



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 01:17 AM UTC

PDB ID : 3G7S / pdb_00003g7s
Title : Crystal structure of a long-chain-fatty-acid-CoA ligase (FadD1) from Archaeoglobus fulgidus
Authors : Palani, K.; Kumaran, D.; Burley, S.K.; Swaminathan, S.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2009-02-10
Resolution : 2.15 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

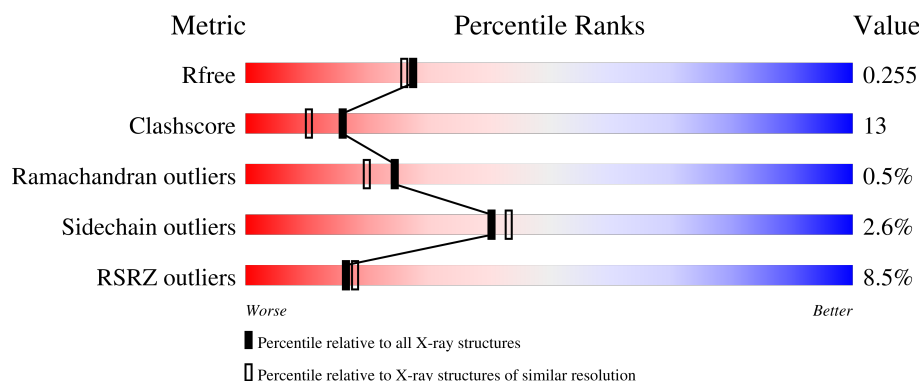
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	549	11% 65% 24% • 9%
1	B	549	4% 64% 25% • 10%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8080 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 Long-chain-fatty-acid--CoA ligase (FadD-1).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	497	Total	C	N	O	S	Se	0	0	0
			3926	2524	641	737	6	18			
1	B	496	Total	C	N	O	S	Se	0	0	0
			3924	2526	641	732	6	19			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MSE	-	expression tag	UNP O30147
A	0	SER	-	expression tag	UNP O30147
A	1	LEU	-	expression tag	UNP O30147
A	541	GLY	-	expression tag	UNP O30147
A	542	HIS	-	expression tag	UNP O30147
A	543	HIS	-	expression tag	UNP O30147
A	544	HIS	-	expression tag	UNP O30147
A	545	HIS	-	expression tag	UNP O30147
A	546	HIS	-	expression tag	UNP O30147
A	547	HIS	-	expression tag	UNP O30147
B	-1	MSE	-	expression tag	UNP O30147
B	0	SER	-	expression tag	UNP O30147
B	1	LEU	-	expression tag	UNP O30147
B	541	GLY	-	expression tag	UNP O30147
B	542	HIS	-	expression tag	UNP O30147
B	543	HIS	-	expression tag	UNP O30147
B	544	HIS	-	expression tag	UNP O30147
B	545	HIS	-	expression tag	UNP O30147
B	546	HIS	-	expression tag	UNP O30147
B	547	HIS	-	expression tag	UNP O30147

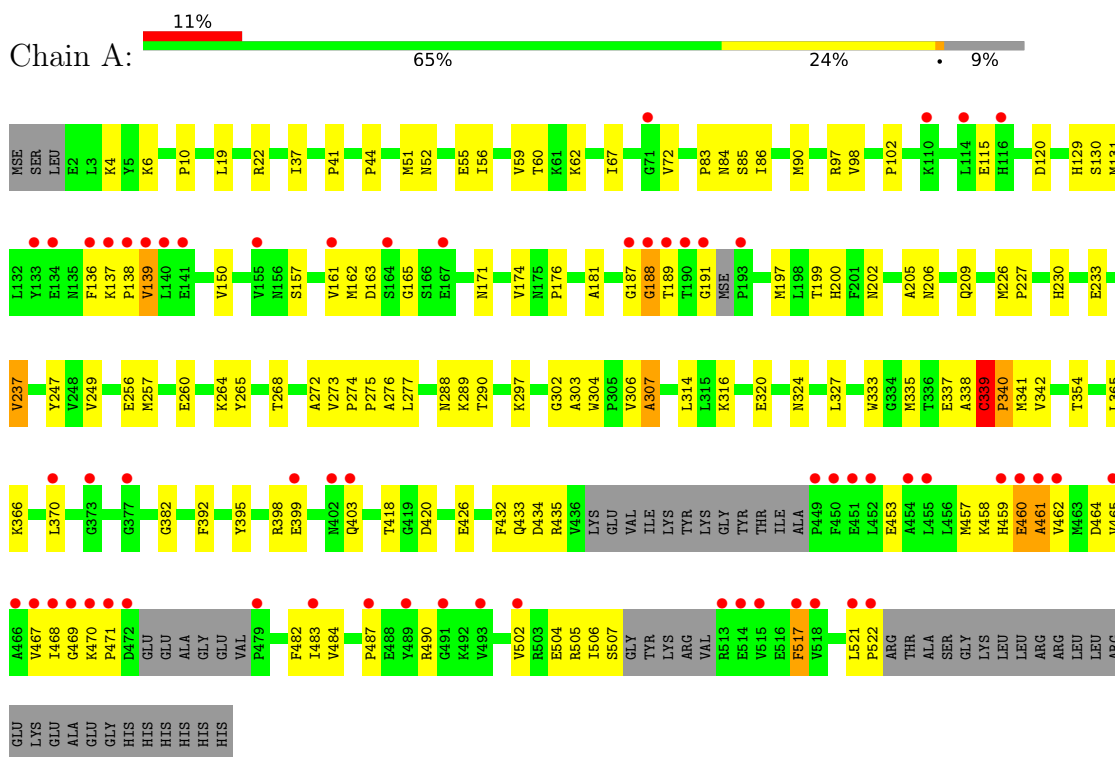
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	92	Total 92	O 92	0	0
2	B	138	Total 138	O 138	0	0

