



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:02 AM UTC

PDB ID : 2AHU / pdb_00002ahu
Title : Crystal structure of Acyl-CoA transferase (YdiF) apoenzyme from Escherichia coli O157:H7.
Authors : Rangarajan, E.S.; Li, Y.; Ajamian, E.; Iannuzzi, P.; Kernaghan, S.D.; Fraser, M.E.; Cygler, M.; Matte, A.; Montreal-Kingston Bacterial Structural Genomics Initiative (BSGI)
Deposited on : 2005-07-28
Resolution : 1.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
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

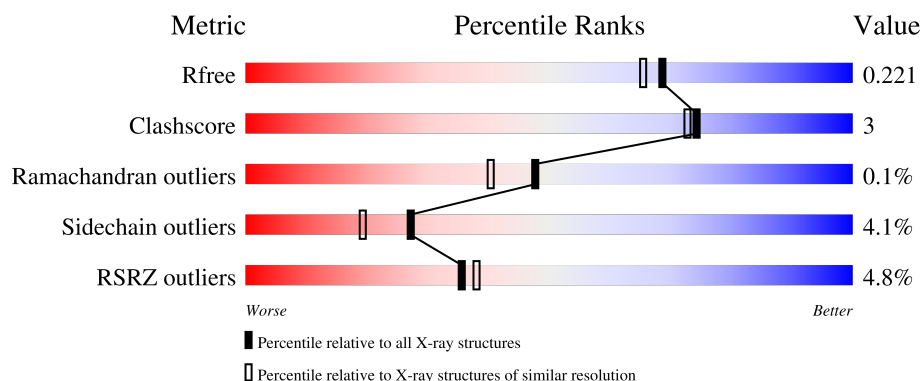
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	531	5% 88% 8% .
1	B	531	4% 87% 10% ..
1	C	531	5% 85% 11% ..
1	D	531	5% 86% 10% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 16967 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 putative enzyme ydiF.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	515	Total	C	N	O	S	Se	0	0	0
			3924	2497	669	742	6	10			
1	B	515	Total	C	N	O	S	Se	0	0	0
			3924	2497	669	742	6	10			
1	C	515	Total	C	N	O	S	Se	0	0	0
			3924	2497	669	742	6	10			
1	D	515	Total	C	N	O	S	Se	0	0	0
			3924	2497	669	742	6	10			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP Q8X5X6
A	204	MSE	MET	modified residue	UNP Q8X5X6
A	223	MSE	MET	modified residue	UNP Q8X5X6
A	224	MSE	MET	modified residue	UNP Q8X5X6
A	229	MSE	MET	modified residue	UNP Q8X5X6
A	299	MSE	MET	modified residue	UNP Q8X5X6
A	359	MSE	MET	modified residue	UNP Q8X5X6
A	397	MSE	MET	modified residue	UNP Q8X5X6
A	499	MSE	MET	modified residue	UNP Q8X5X6
A	512	MSE	MET	modified residue	UNP Q8X5X6
A	522	MSE	MET	modified residue	UNP Q8X5X6
B	1	MSE	MET	modified residue	UNP Q8X5X6
B	204	MSE	MET	modified residue	UNP Q8X5X6
B	223	MSE	MET	modified residue	UNP Q8X5X6
B	224	MSE	MET	modified residue	UNP Q8X5X6
B	229	MSE	MET	modified residue	UNP Q8X5X6
B	299	MSE	MET	modified residue	UNP Q8X5X6
B	359	MSE	MET	modified residue	UNP Q8X5X6
B	397	MSE	MET	modified residue	UNP Q8X5X6
B	499	MSE	MET	modified residue	UNP Q8X5X6
B	512	MSE	MET	modified residue	UNP Q8X5X6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	522	MSE	MET	modified residue	UNP Q8X5X6
C	1	MSE	MET	modified residue	UNP Q8X5X6
C	204	MSE	MET	modified residue	UNP Q8X5X6
C	223	MSE	MET	modified residue	UNP Q8X5X6
C	224	MSE	MET	modified residue	UNP Q8X5X6
C	229	MSE	MET	modified residue	UNP Q8X5X6
C	299	MSE	MET	modified residue	UNP Q8X5X6
C	359	MSE	MET	modified residue	UNP Q8X5X6
C	397	MSE	MET	modified residue	UNP Q8X5X6
C	499	MSE	MET	modified residue	UNP Q8X5X6
C	512	MSE	MET	modified residue	UNP Q8X5X6
C	522	MSE	MET	modified residue	UNP Q8X5X6
D	1	MSE	MET	modified residue	UNP Q8X5X6
D	204	MSE	MET	modified residue	UNP Q8X5X6
D	223	MSE	MET	modified residue	UNP Q8X5X6
D	224	MSE	MET	modified residue	UNP Q8X5X6
D	229	MSE	MET	modified residue	UNP Q8X5X6
D	299	MSE	MET	modified residue	UNP Q8X5X6
D	359	MSE	MET	modified residue	UNP Q8X5X6
D	397	MSE	MET	modified residue	UNP Q8X5X6
D	499	MSE	MET	modified residue	UNP Q8X5X6
D	512	MSE	MET	modified residue	UNP Q8X5X6
D	522	MSE	MET	modified residue	UNP Q8X5X6

