



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 10:11 AM UTC

PDB ID : 4O9A / pdb_00004o9a
Title : Crystal structure of Beta-ketothiolase (PhaA) from Ralstonia eutropha H16
Authors : Kim, E.J.; Kim, J.; Kim, S.; Kim, K.J.
Deposited on : 2014-01-02
Resolution : 1.52 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

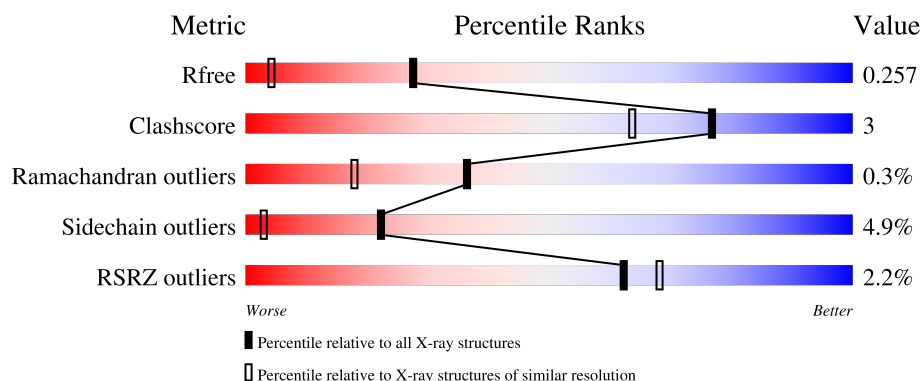
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.52 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	5890 (1.54-1.50)
Clashscore	190562	6116 (1.54-1.50)
Ramachandran outliers	187476	6002 (1.54-1.50)
Sidechain outliers	187428	5999 (1.54-1.50)
RSRZ outliers	180081	5891 (1.54-1.50)

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	398	
1	B	398	
1	C	398	
1	D	398	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11616 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 Acetyl-CoA acetyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	392	Total	C	N	O	S	0	0	0
			2827	1769	501	538	19			
1	B	392	Total	C	N	O	S	0	0	0
			2827	1769	501	538	19			
1	C	392	Total	C	N	O	S	0	0	0
			2827	1769	501	538	19			
1	D	392	Total	C	N	O	S	0	0	0
			2827	1769	501	538	19			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	HIS	-	expression tag	UNP P14611
A	-3	HIS	-	expression tag	UNP P14611
A	-2	HIS	-	expression tag	UNP P14611
A	-1	HIS	-	expression tag	UNP P14611
A	0	HIS	-	expression tag	UNP P14611
A	1	HIS	-	expression tag	UNP P14611
A	88	SER	CYS	engineered mutation	UNP P14611
B	-4	HIS	-	expression tag	UNP P14611
B	-3	HIS	-	expression tag	UNP P14611
B	-2	HIS	-	expression tag	UNP P14611
B	-1	HIS	-	expression tag	UNP P14611
B	0	HIS	-	expression tag	UNP P14611
B	1	HIS	-	expression tag	UNP P14611
B	88	SER	CYS	engineered mutation	UNP P14611
C	-4	HIS	-	expression tag	UNP P14611
C	-3	HIS	-	expression tag	UNP P14611
C	-2	HIS	-	expression tag	UNP P14611
C	-1	HIS	-	expression tag	UNP P14611
C	0	HIS	-	expression tag	UNP P14611
C	1	HIS	-	expression tag	UNP P14611
C	88	SER	CYS	engineered mutation	UNP P14611

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-4	HIS	-	expression tag	UNP P14611
D	-3	HIS	-	expression tag	UNP P14611
D	-2	HIS	-	expression tag	UNP P14611
D	-1	HIS	-	expression tag	UNP P14611
D	0	HIS	-	expression tag	UNP P14611
D	1	HIS	-	expression tag	UNP P14611
D	88	SER	CYS	engineered mutation	UNP P14611

