



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:45 AM UTC

PDB ID : 8IVI / pdb_00008ivi
Title : crystal structure of a medium-long chain fatty acyl-CoA ligase
Authors : Li, S.
Deposited on : 2023-03-27
Resolution : 2.29 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

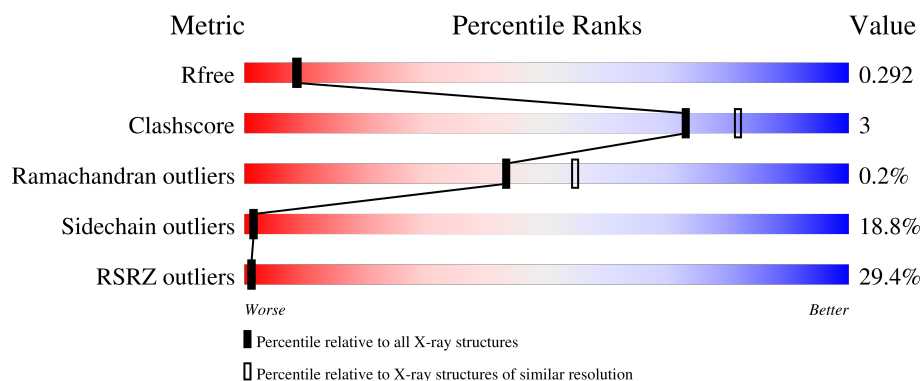
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.29 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	591	
1	B	591	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6266 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 Medium/long-chain-fatty-acid--CoA ligase FadD8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	411	Total	C	N	O	S	0	0	0
			3144	2004	544	585	11			
1	B	408	Total	C	N	O	S	0	0	0
			3122	1994	540	577	11			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP O06417
A	-18	GLY	-	expression tag	UNP O06417
A	-17	SER	-	expression tag	UNP O06417
A	-16	SER	-	expression tag	UNP O06417
A	-15	HIS	-	expression tag	UNP O06417
A	-14	HIS	-	expression tag	UNP O06417
A	-13	HIS	-	expression tag	UNP O06417
A	-12	HIS	-	expression tag	UNP O06417
A	-11	HIS	-	expression tag	UNP O06417
A	-10	HIS	-	expression tag	UNP O06417
A	-9	SER	-	expression tag	UNP O06417
A	-8	SER	-	expression tag	UNP O06417
A	-7	GLY	-	expression tag	UNP O06417
A	-6	LEU	-	expression tag	UNP O06417
A	-5	VAL	-	expression tag	UNP O06417
A	-4	PRO	-	expression tag	UNP O06417
A	-3	ARG	-	expression tag	UNP O06417
A	-2	GLY	-	expression tag	UNP O06417
A	-1	SER	-	expression tag	UNP O06417
A	0	HIS	-	expression tag	UNP O06417
B	-19	MET	-	initiating methionine	UNP O06417
B	-18	GLY	-	expression tag	UNP O06417
B	-17	SER	-	expression tag	UNP O06417
B	-16	SER	-	expression tag	UNP O06417
B	-15	HIS	-	expression tag	UNP O06417