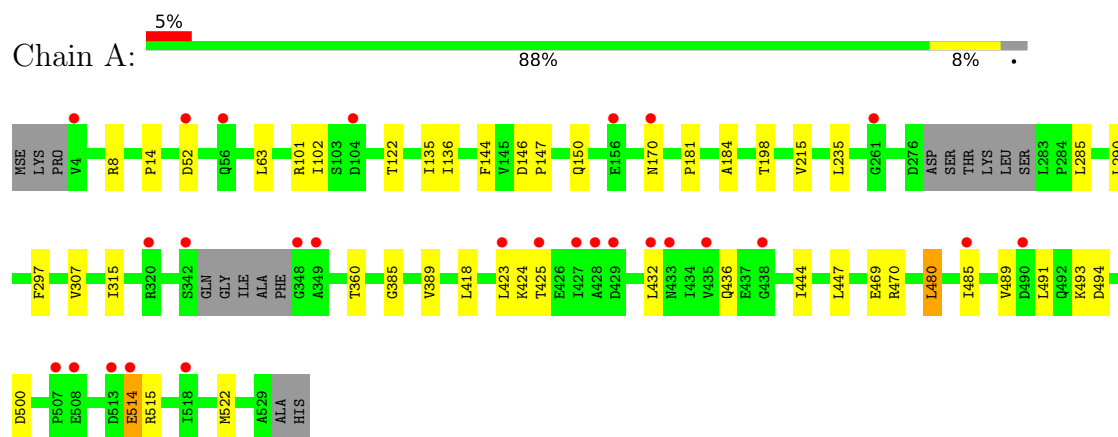
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	291	Total O 291 291	0	0
2	B	285	Total O 285 285	0	0
2	C	362	Total O 362 362	0	0
2	D	333	Total O 333 333	0	0

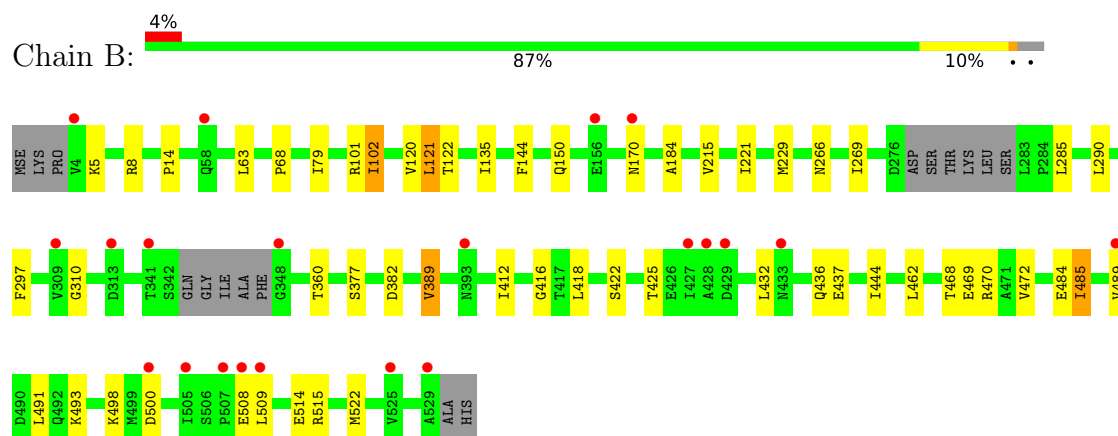
3 Residue-property plots [i](#)

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.