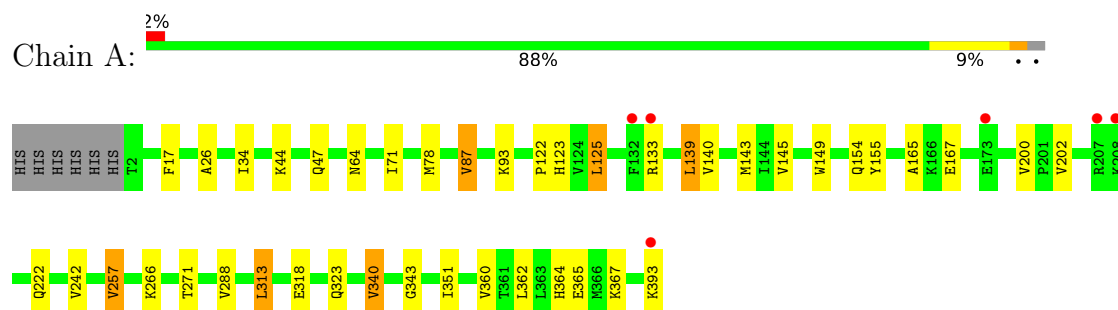
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	79	Total O 79 79	0	0
2	B	102	Total O 102 102	0	0
2	C	62	Total O 62 62	0	0
2	D	65	Total O 65 65	0	0

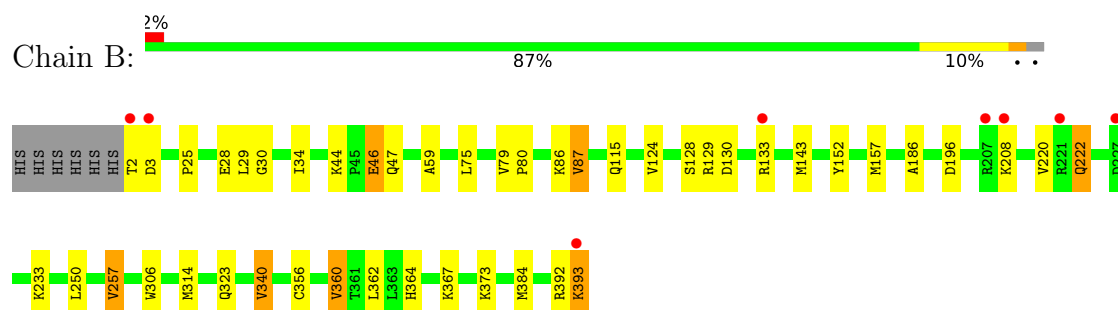
3 Residue-property plots [i](#)

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.

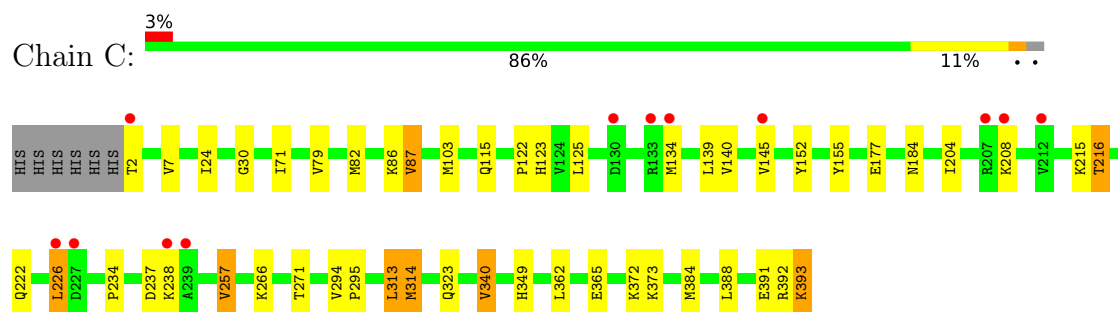
- Molecule 1: Acetyl-CoA acetyltransferase



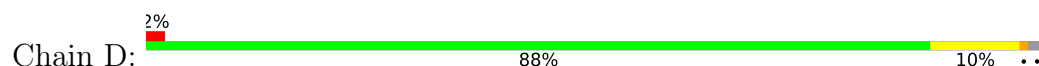
- Molecule 1: Acetyl-CoA acetyltransferase