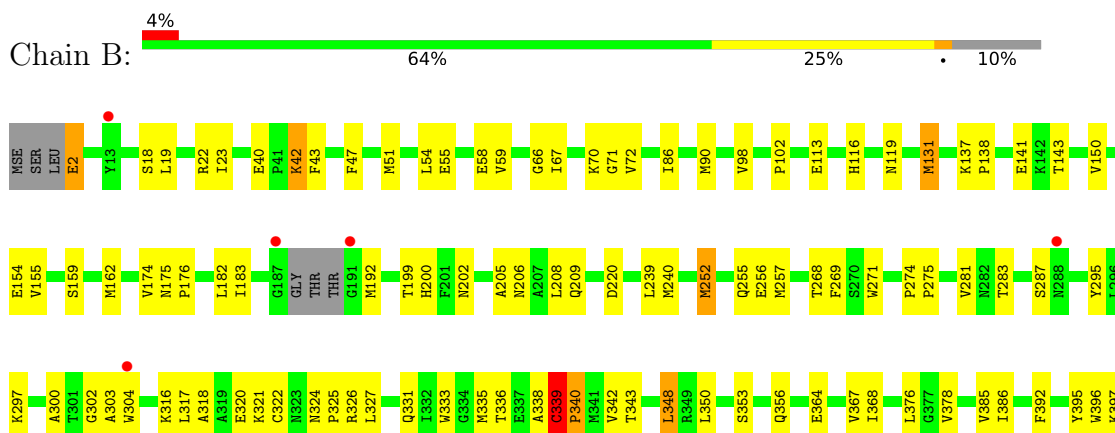
3 Residue-property plots [i](#)

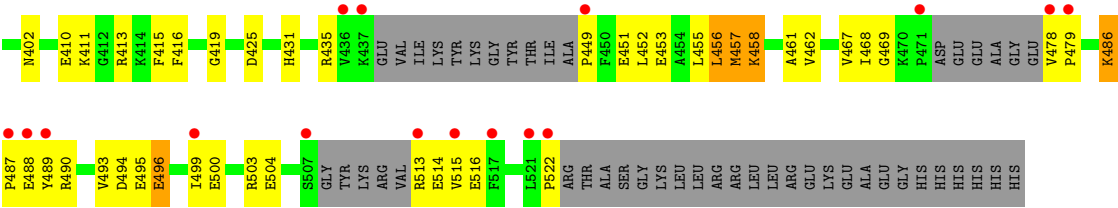
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Long-chain-fatty-acid--CoA ligase (FadD-1)



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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	58.04Å 105.07Å 182.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.57 – 2.15 45.57 – 2.15	Depositor EDS
% Data completeness (in resolution range)	85.8 (45.57-2.15) 86.0 (45.57-2.15)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 2.16Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.222 , 0.256 0.222 , 0.255	Depositor DCC
R_{free} test set	2667 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	22.7	Xtriage
Anisotropy	0.846	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 48.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8080	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% 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	0.46	0/3998	0.93	9/5382 (0.2%)
1	B	0.51	1/3995 (0.0%)	0.96	13/5376 (0.2%)
All	All	0.48	1/7993 (0.0%)	0.95	22/10758 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	457	MSE	SE-CE	-5.78	1.78	1.95