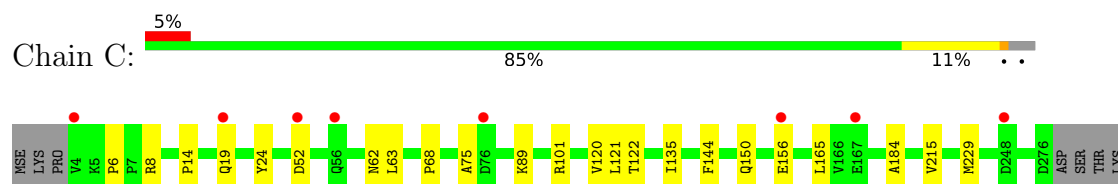
- Molecule 1: putative enzyme ydiF

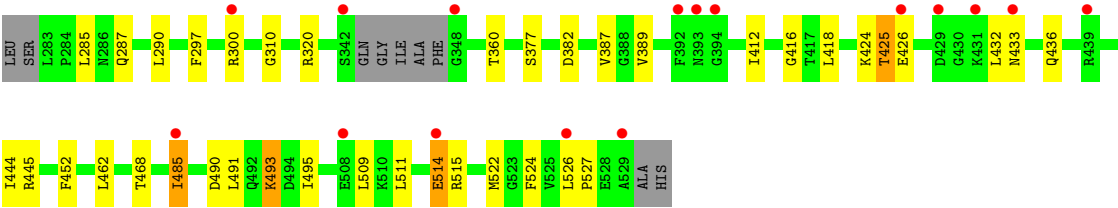


- Molecule 1: putative enzyme ydiF

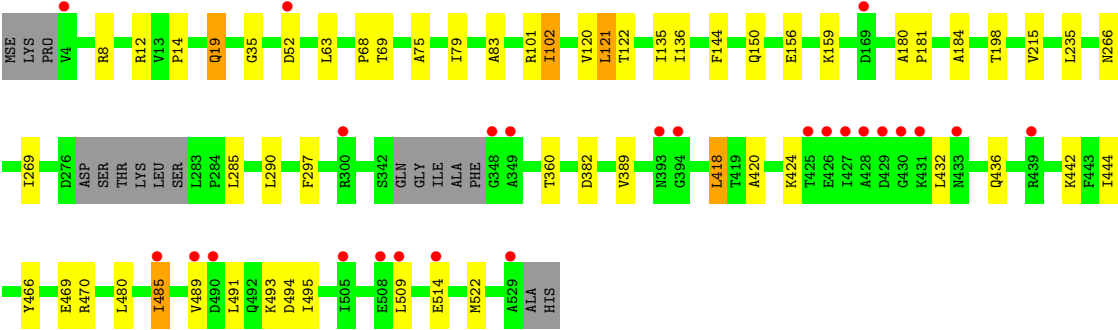
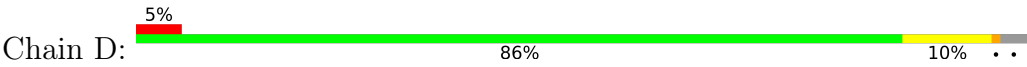


- Molecule 1: putative enzyme ydiF





● Molecule 1: putative enzyme ydiF



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.13Å 133.31Å 105.84Å 90.00° 100.57° 90.00°	Depositor
Resolution (Å)	50.00 – 1.90 50.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	94.3 (50.00-1.90) 94.3 (50.00-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.18 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.187 , 0.220 0.188 , 0.221	Depositor DCC
R_{free} test set	15015 reflections (8.65%)	wwPDB-VP
Wilson B-factor (Å ²)	24.6	Xtriage
Anisotropy	0.217	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 39.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16967	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% 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	0.54	0/3980	0.82	0/5372
1	B	0.53	1/3980 (0.0%)	0.82	0/5372
1	C	0.55	1/3980 (0.0%)	0.81	0/5372
1	D	0.55	0/3980	0.82	0/5372
All	All	0.54	2/15920 (0.0%)	0.82	0/21488