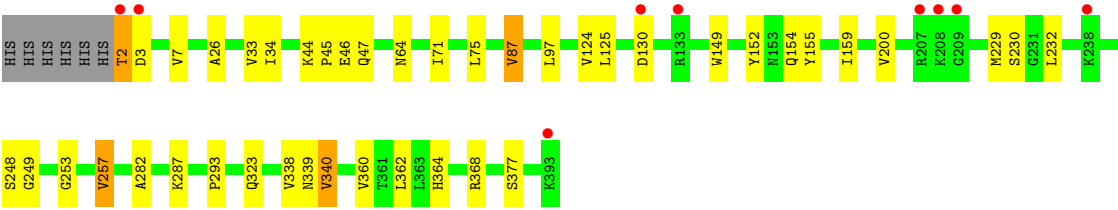


- Molecule 1: Acetyl-CoA acetyltransferase



- Molecule 1: Acetyl-CoA acetyltransferase





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 104.70Å 106.91Å 90.00° 106.12° 90.00°	Depositor
Resolution (Å)	27.86 – 1.52 27.86 – 1.52	Depositor EDS
% Data completeness (in resolution range)	91.2 (27.86-1.52) 91.1 (27.86-1.52)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 1.52Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.218 , 0.254 0.222 , 0.257	Depositor DCC
R_{free} test set	10349 reflections (4.69%)	wwPDB-VP
Wilson B-factor (Å ²)	13.0	Xtriage
Anisotropy	1.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 26.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.031 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11616	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.40% 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	1.36	6/2867 (0.2%)	1.27	13/3876 (0.3%)
1	B	1.35	13/2867 (0.5%)	1.26	10/3876 (0.3%)
1	C	1.29	5/2867 (0.2%)	1.22	9/3876 (0.2%)
1	D	1.27	2/2867 (0.1%)	1.23	16/3876 (0.4%)
All	All	1.32	26/11468 (0.2%)	1.25	48/15504 (0.3%)

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	79	VAL	N-CA	7.00	1.51	1.46
1	C	215	LYS	C-O	-6.94	1.18	1.23
1	C	79	VAL	N-CA	6.56	1.51	1.46
1	A	93	LYS	N-CA	-6.52	1.38	1.46
1	B	59	ALA	C-O	-6.33	1.16	1.24
1	B	29	LEU	N-CA	-6.31	1.38	1.46
1	C	184	ASN	N-CA	5.62	1.53	1.46
1	B	356	CYS	N-CA	-5.62	1.39	1.46
1	A	167	GLU	C-O	-5.52	1.17	1.24
1	B	128	SER	C-O	5.39	1.30	1.24
1	B	196	ASP	N-CA	5.38	1.52	1.46
1	C	216	THR	CA-C	-5.34	1.46	1.52
1	A	34	ILE	CA-CB	-5.24	1.48	1.54
1	B	80	PRO	N-CA	-5.23	1.41	1.46
1	B	3	ASP	CA-C	5.19	1.58	1.52
1	A	288	VAL	C-O	-5.18	1.18	1.24
1	B	220	VAL	N-CA	5.18	1.52	1.46
1	D	159	ILE	N-CA	5.14	1.53	1.46
1	B	367	LYS	N-CA	-5.13	1.40	1.46
1	D	26	ALA	N-CA	5.12	1.51	1.46
1	B	340	VAL	CA-C	5.09	1.60	1.52
1	B	360	VAL	C-O	-5.09	1.18	1.24
1	A	242	VAL	N-CA	5.08	1.52	1.46
1	C	373	LYS	N-CA	-5.07	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	202	VAL	C-O	-5.02	1.18	1.24
1	B	186	ALA	N-CA	5.02	1.52	1.46