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	461	ALA	N-CA-C	-7.63	104.87	114.56
1	A	339	CYS	N-CA-C	6.76	124.75	109.81
1	B	462	VAL	N-CA-C	6.53	117.99	108.58
1	A	320	GLU	N-CA-C	6.53	118.47	111.36
1	A	163	ASP	N-CA-C	-6.20	104.53	111.28
1	B	18	SER	N-CA-C	-6.08	101.49	110.48
1	B	339	CYS	N-CA-C	6.04	123.16	109.81
1	B	150	VAL	N-CA-C	5.98	115.34	106.85
1	B	116	HIS	N-CA-C	5.92	117.82	111.36
1	B	175	ASN	N-CA-C	-5.91	97.01	108.59
1	B	71	GLY	N-CA-C	5.83	121.42	114.48
1	A	342	VAL	N-CA-C	5.61	116.05	111.62
1	A	483	ILE	N-CA-C	5.47	116.36	108.48
1	B	486	LYS	N-CA-C	-5.44	101.50	109.50
1	B	386	ILE	N-CA-C	5.38	117.52	108.81
1	B	220	ASP	N-CA-C	5.28	118.33	110.52
1	B	42	LYS	N-CA-C	5.27	117.99	109.40
1	B	274	PRO	N-CA-C	5.26	117.11	110.70
1	B	23	ILE	N-CA-C	-5.11	105.51	110.42
1	A	307	ALA	CA-C-N	5.04	125.06	119.32
1	A	307	ALA	C-N-CA	5.04	125.06	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	10	PRO	N-CA-C	5.01	118.95	111.14

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	3926	0	3900	105	0
1	B	3924	0	3908	103	0
2	A	92	0	0	3	0
2	B	138	0	0	6	0
All	All	8080	0	7808	207	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 13.