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	229	MSE	SE-CE	5.61	2.12	1.95
1	C	229	MSE	SE-CE	5.28	2.11	1.95

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	3924	0	3981	20	0
1	B	3924	0	3981	24	0
1	C	3924	0	3981	27	0
1	D	3924	0	3981	27	0
2	A	291	0	0	0	0
2	B	285	0	0	0	0
2	C	362	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	333	0	0	0	0
All	All	16967	0	15924	97	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 (97) 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:485:ILE:HD11	1:D:509:LEU:HD11	1.48	0.94
1:C:514:GLU:H	1:C:514:GLU:CD	1.95	0.74
1:A:297:PHE:CZ	1:A:522:MSE:HE1	2.23	0.74
1:C:297:PHE:CZ	1:C:522:MSE:HE1	2.26	0.71
1:C:8:ARG:HG2	1:C:14:PRO:HD3	1.76	0.68
1:D:297:PHE:CE1	1:D:522:MSE:HE1	2.29	0.68
1:C:184:ALA:HB2	1:C:215:VAL:HG21	1.76	0.66
1:B:297:PHE:HZ	1:B:522:MSE:HE1	1.59	0.66
1:C:120:VAL:HG13	1:C:135:ILE:HD11	1.79	0.65
1:A:514:GLU:H	1:A:514:GLU:CD	2.06	0.63
1:B:297:PHE:CZ	1:B:522:MSE:HE1	2.35	0.62
1:A:144:PHE:HB2	1:A:150:GLN:HE21	1.64	0.61
1:B:515:ARG:HB2	1:B:522:MSE:HE3	1.82	0.61
1:D:8:ARG:HG2	1:D:14:PRO:HD3	1.82	0.61
1:D:297:PHE:CZ	1:D:522:MSE:HE1	2.36	0.61
1:D:120:VAL:HG13	1:D:135:ILE:HD11	1.82	0.61
1:D:144:PHE:HB2	1:D:150:GLN:HE21	1.67	0.60
1:A:297:PHE:CE1	1:A:522:MSE:HE1	2.37	0.60
1:D:184:ALA:HB2	1:D:215:VAL:HG21	1.83	0.59
1:D:266:ASN:HB3	1:D:269:ILE:HD12	1.85	0.59
1:A:297:PHE:HZ	1:A:522:MSE:HE1	1.67	0.58
1:B:184:ALA:HB2	1:B:215:VAL:HG21	1.84	0.58
1:C:297:PHE:HZ	1:C:522:MSE:HE1	1.69	0.58
1:C:144:PHE:HB2	1:C:150:GLN:HE21	1.69	0.57
1:B:79:ILE:O	1:B:102:ILE:HD11	2.05	0.57
1:A:8:ARG:HG2	1:A:14:PRO:HD3	1.86	0.56
1:B:485:ILE:HG12	1:B:509:LEU:HD11	1.88	0.56
1:A:198:THR:HG23	1:A:235:LEU:HD13	1.88	0.56
1:C:122:THR:HG23	1:C:360:THR:HG23	1.87	0.56
1:A:184:ALA:HB2	1:A:215:VAL:HG21	1.87	0.56
1:B:5:LYS:HG2	1:B:221:ILE:HG12	1.88	0.55
1:B:144:PHE:HB2	1:B:150:GLN:HE21	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:62:ASN:HB3	1:C:89:LYS:HD2	1.89	0.55
1:C:297:PHE:CE1	1:C:522:MSE:HE1	2.41	0.55
1:B:122:THR:HG23	1:B:360:THR:HG23	1.89	0.54
1:B:472:VAL:HB	1:B:484:GLU:HB2	1.90	0.54
1:A:515:ARG:HB2	1:A:522:MSE:HE3	1.90	0.54
1:D:156:GLU:O	1:D:159:LYS:HE3	2.08	0.53
1:A:181:PRO:HB2	1:A:215:VAL:HG22	1.91	0.53
1:C:515:ARG:HB2	1:C:522:MSE:HE3	1.91	0.53
1:D:68:PRO:HA	1:D:121:LEU:HD13	1.90	0.52
1:C:424:LYS:HB2	1:C:436:GLN:HB3	1.91	0.52
1:B:444:ILE:HA	1:B:500:ASP:HB2	1.92	0.51
1:B:514:GLU:H	1:B:514:GLU:CD	2.18	0.51
1:A:489:VAL:HG13	1:A:494:ASP:HB2	1.92	0.51
1:C:310:GLY:HA3	1:C:377:SER:OG	2.11	0.51
