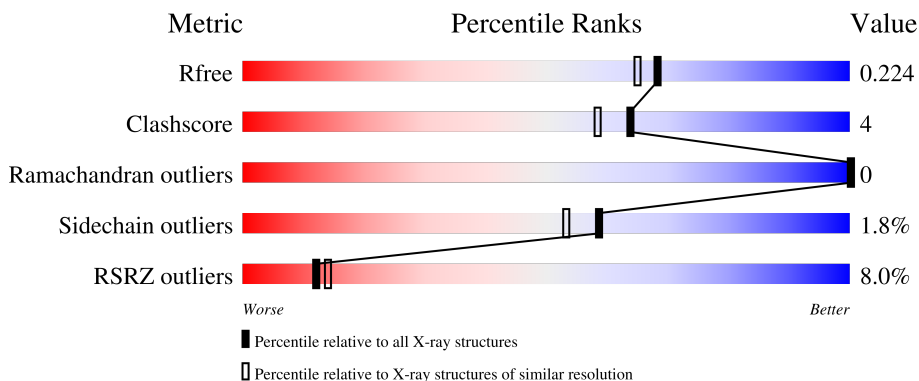
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

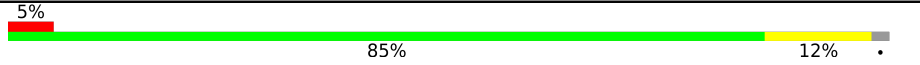



The reported resolution of this entry is 1.92 Å.

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}	130704	7937 (1.94-1.90)
Clashscore	141614	8644 (1.94-1.90)
Ramachandran outliers	138981	8530 (1.94-1.90)
Sidechain outliers	138945	8530 (1.94-1.90)
RSRZ outliers	127900	7793 (1.94-1.90)

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	350	
1	B	350	
1	C	350	
1	D	350	

2 Entry composition [i](#)

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

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

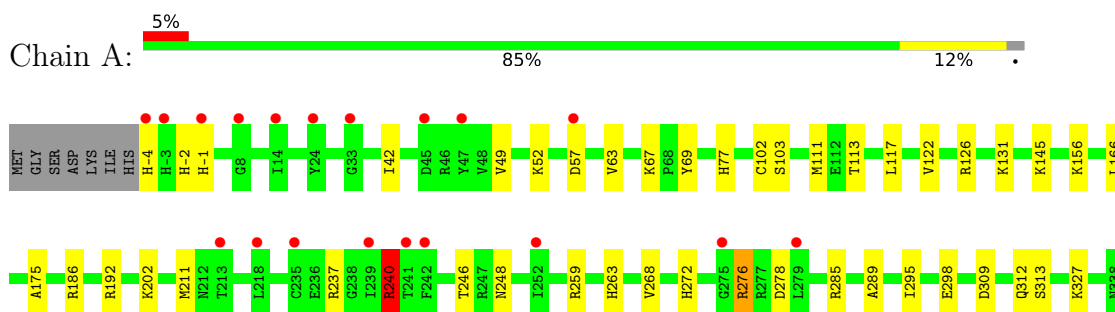
- Molecule 2 is water.

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

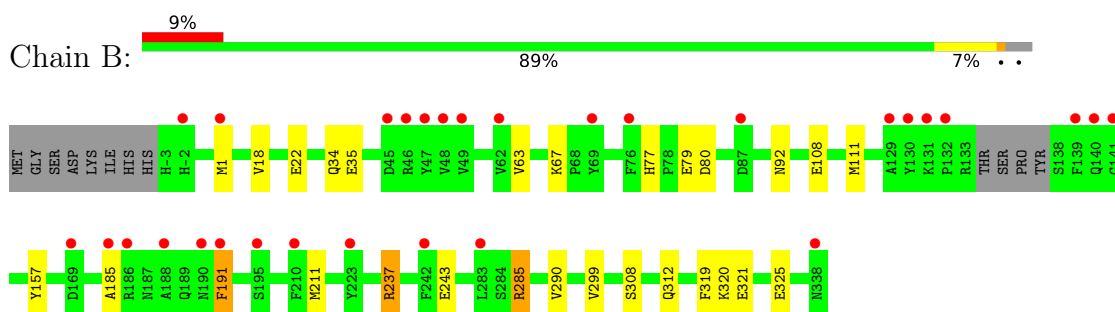
3 Residue-property plots [i](#)

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.