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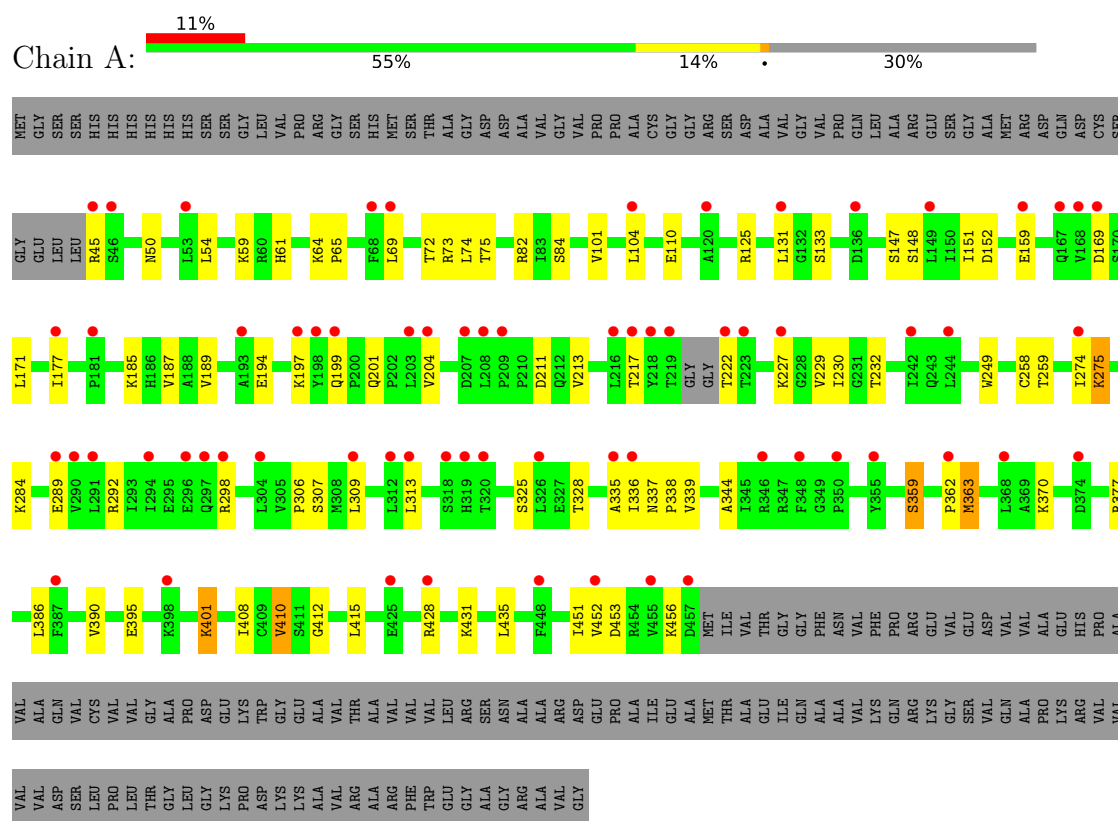
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP O06417
B	-13	HIS	-	expression tag	UNP O06417
B	-12	HIS	-	expression tag	UNP O06417
B	-11	HIS	-	expression tag	UNP O06417
B	-10	HIS	-	expression tag	UNP O06417
B	-9	SER	-	expression tag	UNP O06417
B	-8	SER	-	expression tag	UNP O06417
B	-7	GLY	-	expression tag	UNP O06417
B	-6	LEU	-	expression tag	UNP O06417
B	-5	VAL	-	expression tag	UNP O06417
B	-4	PRO	-	expression tag	UNP O06417
B	-3	ARG	-	expression tag	UNP O06417
B	-2	GLY	-	expression tag	UNP O06417
B	-1	SER	-	expression tag	UNP O06417
B	0	HIS	-	expression tag	UNP O06417

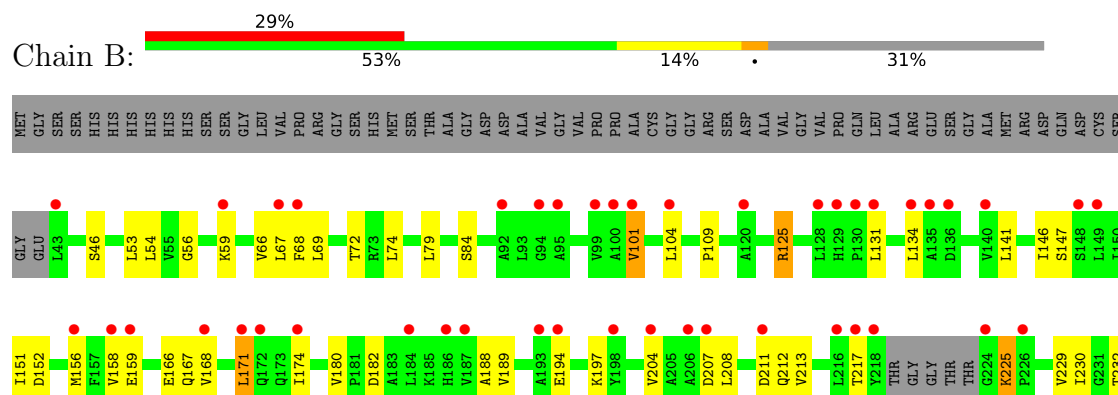
3 Residue-property plots

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: Medium/long-chain-fatty-acid--CoA ligase FadD8