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	3	ASP	N-CA-CB	-8.80	96.10	110.71
1	D	34	ILE	N-CA-C	-7.88	103.13	110.53
1	A	351	ILE	N-CA-C	7.56	118.30	110.36
1	B	34	ILE	N-CA-C	-7.42	103.55	110.53
1	B	3	ASP	N-CA-CB	-7.41	98.09	110.32
1	B	257	VAL	N-CA-CB	-7.32	100.15	112.44
1	D	257	VAL	N-CA-CB	-6.76	99.42	111.93
1	A	143	MET	N-CA-C	-6.60	104.17	111.36
1	C	340	VAL	CG1-CB-CG2	6.59	125.29	110.80
1	C	271	THR	CA-C-N	-6.50	113.59	120.03
1	C	271	THR	C-N-CA	-6.50	113.59	120.03
1	A	257	VAL	CG1-CB-CG2	6.46	125.02	110.80
1	D	26	ALA	CA-C-N	-6.45	112.98	119.56
1	D	26	ALA	C-N-CA	-6.45	112.98	119.56
1	B	86	LYS	N-CA-C	-6.38	102.71	110.88
1	B	257	VAL	CG1-CB-CG2	6.27	124.59	110.80
1	B	340	VAL	CA-CB-CG2	6.11	120.79	110.40
1	A	26	ALA	CA-C-N	-6.08	113.42	119.56
1	A	26	ALA	C-N-CA	-6.08	113.42	119.56
1	A	125	LEU	CA-C-N	-5.98	113.62	119.78
1	A	125	LEU	C-N-CA	-5.98	113.62	119.78
1	A	271	THR	CA-C-N	-5.96	113.83	119.85
1	A	271	THR	C-N-CA	-5.96	113.83	119.85
1	D	282	ALA	CA-C-N	5.93	125.68	121.65
1	D	282	ALA	C-N-CA	5.93	125.68	121.65
1	A	257	VAL	N-CA-CB	-5.77	101.26	111.93
1	C	134	MET	N-CA-C	5.74	117.83	108.76
1	C	86	LYS	N-CA-C	-5.67	103.62	110.88
1	D	33	VAL	N-CA-C	5.66	118.16	111.09
1	B	233	LYS	CA-C-N	-5.63	113.96	119.76
1	B	233	LYS	C-N-CA	-5.63	113.96	119.76
1	A	340	VAL	N-CA-CB	-5.62	101.03	110.65
1	D	368	ARG	NE-CZ-NH2	5.60	124.24	119.20
1	D	230	SER	CB-CA-C	-5.54	99.71	110.46
1	D	253	GLY	N-CA-C	5.43	118.40	110.63
1	D	257	VAL	CG1-CB-CG2	5.38	122.64	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	349	HIS	N-CA-CB	-5.38	104.42	111.09
1	A	165	ALA	N-CA-C	-5.36	105.52	111.36
1	D	340	VAL	CG1-CB-CG2	5.32	122.50	110.80
1	C	257	VAL	CG1-CB-CG2	5.30	122.46	110.80
1	B	257	VAL	CA-CB-CG1	5.28	119.37	110.40
1	C	257	VAL	N-CA-CB	-5.28	102.17	111.93
1	B	340	VAL	CG1-CB-CG2	5.26	122.38	110.80
1	D	287	LYS	N-CA-C	5.26	117.76	111.71
1	C	340	VAL	N-CA-CB	-5.20	100.13	111.05
1	D	229	MET	CA-C-N	5.20	127.97	120.38
1	D	229	MET	C-N-CA	5.20	127.97	120.38
1	A	34	ILE	N-CA-C	-5.03	105.80	110.53

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2827	0	2895	15	0
1	B	2827	0	2895	22	0
1	C	2827	0	2895	23	0
1	D	2827	0	2895	18	0
2	A	79	0	0	0	0
2	B	102	0	0	2	0
2	C	62	0	0	0	0
2	D	65	0	0	3	0
All	All	11616	0	11580	67	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 3.