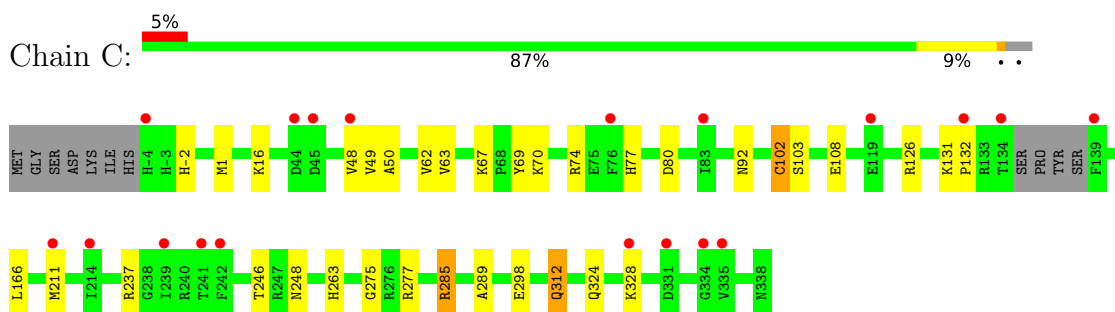
- Molecule 1: Phospho-2-dehydro-3-deoxyheptonate aldolase



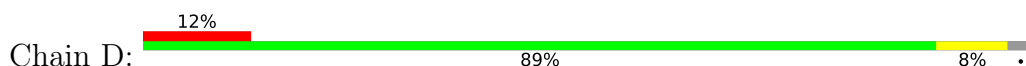
- Molecule 1: Phospho-2-dehydro-3-deoxyheptonate aldolase

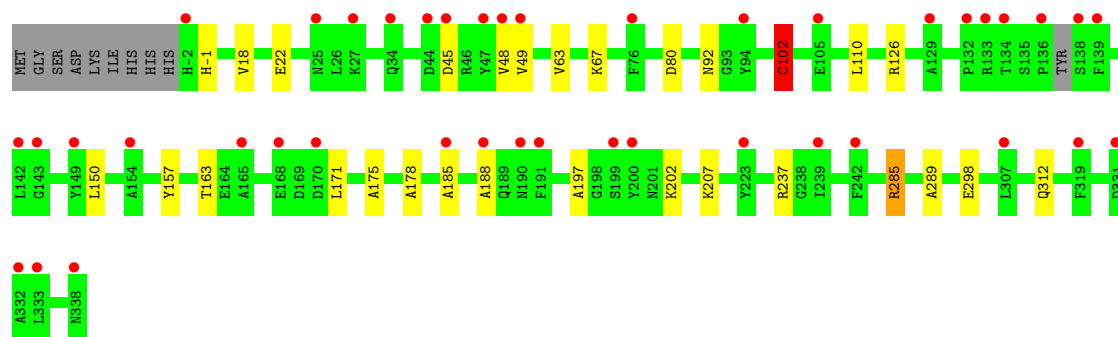


- Molecule 1: Phospho-2-dehydro-3-deoxyheptonate aldolase



- 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 49.91 – 1.92	Depositor EDS
% Data completeness (in resolution range)	98.5 (47.76-1.92) 98.5 (49.91-1.92)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.99 (at 1.92Å)	Xtrriage
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 (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	36.2	Xtrriage
Anisotropy	0.088	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 58.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.016 for k,h,-l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11010	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtrriage'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 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	0.86	1/2704 (0.0%)	0.90	6/3649 (0.2%)
1	B	0.77	1/2666 (0.0%)	0.84	2/3598 (0.1%)
1	C	0.76	1/2649 (0.0%)	0.76	2/3578 (0.1%)
1	D	0.67	2/2578 (0.1%)	0.72	2/3494 (0.1%)
All	All	0.77	5/10597 (0.0%)	0.81	12/14319 (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 (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	157	TYR	C-O	6.71	1.36	1.23
1	D	102	CYS	CB-SG	-5.94	1.72	1.81
1	C	102	CYS	CB-SG	-5.78	1.72	1.81
1	B	243	GLU	CB-CG	5.47	1.62	1.52
1	A	240	ARG	CD-NE	-5.30	1.37	1.46