- Molecule 1: Medium/long-chain-fatty-acid--CoA ligase FadD8



ALA	VAL	GLY	Y449	L386	D322	L242
ARG	ARG	ARG	Y450	F387	L323	
GLU	GLU	GLU	I451	A388	S324	W247
PRO	PRO	PRO	D452	R389	S325	
ALA	ALA	ALA	D453	V390	L326	F250
ILE	ILE	ILE	R454	A391	E327	
LYS	LYS	LYS	Y455	L392	T328	
GLU	GLU	GLU	ASP	L393	V329	
ALA	ALA	ALA	NET	D394	V330	
THR	THR	THR	THR	E395	Y331	W257
ALA	ALA	ALA	VAL	H396	G332	C258
GLU	GLU	GLU	THR	G397	A333	T259
ILE	ILE	ILE	THR	K398	S334	Y260
GLN	GLN	GLN	GLY	P399	A335	L261
ALA	ALA	ALA	PHE	V400	T336	S262
ALA	ALA	ALA	ASN	K401	N337	H263
VAL	VAL	VAL	VAL	Q402	P338	A264
LYS	LYS	LYS	PHE	G403	V339	C265
GLN	GLN	GLN	PRO	A404	R340	A266
ARG	ARG	ARG	ARG	G406	L341	A267
LYS	LYS	LYS	GLU	E407	A344	F268
GLY	GLY	GLY	VAL	I408	T345	E278
SER	SER	SER	GLU	G409	R346	W279
VAL	VAL	VAL	VAL	V410	F347	L280
GLN	GLN	GLN	VAL	L414	G348	V281
ALA	ALA	ALA	VAL	L415	G349	L282
PRO	PRO	PRO	ALA	A416	P350	A283
LYS	LYS	LYS	GLU	G417	T351	K284
ARG	ARG	ARG	HIS	G418	F352	
VAL	VAL	VAL	PRO	A419	A353	A288
ALA	ALA	ALA	ALA	Y419	Q354	E289
VAL	VAL	VAL	VAL	W420	V355	V290
VAL	VAL	VAL	ALA	W421	Y356	L291
ASP	ASP	ASP	GLN	L422	G357	R292
SER	SER	SER	VAL	F423	G358	L293
LEU	LEU	LEU	CYS	D424	S359	L294
LEU	LEU	LEU	VAL	E425	E360	
THR	THR	THR	VAL	T426	A361	I299
GLY	GLY	GLY	GLY	S427	P362	T300
LEU	LEU	LEU	ALA	R428	G363	A301
PRO	PRO	PRO	PRO	T429	V364	T302
GLY	GLY	GLY	ASP	F430	L365	M303
LYS	LYS	LYS	GLU	K431	T366	L304
PRO	PRO	PRO	ASP	D432	Y367	V305
ASP	ASP	ASP	TRP	G433	L368	P306
LYS	LYS	LYS	GLY	W434	A366	S307
LYS	LYS	LYS	GLU	L435	H372	M308
ALA	ALA	ALA	ALA	H436	H373	L309
VAL	VAL	VAL	VAL	VAL	D374	
ARG	ARG	ARG	THR	THR	E375	L312
ALA	ALA	ALA	VAL	VAL	K376	L313
ARG	ARG	ARG	VAL	VAL	A441	D314
PHE	PHE	PHE	VAL	VAL	R442	H315
TRP	TRP	TRP	VAL	VAL	E443	P316
GLU	GLU	GLU	LEU	LEU	D444	D317
GLY	GLY	GLY	ARG	ARG	S445	S318
ALA	ALA	ALA	SER	SER	D446	G382
GLY	GLY	GLY	ASN	ASN	G447	T320
ARG	ARG	ARG	ALA	ALA	F448	P321

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	66.23Å 105.00Å 135.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	52.50 – 2.29 52.50 – 2.29	Depositor EDS
% Data completeness (in resolution range)	99.3 (52.50-2.29) 92.4 (52.50-2.29)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 2.29Å)	Xtriage
Refinement program	PHENIX (1.18.2_3874: ???)	Depositor
R, R_{free}	0.247 , 0.275 0.283 , 0.292	Depositor DCC
R_{free} test set	2000 reflections (4.62%)	wwPDB-VP
Wilson B-factor (Å ²)	60.9	Xtriage
Anisotropy	0.383	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 47.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6266	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.88% 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	0.50	1/3215 (0.0%)	0.85	9/4378 (0.2%)
1	B	0.48	0/3193	0.88	3/4348 (0.1%)
All	All	0.49	1/6408 (0.0%)	0.86	12/8726 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	412	GLY	C-N	5.74	1.38	1.33