1:C:300:ARG:HD3	1:C:527:PRO:HB2	1.93	0.51
1:D:418:LEU:HD22	1:D:470:ARG:HD2	1.92	0.50
1:A:424:LYS:HB2	1:A:436:GLN:HB3	1.94	0.50
1:D:79:ILE:HD12	1:D:102:ILE:HD13	1.92	0.50
1:D:19:GLN:NE2	1:D:19:GLN:H	2.09	0.49
1:B:120:VAL:HG13	1:B:135:ILE:HD11	1.94	0.49
1:C:416:GLY:O	1:C:468:THR:HA	2.13	0.48
1:D:489:VAL:HG13	1:D:494:ASP:HB2	1.95	0.48
1:B:8:ARG:HG2	1:B:14:PRO:HD3	1.95	0.47
1:C:412:ILE:HD11	1:C:462:LEU:HD13	1.95	0.47
1:D:297:PHE:HE1	1:D:522:MSE:HE1	1.77	0.47
1:D:35:GLY:O	1:D:69:THR:HB	2.14	0.47
1:D:382:ASP:HA	1:D:444:ILE:O	2.15	0.47
1:C:426:GLU:HG2	1:C:433:ASN:HB3	1.96	0.47
1:C:490:ASP:HB3	1:C:493:LYS:HG2	1.97	0.47
1:D:514:GLU:H	1:D:514:GLU:CD	2.23	0.46
1:B:382:ASP:HA	1:B:444:ILE:O	2.15	0.46
1:C:382:ASP:HA	1:C:444:ILE:O	2.16	0.46
1:D:122:THR:HG23	1:D:360:THR:HG23	1.97	0.46
1:A:444:ILE:HD11	1:A:447:LEU:HD23	1.97	0.46
1:A:418:LEU:HD22	1:A:470:ARG:HD2	1.97	0.45
1:B:310:GLY:HA3	1:B:377:SER:OG	2.17	0.45
1:A:136:ILE:HD11	1:D:136:ILE:HD11	1.97	0.45
1:C:68:PRO:HA	1:C:121:LEU:HD13	1.99	0.44
1:B:68:PRO:HA	1:B:121:LEU:HD13	2.00	0.44
1:C:6:PRO:HD3	1:C:24:TYR:CE1	2.53	0.44
1:D:424:LYS:HB2	1:D:436:GLN:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:VAL:HG21	1:A:315:ILE:CG2	2.47	0.44
1:A:122:THR:HG23	1:A:360:THR:HG23	2.00	0.43
1:C:387:VAL:HB	1:C:452:PHE:HB3	1.99	0.43
1:D:83:ALA:HB2	1:D:102:ILE:HG13	2.01	0.43
1:C:485:ILE:HG23	1:C:495:ILE:CD1	2.48	0.43
1:D:198:THR:HG23	1:D:235:LEU:HD13	2.00	0.43
1:C:19:GLN:NE2	1:C:19:GLN:H	2.15	0.43
1:B:416:GLY:O	1:B:468:THR:HA	2.19	0.43
1:A:385:GLY:HA2	1:A:480:LEU:HD21	2.00	0.43
1:B:412:ILE:HD11	1:B:462:LEU:HD13	2.01	0.43
1:B:266:ASN:HB3	1:B:269:ILE:HD12	2.02	0.42
1:B:437:GLU:HG2	1:B:498:LYS:HE2	2.00	0.42
1:D:466:TYR:CE1	1:D:480:LEU:HD21	2.54	0.42
1:D:485:ILE:HG23	1:D:495:ILE:CD1	2.48	0.42
1:C:287:GLN:HE21	1:C:425:THR:HB	1.85	0.41
1:C:524:PHE:CE1	1:C:526:LEU:HD23	2.55	0.41
1:D:420:ALA:HB2	1:D:442:LYS:HD2	2.01	0.41
1:B:418:LEU:HD22	1:B:470:ARG:HD2	2.02	0.41
1:B:515:ARG:CB	1:B:522:MSE:HE3	2.50	0.41
1:C:514:GLU:CD	1:C:514:GLU:N	2.73	0.41
1:D:180:ALA:HA	1:D:181:PRO:HD3	1.90	0.40
1:A:146:ASP:HA	1:A:147:PRO:HD3	1.99	0.40
1:A:444:ILE:HA	1:A:500:ASP:HB2	2.04	0.40
1:B:422:SER:HB3	1:B:436:GLN:OE1	2.21	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	509/531 (96%)	499 (98%)	10 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	509/531 (96%)	495 (97%)	13 (3%)	1 (0%)	43	36
1	C	509/531 (96%)	497 (98%)	11 (2%)	1 (0%)	43	36
1	D	509/531 (96%)	497 (98%)	11 (2%)	1 (0%)	43	36
All	All	2036/2124 (96%)	1988 (98%)	45 (2%)	3 (0%)	48	40