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	285	ARG	NE-CZ-NH2	-15.51	112.54	120.30
1	B	285	ARG	NE-CZ-NH1	14.67	127.63	120.30
1	A	240	ARG	NE-CZ-NH2	-13.40	113.60	120.30
1	A	240	ARG	NE-CZ-NH1	10.33	125.46	120.30
1	A	285	ARG	NE-CZ-NH2	-9.70	115.45	120.30
1	D	285	ARG	NE-CZ-NH1	8.05	124.32	120.30
1	D	285	ARG	NE-CZ-NH2	-7.13	116.73	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	285	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	C	285	ARG	NE-CZ-NH2	-5.41	117.60	120.30
1	C	74	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	A	259	ARG	NE-CZ-NH2	-5.25	117.68	120.30
1	A	259	ARG	NE-CZ-NH1	5.19	122.89	120.30

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	37	0
1	B	2611	0	2625	19	0
1	C	2600	0	2603	26	0
1	D	2531	0	2479	16	0
2	A	197	0	0	6	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	88	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 (88) 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:C:102:CYS:SG	1:C:298:GLU:OE2	2.32	0.86
1:A:298[B]:GLU:CD	1:A:313:SER:OG	2.17	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:CYS:SG	1:A:298[A]:GLU:OE1	2.43	0.77
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
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: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:79:GLU:H	1:B:79:GLU:CD	2.06	0.58
1:B:34:GLN:HG2	1:C:-2:HIS:CE1	2.39	0.58
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: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:A:327:LYS:NZ	2:A:508:HOH:O	2.38	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:-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	0.50
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:ASP:OD2	1:B:92:ASN:CB	2.61	0.48
1:A:240:ARG:HB3	1:C:211:MET:HE2	1.96	0.47
1:A:111:MET:HE1	1:A:156:LYS:HD3	1.97	0.47
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:B:191:PHE:CD1	1:B:191:PHE:C	2.90	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: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:C:1:MET:HB3	1:C:1:MET:HE3	1.85	0.42
1:D:18:VAL:O	1:D:22:GLU:HG3	2.19	0.42
1:A:67:LYS:NZ	2:A:372:HOH:O	2.27	0.42
1:A:67:LYS:HE2	1:A:69:TYR:CE1	2.55	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:77:HIS:HB3	1:A:263:HIS:CD2	2.55	0.42
1:A:240:ARG:HB3	1:C:211:MET:CE	2.50	0.41
1:B:1:MET:HB3	1:B:1:MET:HE2	1.87	0.41
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:48:VAL:HG22	1:C:49:VAL:N	2.36	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%)	278 (98%)	6 (2%)	53	46
1	B	279/297 (94%)	271 (97%)	8 (3%)	42	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	276/297 (93%)	274 (99%)	2 (1%)	84	83
1	D	257/297 (86%)	253 (98%)	4 (2%)	62	58
All	All	1096/1188 (92%)	1076 (98%)	20 (2%)	59	53

All (20) 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	276	ARG
1	A	312	GLN
1	B	67	LYS
1	B	108	GLU
1	B	191	PHE
1	B	211	MET
1	B	237	ARG
1	B	290	VAL
1	B	308	SER
1	B	312	GLN
1	C	237	ARG
1	C	312	GLN
1	D	67	LYS
1	D	102	CYS
1	D	237	ARG
1	D	312	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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](#)