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	433	GLY	N-CA-C	-8.29	104.43	115.21
1	A	363	MET	N-CA-C	8.21	128.28	110.80
1	B	152	ASP	N-CA-C	-7.70	99.95	109.65
1	A	152	ASP	N-CA-C	-7.69	99.96	109.65
1	A	359	SER	N-CA-C	-6.99	104.56	113.23
1	B	432	ASP	N-CA-C	-6.86	103.27	112.94
1	A	412	GLY	CA-C-N	-5.61	115.11	120.83
1	A	412	GLY	C-N-CA	-5.61	115.11	120.83
1	A	249	TRP	CA-C-N	-5.32	114.48	119.85
1	A	249	TRP	C-N-CA	-5.32	114.48	119.85
1	A	274	ILE	N-CA-C	-5.26	105.41	110.72
1	A	362	PRO	N-CA-C	5.03	122.82	112.47

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	3144	0	3156	17	0
1	B	3122	0	3140	24	0
All	All	6266	0	6296	40	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 (40) 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:194:GLU:OE2	1:A:197:LYS:NZ	2.26	0.68
1:B:68:PHE:HB2	1:B:280:ILE:HA	1.79	0.64
1:B:305:VAL:HG22	1:B:308:MET:HG3	1.84	0.60
1:B:419:TYR:H	1:B:426:THR:HG22	1.67	0.58
1:A:65:PRO:HA	1:A:75:THR:HA	1.88	0.56
1:B:68:PHE:HE1	1:B:278:GLU:HB2	1.70	0.54
1:A:61:HIS:HB3	1:A:64:LYS:HB3	1.92	0.52
1:A:386:LEU:HD22	1:B:56:GLY:HA3	1.93	0.51
1:A:213:VAL:HG13	1:A:230:ILE:HG23	1.92	0.51
1:A:306:PRO:HG3	1:A:335:ALA:HB1	1.94	0.49
1:A:401:LYS:HB2	1:A:401:LYS:HE2	1.56	0.49
1:B:141:LEU:HD22	1:B:146:ILE:HG13	1.94	0.49
1:B:213:VAL:HG13	1:B:230:ILE:HG23	1.95	0.49
1:B:69:LEU:HD22	1:B:109:PRO:HD3	1.96	0.48
1:B:225:LYS:HB2	1:B:225:LYS:HE3	1.30	0.46
1:B:208:LEU:HD22	1:B:212:GLN:HG2	1.98	0.45
1:A:328:THR:HG23	1:A:370:LYS:HD3	1.98	0.45
1:B:376:LYS:H	1:B:376:LYS:HG3	1.45	0.45
1:A:390:VAL:HG22	1:A:410:VAL:HG13	1.97	0.45
1:B:294:ILE:HA	1:B:299:ILE:HB	1.99	0.45
1:B:174:ILE:HB	1:B:188:ALA:HB2	1.99	0.44
1:B:171:LEU:HD23	1:B:171:LEU:HA	1.89	0.44
1:A:313:LEU:HD11	1:A:344:ALA:HB2	1.98	0.44
1:B:104:LEU:HB3	1:B:151:ILE:HG22	2.00	0.43
1:A:104:LEU:HB3	1:A:151:ILE:HG22	1.99	0.43
1:B:101:VAL:HG21	1:B:125:ARG:HH21	1.84	0.43
1:A:298:ARG:HD3	1:A:325:SER:HB3	2.00	0.42
1:B:340:ARG:HE	1:B:340:ARG:HB3	1.43	0.42
1:B:401:LYS:HE2	1:B:401:LYS:HB2	1.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:211:ASP:HA	1:B:232:THR:HB	2.02	0.42
1:A:275:LYS:HB3	1:A:275:LYS:HE3	1.59	0.42
1:B:354:GLN:HB3	1:B:368:LEU:HB2	2.01	0.42
1:A:171:LEU:HD12	1:A:171:LEU:HA	1.90	0.42
1:A:410:VAL:HB	1:A:415:LEU:HD11	2.01	0.42
1:B:79:LEU:HD12	1:B:79:LEU:HA	1.83	0.41
1:A:337:ASN:HA	1:A:338:PRO:HD2	1.95	0.41
1:B:141:LEU:HB2	1:B:168:VAL:HG21	2.02	0.41
1:A:194:GLU:CD	1:A:197:LYS:NZ	2.78	0.41
1:B:400:VAL:HB	1:B:404:GLU:HB3	2.03	0.41
1:B:341:LEU:HB3	1:B:378:LEU:HD22	2.03	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	407/591 (69%)	395 (97%)	11 (3%)	1 (0%)	43	55
1	B	404/591 (68%)	369 (91%)	34 (8%)	1 (0%)	43	55
All	All	811/1182 (69%)	764 (94%)	45 (6%)	2 (0%)	43	55