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	75	ALA
1	C	75	ALA
1	B	389	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	418/420 (100%)	400 (96%)	18 (4%)	26	18
1	B	418/420 (100%)	402 (96%)	16 (4%)	29	21
1	C	418/420 (100%)	399 (96%)	19 (4%)	24	17
1	D	418/420 (100%)	402 (96%)	16 (4%)	29	21
All	All	1672/1680 (100%)	1603 (96%)	69 (4%)	27	19

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	ASP
1	A	63	LEU
1	A	101	ARG
1	A	102	ILE
1	A	135	ILE
1	A	170	ASN
1	A	285	LEU
1	A	290	LEU

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Mol	Chain	Res	Type
1	A	389	VAL
1	A	423	LEU
1	A	425	THR
1	A	432	LEU
1	A	469	GLU
1	A	480	LEU
1	A	485	ILE
1	A	491	LEU
1	A	493	LYS
1	A	514	GLU
1	B	63	LEU
1	B	101	ARG
1	B	102	ILE
1	B	121	LEU
1	B	170	ASN
1	B	285	LEU
1	B	290	LEU
1	B	389	VAL
1	B	425	THR
1	B	432	LEU
1	B	469	GLU
1	B	485	ILE
1	B	489	VAL
1	B	491	LEU
1	B	493	LYS
1	B	508	GLU
1	C	52	ASP
1	C	63	LEU
1	C	101	ARG
1	C	156	GLU
1	C	165	LEU
1	C	285	LEU
1	C	290	LEU
1	C	320	ARG
1	C	389	VAL
1	C	418	LEU
1	C	425	THR
1	C	432	LEU
1	C	445	ARG
1	C	485	ILE
1	C	491	LEU
1	C	493	LYS

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Mol	Chain	Res	Type
1	C	509	LEU
1	C	511	LEU
1	C	514	GLU
1	D	12	ARG
1	D	19	GLN
1	D	52	ASP
1	D	63	LEU
1	D	101	ARG
1	D	102	ILE
1	D	121	LEU
1	D	285	LEU
1	D	290	LEU
1	D	389	VAL
1	D	418	LEU
1	D	432	LEU
1	D	469	GLU
1	D	485	ILE
1	D	491	LEU
1	D	493	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	GLN
1	A	150	GLN
1	A	170	ASN
1	A	287	GLN
1	A	350	ASN
1	A	383	GLN
1	B	58	GLN
1	B	123	GLN
1	B	150	GLN
1	B	287	GLN
1	B	350	ASN
1	B	383	GLN
1	B	492	GLN
1	C	19	GLN
1	C	58	GLN
1	C	84	GLN
1	C	123	GLN
1	C	150	GLN
1	C	170	ASN