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%)	0.66	19 (5%) 25 28	33, 44, 55, 76	0
1	B	338/350 (96%)	0.68	30 (8%) 9 11	31, 45, 61, 77	0
1	C	339/350 (96%)	0.62	19 (5%) 24 27	35, 45, 55, 71	0
1	D	340/350 (97%)	0.89	41 (12%) 4 5	34, 45, 61, 82	0
All	All	1360/1400 (97%)	0.72	109 (8%) 12 14	31, 45, 58, 82	0

All (109) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	47	TYR	8.4
1	B	139	PHE	6.8
1	D	191	PHE	5.4
1	A	33	GLY	4.9
1	D	132	PRO	4.9
1	D	139	PHE	4.9
1	D	-2	HIS	4.6
1	D	25	ASN	4.5
1	D	48	VAL	4.4
1	C	134	THR	4.4
1	B	47	TYR	4.3
1	A	239	ILE	4.0
1	B	223	TYR	3.9
1	D	242	PHE	3.9
1	C	239	ILE	3.8
1	D	154	ALA	3.8
1	D	190	ASN	3.7
1	C	-4	HIS	3.7
1	B	-2	HIS	3.6
1	D	143	GLY	3.6
1	C	48	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	14	ILE	3.4
1	B	185	ALA	3.3
1	C	242	PHE	3.3
1	D	134	THR	3.3
1	D	76	PHE	3.3
1	D	27	LYS	3.2
1	C	139	PHE	3.2
1	D	307	LEU	3.2
1	B	132	PRO	3.2
1	B	49	VAL	3.1
1	A	-3	HIS	3.0
1	D	136	PRO	3.0
1	A	57	ASP	3.0
1	C	44	ASP	2.9
1	D	199	SER	2.9
1	B	45	ASP	2.9
1	A	242	PHE	2.9
1	D	45	ASP	2.8
1	A	-4	HIS	2.8
1	D	138	SER	2.8
1	C	331	ASP	2.8
1	D	49	VAL	2.7
1	B	195	SER	2.7
1	B	338	ASN	2.7
1	A	24	TYR	2.7
1	A	47	TYR	2.7
1	A	235	CYS	2.7
1	D	185	ALA	2.6
1	B	87	ASP	2.6
1	B	242	PHE	2.6
1	B	141	GLY	2.6
1	C	334	GLY	2.6
1	A	-1	HIS	2.6
1	B	140	GLN	2.6
1	C	335	VAL	2.6
1	D	149	TYR	2.5
1	A	8	GLY	2.5
1	B	169	ASP	2.5
1	B	76	PHE	2.5
1	B	191	PHE	2.5
1	C	211	MET	2.5
1	B	188	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	142	LEU	2.5
1	B	1	MET	2.4
1	B	131	LYS	2.4
1	B	283	LEU	2.4
1	B	62	VAL	2.4
1	C	132	PRO	2.4
1	D	34	GLN	2.4
1	D	105	GLU	2.4
1	A	252	ILE	2.4
1	C	45	ASP	2.4
1	D	223	TYR	2.3
1	D	44	ASP	2.3
1	D	319	PHE	2.3
1	D	94	TYR	2.3
1	B	210	PHE	2.3
1	C	214	ILE	2.3
1	D	239	ILE	2.3
1	D	188	ALA	2.3
1	C	76	PHE	2.3
1	C	83	ILE	2.3
1	D	133	ARG	2.3
1	D	331	ASP	2.3
1	B	48	VAL	2.2
1	C	328	LYS	2.2
1	D	332	ALA	2.2
1	D	338	ASN	2.2
1	B	46	ARG	2.2
1	C	241	THR	2.2
1	D	129	ALA	2.2
1	D	165	ALA	2.2
1	D	168	GLU	2.2
1	A	213	THR	2.2
1	D	333	LEU	2.1
1	D	170	ASP	2.1
1	C	119	GLU	2.1
1	A	275	GLY	2.1
1	A	279	LEU	2.1
1	B	129	ALA	2.1
1	B	190	ASN	2.1
1	D	200	TYR	2.1
1	B	130	TYR	2.1
1	A	45	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	218	LEU	2.0
1	B	69	TYR	2.0
1	B	186	ARG	2.0
1	A	241	THR	2.0

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.