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	363	MET
1	B	362	PRO

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	332/466 (71%)	277 (83%)	55 (17%)	2	2
1	B	329/466 (71%)	260 (79%)	69 (21%)	1	1
All	All	661/932 (71%)	537 (81%)	124 (19%)	1	1

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	ARG
1	A	50	ASN
1	A	54	LEU
1	A	59	LYS
1	A	69	LEU
1	A	72	THR
1	A	73	ARG
1	A	74	LEU
1	A	82	ARG
1	A	84	SER
1	A	101	VAL
1	A	110	GLU
1	A	125	ARG
1	A	131	LEU
1	A	133	SER
1	A	147	SER
1	A	148	SER
1	A	159	GLU
1	A	169	ASP
1	A	177	ILE
1	A	185	LYS
1	A	187	VAL
1	A	189	VAL
1	A	199	GLN
1	A	201	GLN
1	A	204	VAL
1	A	211	ASP

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Mol	Chain	Res	Type
1	A	217	THR
1	A	222	THR
1	A	227	LYS
1	A	229	VAL
1	A	232	THR
1	A	258	CYS
1	A	259	THR
1	A	275	LYS
1	A	284	LYS
1	A	289	GLU
1	A	292	ARG
1	A	307	SER
1	A	309	LEU
1	A	336	ILE
1	A	339	VAL
1	A	359	SER
1	A	377	ARG
1	A	395	GLU
1	A	401	LYS
1	A	408	ILE
1	A	410	VAL
1	A	428	ARG
1	A	431	LYS
1	A	435	LEU
1	A	451	ILE
1	A	452	VAL
1	A	453	ASP
1	A	456	LYS
1	B	46	SER
1	B	53	LEU
1	B	54	LEU
1	B	59	LYS
1	B	66	VAL
1	B	67	LEU
1	B	72	THR
1	B	74	LEU
1	B	84	SER
1	B	101	VAL
1	B	125	ARG
1	B	131	LEU
1	B	134	LEU
1	B	147	SER

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Mol	Chain	Res	Type
1	B	156	MET
1	B	158	VAL
1	B	159	GLU
1	B	166	GLU
1	B	167	GLN
1	B	171	LEU
1	B	180	VAL
1	B	182	ASP
1	B	189	VAL
1	B	194	GLU
1	B	197	LYS
1	B	204	VAL
1	B	207	ASP
1	B	217	THR
1	B	225	LYS
1	B	229	VAL
1	B	258	CYS
1	B	259	THR
1	B	278	GLU
1	B	280	ILE
1	B	281	VAL
1	B	282	LEU
1	B	284	LYS
1	B	291	LEU
1	B	292	ARG
1	B	293	ILE
1	B	304	LEU
1	B	305	VAL
1	B	307	SER
1	B	312	LEU
1	B	334	SER
1	B	340	ARG
1	B	341	LEU
1	B	358	GLN
1	B	360	GLU
1	B	362	PRO
1	B	368	LEU
1	B	375	GLU
1	B	376	LYS
1	B	379	THR
1	B	386	LEU
1	B	394	ASP

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Mol	Chain	Res	Type
1	B	395	GLU
1	B	396	HIS
1	B	401	LYS
1	B	404	GLU
1	B	408	ILE
1	B	410	VAL
1	B	415	LEU
1	B	422	LEU
1	B	424	ASP
1	B	428	ARG
1	B	431	LYS
1	B	432	ASP
1	B	446	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	ASN
1	A	88	GLN
1	A	119	GLN
1	A	154	ASN
1	A	167	GLN
1	A	172	GLN
1	A	252	ASN
1	A	263	HIS
1	A	358	GLN
1	B	154	ASN
1	B	172	GLN
1	B	358	GLN
1	B	421	ASN