All (67) 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:44:LYS:H	1:D:47:GLN:HE21	1.35	0.72
1:D:364:HIS:HE1	2:D:445:HOH:O	1.75	0.69
1:B:364:HIS:HE1	2:B:453:HOH:O	1.79	0.65
1:B:222:GLN:HE21	1:B:222:GLN:H	1.47	0.61
1:B:392:ARG:O	1:B:393:LYS:CD	2.48	0.60
1:A:140:VAL:CG1	1:A:145:VAL:HG21	2.31	0.60
1:B:157:MET:HE2	1:B:157:MET:HA	1.83	0.59
1:A:313:LEU:HD21	1:A:365:GLU:HG3	1.85	0.58
1:A:64:ASN:ND2	1:B:384:MET:HE1	2.19	0.57
1:C:313:LEU:HD21	1:C:365:GLU:HG3	1.86	0.57
1:A:44:LYS:H	1:A:47:GLN:NE2	2.03	0.57
1:C:392:ARG:O	1:C:393:LYS:HD3	2.06	0.56
1:B:392:ARG:O	1:B:393:LYS:HD2	2.07	0.55
1:C:140:VAL:CG1	1:C:145:VAL:HG21	2.37	0.54
1:D:2:THR:N	2:D:441:HOH:O	2.42	0.53
1:A:149:TRP:HE1	1:A:154:GLN:NE2	2.06	0.53
1:C:392:ARG:O	1:C:393:LYS:CD	2.57	0.53
1:A:123:HIS:HB3	1:A:139:LEU:HD23	1.92	0.52
1:D:45:PRO:HB3	1:D:75:LEU:HD23	1.92	0.51
1:D:44:LYS:H	1:D:47:GLN:NE2	2.07	0.51
1:A:64:ASN:HD22	1:B:384:MET:HE1	1.76	0.51
1:C:7:VAL:O	1:C:7:VAL:HG12	2.11	0.50
1:C:140:VAL:HG11	1:C:145:VAL:HG21	1.93	0.50
1:C:24:ILE:HD11	1:C:204:ILE:HD12	1.94	0.49
1:C:24:ILE:HD11	1:C:204:ILE:CD1	2.42	0.49
1:C:384:MET:HE1	1:D:64:ASN:ND2	2.28	0.49
1:B:392:ARG:O	1:B:393:LYS:HD3	2.13	0.48
1:D:293:PRO:HB3	1:D:377:SER:OG	2.13	0.48
1:D:7:VAL:HG12	1:D:7:VAL:O	2.14	0.48
1:D:360:VAL:O	1:D:364:HIS:HD2	1.97	0.47
1:B:364:HIS:CE1	2:B:453:HOH:O	2.62	0.46
1:C:123:HIS:HB3	1:C:139:LEU:HD22	1.98	0.46
1:B:46:GLU:H	1:B:46:GLU:HG3	1.27	0.45
1:B:306:TRP:CE2	1:B:373:LYS:HD3	2.51	0.45
1:D:364:HIS:CE1	2:D:445:HOH:O	2.60	0.45
1:B:143:MET:HE1	1:B:250:LEU:HD13	1.99	0.45
1:C:152:TYR:CZ	1:D:71:ILE:HD12	2.52	0.45
1:A:318:GLU:CD	1:A:343:GLY:HA3	2.42	0.44
1:C:30:GLY:HA3	1:C:115:GLN:NE2	2.32	0.44
1:C:388:LEU:C	1:C:388:LEU:HD23	2.42	0.44
1:A:140:VAL:HG13	1:A:145:VAL:HG21	2.00	0.44
1:C:177:GLU:HG2	1:C:226:LEU:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:LYS:HB2	1:B:47:GLN:HG2	2.00	0.43
1:C:384:MET:HE1	1:D:64:ASN:HD22	1.83	0.43
1:D:149:TRP:HE1	1:D:154:GLN:NE2	2.16	0.43
1:B:30:GLY:HA3	1:B:115:GLN:NE2	2.34	0.43
1:A:122:PRO:CG	1:B:124:VAL:HG21	2.49	0.42
1:B:25:PRO:HD2	1:B:28:GLU:CD	2.44	0.42
1:C:2:THR:CG2	1:C:103:MET:HA	2.49	0.42
1:C:82:MET:HE1	1:D:97:LEU:HD21	2.01	0.42
1:A:17:PHE:CZ	1:B:129:ARG:HD3	2.54	0.42
1:C:234:PRO:HB2	1:C:237:ASP:O	2.20	0.42
1:D:248:SER:OG	1:D:249:GLY:N	2.49	0.42
1:A:44:LYS:H	1:A:47:GLN:HE21	1.67	0.42
1:A:140:VAL:HG11	1:A:145:VAL:HG21	2.01	0.41
1:C:314:MET:SD	1:C:314:MET:N	2.93	0.41
1:B:75:LEU:HD12	1:B:75:LEU:N	2.34	0.41
1:C:372:LYS:O	1:C:391:GLU:HA	2.20	0.41
1:B:222:GLN:HE21	1:B:222:GLN:N	2.17	0.41
1:C:294:VAL:HB	1:C:295:PRO:CD	2.51	0.41
1:D:338:VAL:O	1:D:339:ASN:C	2.64	0.41
1:C:122:PRO:HB2	1:D:124:VAL:HG22	2.03	0.41
1:C:71:ILE:HD12	1:D:152:TYR:CZ	2.56	0.40
1:A:71:ILE:HD12	1:B:152:TYR:CZ	2.56	0.40
1:A:360:VAL:O	1:A:364:HIS:HD2	2.04	0.40
1:B:314:MET:N	1:B:314:MET:SD	2.95	0.40
1:B:360:VAL:O	1:B:364:HIS:HD2	2.05	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	390/398 (98%)	379 (97%)	10 (3%)	1 (0%)	36 18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	390/398 (98%)	380 (97%)	9 (2%)	1 (0%)	36	18
1	C	390/398 (98%)	379 (97%)	10 (3%)	1 (0%)	36	18
1	D	390/398 (98%)	375 (96%)	14 (4%)	1 (0%)	36	18
All	All	1560/1592 (98%)	1513 (97%)	43 (3%)	4 (0%)	36	18