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Mol	Chain	Res	Type
1	C	287	GLN
1	C	350	ASN
1	C	383	GLN
1	D	19	GLN
1	D	62	ASN
1	D	84	GLN
1	D	123	GLN
1	D	150	GLN
1	D	350	ASN
1	D	383	GLN
1	D	436	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	505/531 (95%)	0.35	27 (5%) 32 34	16, 26, 41, 58	0
1	B	505/531 (95%)	0.33	21 (4%) 40 43	16, 25, 45, 54	0
1	C	505/531 (95%)	0.21	24 (4%) 35 38	17, 24, 36, 44	0
1	D	505/531 (95%)	0.20	25 (4%) 34 36	15, 23, 41, 51	0
All	All	2020/2124 (95%)	0.27	97 (4%) 35 38	15, 25, 41, 58	0

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	4	VAL	4.6
1	B	348	GLY	4.6
1	D	529	ALA	4.5
1	A	428	ALA	4.2
1	D	428	ALA	4.1
1	B	393	ASN	4.1
1	A	485	ILE	3.8
1	D	514	GLU	3.8
1	D	393	ASN	3.6
1	C	429	ASP	3.6
1	B	428	ALA	3.4
1	C	56	GLN	3.3
1	A	348	GLY	3.2
1	A	170	ASN	3.2
1	A	427	ILE	3.1
1	B	427	ILE	3.1
1	D	425	THR	3.1
1	B	529	ALA	3.1
1	A	432	LEU	3.0
1	C	508	GLU	3.0
1	A	435	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	431	LYS	2.8
1	C	392	PHE	2.8
1	D	348	GLY	2.8
1	B	433	ASN	2.7
1	C	393	ASN	2.7
1	C	514	GLU	2.7
1	B	525	VAL	2.7
1	A	429	ASP	2.7
1	C	342	SER	2.7
1	B	505	ILE	2.7
1	D	4	VAL	2.7
1	D	427	ILE	2.6
1	A	433	ASN	2.6
1	B	429	ASP	2.6
1	D	433	ASN	2.5
1	B	4	VAL	2.5
1	C	348	GLY	2.5
1	A	425	THR	2.5
1	C	529	ALA	2.5
1	A	104	ASP	2.5
1	B	508	GLU	2.4
1	A	349	ALA	2.4
1	A	52	ASP	2.4
1	D	426	GLU	2.4
1	B	509	LEU	2.4
1	D	509	LEU	2.4
1	A	513	ASP	2.4
1	B	489	VAL	2.4
1	A	56	GLN	2.4
1	B	341	THR	2.4
1	B	507	PRO	2.4
1	D	430	GLY	2.4
1	C	52	ASP	2.3
1	A	508	GLU	2.3
1	A	514	GLU	2.3
1	D	505	ILE	2.3
1	D	394	GLY	2.3
1	A	156	GLU	2.3
1	B	170	ASN	2.3
1	C	485	ILE	2.3
1	C	394	GLY	2.3
1	B	313	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	248	ASP	2.3
1	C	426	GLU	2.3
1	D	52	ASP	2.3
1	B	58	GLN	2.3
1	A	320	ARG	2.2
1	D	439	ARG	2.2
1	C	156	GLU	2.2
1	C	167	GLU	2.2
1	B	309	VAL	2.2
1	C	431	LYS	2.2
1	C	439	ARG	2.2
1	C	526	LEU	2.2
1	B	500	ASP	2.2
1	C	300	ARG	2.2
1	A	423	LEU	2.2
1	A	342	SER	2.2
1	A	518	ILE	2.2
1	D	485	ILE	2.2
1	B	156	GLU	2.2
1	A	261	GLY	2.2
1	D	349	ALA	2.2
1	D	300	ARG	2.1
1	A	490	ASP	2.1
1	C	76	ASP	2.1
1	D	169	ASP	2.1
1	D	490	ASP	2.1
1	C	19	GLN	2.1
1	D	429	ASP	2.1
1	A	4	VAL	2.0
1	A	507	PRO	2.0
1	D	508	GLU	2.0
1	A	438	GLY	2.0
1	C	433	ASN	2.0
1	D	489	VAL	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.