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	411/591 (69%)	1.29	67 (16%) 4 5	48, 65, 84, 109	0
1	B	408/591 (69%)	1.91	174 (42%) 0 0	58, 81, 114, 127	0
All	All	819/1182 (69%)	1.60	241 (29%) 1 1	48, 72, 106, 127	0

All (241) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	335	ALA	6.4
1	A	69	LEU	4.8
1	B	377	ARG	4.6
1	B	348	PHE	4.4
1	B	430	PHE	4.4
1	B	445	SER	4.4
1	B	68	PHE	4.4
1	B	43	LEU	4.3
1	A	335	ALA	4.3
1	B	378	LEU	4.2
1	B	302	THR	4.2
1	B	323	LEU	4.0
1	B	444	ASP	4.0
1	B	328	THR	3.9
1	B	452	VAL	3.8
1	B	67	LEU	3.8
1	B	206	ALA	3.8
1	B	291	LEU	3.8
1	B	304	LEU	3.8
1	B	356	TYR	3.7
1	B	168	VAL	3.7
1	B	365	ILE	3.7
1	B	402	GLN	3.7
1	B	334	SER	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	292	ARG	3.6
1	B	333	ALA	3.6
1	B	341	LEU	3.5
1	A	374	ASP	3.5
1	B	322	ASP	3.5
1	B	442	ARG	3.5
1	B	224	GLY	3.5
1	B	433	GLY	3.5
1	B	368	LEU	3.5
1	B	448	PHE	3.4
1	B	305	VAL	3.4
1	B	450	TYR	3.4
1	A	222	THR	3.3
1	B	408	ILE	3.3
1	B	360	GLU	3.3
1	A	455	VAL	3.3
1	B	446	ASP	3.3
1	B	431	LYS	3.3
1	B	338	PRO	3.2
1	A	68	PHE	3.2
1	A	298	ARG	3.2
1	B	434	TRP	3.2
1	B	326	LEU	3.2
1	A	168	VAL	3.2
1	B	406	GLY	3.1
1	B	391	ALA	3.1
1	B	336	ILE	3.1
1	B	218	TYR	3.0
1	B	257	MET	3.0
1	B	449	TYR	3.0
1	A	223	THR	3.0
1	A	320	THR	3.0
1	B	350	PRO	3.0
1	A	309	LEU	3.0
1	B	293	ILE	2.9
1	B	367	TYR	2.9
1	B	193	ALA	2.9
1	B	320	THR	2.9
1	B	405	VAL	2.9
1	B	211	ASP	2.9
1	B	92	ALA	2.9
1	B	134	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	441	ALA	2.9
1	B	339	VAL	2.9
1	B	381	CYS	2.9
1	A	457	ASP	2.9
1	A	198	TYR	2.8
1	B	184	LEU	2.8
1	B	364	VAL	2.8
1	B	156	MET	2.8
1	A	169	ASP	2.8
1	B	432	ASP	2.8
1	B	393	LEU	2.8
1	B	264	ALA	2.8
1	B	443	GLU	2.8
1	B	318	SER	2.8
1	B	325	SER	2.8
1	B	198	TYR	2.8
1	B	419	TYR	2.8
1	B	451	ILE	2.8
1	B	421	ASN	2.8
1	A	348	PHE	2.8
1	B	400	VAL	2.8
1	B	315	HIS	2.7
1	A	177	ILE	2.7
1	A	209	PRO	2.7
1	A	289	GLU	2.7
1	A	428	ARG	2.7
1	B	95	ALA	2.7
1	A	136	ASP	2.7
1	A	304	LEU	2.7
1	B	346	ARG	2.7
1	A	355	TYR	2.7
1	B	268	PHE	2.7
1	B	387	PHE	2.7
1	B	140	VAL	2.7
1	B	204	VAL	2.7
1	B	455	VAL	2.7
1	B	362	PRO	2.7
1	B	363	MET	2.7
1	A	199	GLN	2.7
1	B	158	VAL	2.7
1	A	203	LEU	2.7
1	B	149	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	362	PRO	2.6
1	B	172	GLN	2.6
1	B	388	ALA	2.6
1	B	159	GLU	2.6
1	B	428	ARG	2.6
1	A	319	HIS	2.6
1	B	263	HIS	2.6