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	87	VAL
1	B	87	VAL
1	C	87	VAL
1	D	87	VAL

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	284/290 (98%)	268 (94%)	16 (6%)	19	2
1	B	284/290 (98%)	272 (96%)	12 (4%)	26	4
1	C	284/290 (98%)	268 (94%)	16 (6%)	19	2
1	D	284/290 (98%)	272 (96%)	12 (4%)	26	4
All	All	1136/1160 (98%)	1080 (95%)	56 (5%)	22	3

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	MET
1	A	87	VAL
1	A	125	LEU
1	A	133	ARG
1	A	139	LEU
1	A	155	TYR
1	A	200	VAL

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Mol	Chain	Res	Type
1	A	222	GLN
1	A	257	VAL
1	A	266	LYS
1	A	313	LEU
1	A	323	GLN
1	A	340	VAL
1	A	362	LEU
1	A	367	LYS
1	A	393	LYS
1	B	2	THR
1	B	46	GLU
1	B	87	VAL
1	B	130	ASP
1	B	133	ARG
1	B	208	LYS
1	B	222	GLN
1	B	257	VAL
1	B	323	GLN
1	B	340	VAL
1	B	362	LEU
1	B	393	LYS
1	C	87	VAL
1	C	125	LEU
1	C	155	TYR
1	C	208	LYS
1	C	216	THR
1	C	222	GLN
1	C	226	LEU
1	C	238	LYS
1	C	257	VAL
1	C	266	LYS
1	C	313	LEU
1	C	314	MET
1	C	323	GLN
1	C	340	VAL
1	C	362	LEU
1	C	393	LYS
1	D	2	THR
1	D	46	GLU
1	D	87	VAL
1	D	125	LEU
1	D	130	ASP

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Mol	Chain	Res	Type
1	D	155	TYR
1	D	200	VAL
1	D	232	LEU
1	D	257	VAL
1	D	323	GLN
1	D	340	VAL
1	D	362	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	GLN
1	A	115	GLN
1	A	154	GLN
1	A	329	GLN
1	A	330	GLN
1	A	364	HIS
1	B	115	GLN
1	B	154	GLN
1	B	184	ASN
1	B	222	GLN
1	B	329	GLN
1	B	330	GLN
1	B	341	ASN
1	B	364	HIS
1	C	115	GLN
1	C	154	GLN
1	C	341	ASN
1	C	364	HIS
1	D	47	GLN
1	D	154	GLN
1	D	364	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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	392/398 (98%)	0.10	6 (1%) 72 77	10, 16, 30, 59	0
1	B	392/398 (98%)	0.10	8 (2%) 65 71	9, 17, 32, 55	0
1	C	392/398 (98%)	0.27	12 (3%) 51 58	10, 18, 34, 58	0
1	D	392/398 (98%)	0.27	9 (2%) 61 67	11, 19, 33, 66	0
All	All	1568/1592 (98%)	0.18	35 (2%) 62 68	9, 17, 33, 66	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	2	THR	5.3
1	C	208	LYS	5.1
1	B	2	THR	4.7
1	D	393	LYS	3.3
1	C	130	ASP	3.2
1	A	393	LYS	3.2
1	B	207	ARG	3.2
1	A	208	LYS	3.2
1	C	207	ARG	2.9
1	C	227	ASP	2.9
1	B	208	LYS	2.8
1	A	133	ARG	2.8
1	C	239	ALA	2.7
1	C	2	THR	2.7
1	D	133	ARG	2.6
1	D	208	LYS	2.5
1	B	133	ARG	2.5
1	D	3	ASP	2.4
1	A	173	GLU	2.4
1	C	226	LEU	2.4
1	C	238	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	132	PHE	2.4
1	A	207	ARG	2.3
1	C	212	VAL	2.3
1	D	209	GLY	2.3
1	D	238	LYS	2.3
1	C	134	MET	2.2
1	B	393	LYS	2.2
1	D	130	ASP	2.2
1	B	3	ASP	2.1
1	B	221	ARG	2.1
1	C	133	ARG	2.1
1	D	207	ARG	2.1
1	C	145	VAL	2.0
1	B	227	ASP	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 ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.