1	B	131	LEU	2.6
1	B	423	PRO	2.6
1	A	46	SER	2.6
1	A	167	GLN	2.6
1	B	383	ARG	2.6
1	B	447	GLY	2.6
1	B	380	SER	2.6
1	B	59	LYS	2.6
1	A	326	LEU	2.5
1	B	372	ASP	2.5
1	A	227	LYS	2.5
1	B	435	LEU	2.5
1	A	149	LEU	2.5
1	B	386	LEU	2.5
1	B	394	ASP	2.5
1	B	130	PRO	2.5
1	A	425	GLU	2.5
1	B	359	SER	2.5
1	A	398	LYS	2.5
1	B	374	ASP	2.5
1	B	247	TRP	2.4
1	B	422	LEU	2.4
1	B	120	ALA	2.4
1	B	226	PRO	2.4
1	B	316	PRO	2.4
1	B	321	ARG	2.4
1	B	349	GLY	2.4
1	B	294	ILE	2.4
1	B	376	LYS	2.4
1	A	159	GLU	2.4
1	B	332	GLY	2.4
1	B	403	GLY	2.4
1	B	242	ILE	2.4
1	B	390	VAL	2.4
1	A	131	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	312	LEU	2.4
1	B	415	LEU	2.4
1	B	330	TYR	2.4
1	A	274	ILE	2.4
1	B	104	LEU	2.4
1	B	392	LEU	2.4
1	A	181	PRO	2.3
1	A	350	PRO	2.3
1	B	250	PRO	2.3
1	B	417	GLY	2.3
1	B	128	LEU	2.3
1	B	355	TYR	2.3
1	B	94	GLY	2.3
1	B	300	THR	2.3
1	A	294	ILE	2.3
1	A	452	VAL	2.3
1	B	410	VAL	2.3
1	A	208	LEU	2.3
1	B	136	ASP	2.3
1	B	344	ALA	2.3
1	B	194	GLU	2.3
1	A	387	PHE	2.3
1	B	313	LEU	2.3
1	A	207	ASP	2.3
1	B	100	ALA	2.3
1	B	217	THR	2.3
1	A	216	LEU	2.2
1	B	101	VAL	2.3
1	B	317	ASP	2.2
1	A	45	ARG	2.2
1	A	219	THR	2.2
1	B	186	HIS	2.2
1	B	396	HIS	2.2
1	A	297	GLN	2.2
1	B	427	SER	2.2
1	B	351	ILE	2.2
1	B	329	VAL	2.2
1	B	289	GLU	2.2
1	B	261	LEU	2.2
1	A	448	PHE	2.2
1	B	352	PHE	2.2
1	B	253	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	303	MET	2.2
1	B	265	GLY	2.2
1	B	436	HIS	2.2
1	B	266	ALA	2.2
1	A	104	LEU	2.2
1	A	368	LEU	2.2
1	B	280	ILE	2.2
1	B	99	VAL	2.2
1	B	439	ASP	2.2
1	B	399	PRO	2.2
1	A	193	ALA	2.2
1	A	291	LEU	2.1
1	A	336	ILE	2.1
1	A	204	VAL	2.1
1	B	424	ASP	2.1
1	A	120	ALA	2.1
1	A	53	LEU	2.1
1	B	174	ILE	2.1
1	B	440	LEU	2.1
1	B	397	GLY	2.1
1	B	259	THR	2.1
1	A	312	LEU	2.1
1	B	216	LEU	2.1
1	B	453	ASP	2.1
1	B	340	ARG	2.1
1	B	148	SER	2.1
1	B	429	THR	2.1
1	A	296	GLU	2.1
1	B	129	HIS	2.1
1	B	373	HIS	2.1
1	B	187	VAL	2.1
1	A	346	ARG	2.1
1	A	318	SER	2.0
1	B	135	ALA	2.0
1	B	267	ALA	2.0
1	B	288	ALA	2.0
1	B	319	HIS	2.0
1	B	309	LEU	2.0
1	B	414	LEU	2.0
1	A	242	ILE	2.0
1	A	218	TYR	2.0
1	A	290	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	382	GLY	2.0
1	A	217	THR	2.0
1	A	244	LEU	2.0
1	A	313	LEU	2.0
1	B	171	LEU	2.0
1	B	207	ASP	2.0
1	A	197	LYS	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 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.