All (207) 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:457:MSE:HE2	1:A:465:VAL:HG12	1.32	1.07
1:A:457:MSE:HE1	1:A:464:ASP:HA	1.31	1.07
1:A:457:MSE:HE1	1:A:464:ASP:CA	1.95	0.96
1:A:137:LYS:HB3	1:A:138:PRO:HD3	1.48	0.95
1:B:338:ALA:C	1:B:340:PRO:HA	1.94	0.91
1:B:395:TYR:N	1:B:402:ASN:HD21	1.71	0.89
1:A:51:MSE:HE1	1:A:59:VAL:HG21	1.56	0.88
1:B:395:TYR:H	1:B:402:ASN:ND2	1.71	0.88
1:B:19:LEU:H	1:B:200:HIS:HD2	1.22	0.87
1:B:40:GLU:HB2	1:B:257:MSE:HE2	1.58	0.85
1:B:395:TYR:H	1:B:402:ASN:HD21	0.88	0.85
1:A:457:MSE:CE	1:A:465:VAL:HG12	2.06	0.84
1:A:129:HIS:CD2	1:A:131:MSE:HG2	2.12	0.83
1:A:19:LEU:H	1:A:200:HIS:HD2	1.29	0.77
1:B:339:CYS:N	1:B:340:PRO:HA	1.99	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:335:MSE:O	1:B:340:PRO:HB2	1.88	0.74
1:A:56:ILE:HG23	1:A:90:MSE:HE1	1.70	0.73
1:A:199:THR:H	1:A:202:ASN:HD22	1.37	0.71
1:B:40:GLU:HB2	1:B:257:MSE:CE	2.19	0.71
1:A:174:VAL:O	1:A:176:PRO:HD3	1.90	0.70
1:A:457:MSE:HE2	1:A:465:VAL:CG1	2.19	0.69
1:B:452:LEU:HD22	1:B:515:VAL:HG23	1.74	0.69
1:B:324:ASN:ND2	1:B:327:LEU:HB2	2.07	0.69
1:B:503:ARG:HD2	1:B:514:GLU:OE1	1.94	0.67
1:A:129:HIS:HD2	1:A:131:MSE:HG2	1.60	0.66
1:A:457:MSE:CE	1:A:465:VAL:N	2.59	0.65
1:B:479:PRO:HG2	1:B:515:VAL:HA	1.79	0.65
1:A:19:LEU:H	1:A:200:HIS:CD2	2.14	0.65
1:B:19:LEU:H	1:B:200:HIS:CD2	2.10	0.65
1:A:470:LYS:HG2	1:A:471:PRO:HD2	1.80	0.65
1:A:370:LEU:CD2	1:A:382:GLY:HA2	2.27	0.64
1:B:335:MSE:C	1:B:340:PRO:HB2	2.22	0.64
1:A:256:GLU:O	1:A:260:GLU:HG3	1.98	0.63
1:B:159:SER:HA	1:B:162:MSE:HE3	1.80	0.63
1:A:67:ILE:HD12	1:A:72:VAL:HB	1.81	0.62
1:A:468:ILE:HD12	1:A:482:PHE:CE1	2.35	0.62
1:A:502:VAL:O	1:A:506:ILE:HG22	1.99	0.62
1:A:324:ASN:ND2	1:A:327:LEU:HB2	2.15	0.62
1:B:411:LYS:HD2	1:B:413:ARG:NH2	2.15	0.61
1:B:2:GLU:HG3	1:B:378:VAL:HB	1.82	0.61
1:B:43:PHE:CD1	1:B:131:MSE:HE1	2.36	0.61
1:B:86:ILE:O	1:B:90:MSE:HG2	2.02	0.59
1:B:396:TRP:CE2	1:B:397:LYS:HG2	2.38	0.59
1:B:40:GLU:CB	1:B:257:MSE:HE2	2.29	0.59
1:A:129:HIS:HD2	1:A:131:MSE:H	1.51	0.59
1:B:154:GLU:HG2	1:B:155:VAL:HG23	1.85	0.59
1:B:119:ASN:HD21	1:B:143:THR:HA	1.68	0.59
1:B:335:MSE:O	1:B:340:PRO:CB	2.52	0.58
1:A:457:MSE:CE	1:A:464:ASP:HA	2.21	0.56
1:B:453:GLU:HG2	1:B:467:VAL:HG23	1.88	0.56
1:A:335:MSE:HE2	1:A:418:THR:HB	1.88	0.56
1:B:287:SER:O	1:B:321:LYS:NZ	2.39	0.56
1:B:419:GLY:HA3	1:B:435:ARG:HH21	1.71	0.56
1:A:399:GLU:O	1:A:403:GLN:HG3	2.06	0.56
1:A:289:LYS:HE2	1:A:290:THR:O	2.06	0.55
1:B:490:ARG:NH2	1:B:522:PRO:HG3	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:449:PRO:HG2	2:B:549:HOH:O	2.06	0.55
1:A:136:PHE:O	1:A:139:VAL:HG12	2.06	0.55
1:B:478:VAL:HG13	1:B:516:GLU:HG3	1.89	0.55
1:A:457:MSE:CE	1:A:465:VAL:H	2.20	0.54
1:A:51:MSE:HE1	1:A:59:VAL:CG2	2.35	0.54
1:A:420:ASP:OD1	1:A:435:ARG:HG2	2.07	0.54
1:B:47:PHE:HE1	1:B:59:VAL:HG11	1.72	0.54
1:B:268:THR:HB	1:B:297:LYS:HE2	1.89	0.54
1:B:331:GLN:NE2	1:B:356:GLN:HE21	2.06	0.54
1:A:86:ILE:O	1:A:90:MSE:HG2	2.07	0.54
1:A:338:ALA:C	1:A:340:PRO:HA	2.34	0.53
1:B:98:VAL:O	1:B:98:VAL:HG12	2.07	0.53
1:B:154:GLU:H	1:B:154:GLU:CD	2.16	0.53
1:A:189:THR:HG22	1:A:191:GLY:H	1.74	0.53
1:B:455:LEU:HA	1:B:458:LYS:HD2	1.90	0.52
1:B:495:GLU:O	1:B:499:ILE:HG12	2.09	0.52
1:A:457:MSE:HE1	1:A:464:ASP:C	2.34	0.52
1:A:482:PHE:HD2	1:A:521:LEU:HD12	1.74	0.52
1:B:205:ALA:O	1:B:209:GLN:HG3	2.10	0.52
1:A:67:ILE:HG22	1:A:161:VAL:HG11	1.92	0.52
1:B:202:ASN:HB3	1:B:339:CYS:SG	2.50	0.51
1:A:226:MSE:HE1	1:A:276:ALA:HB2	1.93	0.51
1:B:367:VAL:HG12	1:B:376:LEU:HD12	1.92	0.51
1:B:411:LYS:HD2	1:B:413:ARG:HH21	1.76	0.51
1:A:470:LYS:HG2	1:A:471:PRO:CD	2.41	0.51
1:A:19:LEU:N	1:A:200:HIS:HD2	2.06	0.50
1:A:370:LEU:HD21	1:A:382:GLY:HA2	1.92	0.50
1:A:115:GLU:HB2	1:A:139:VAL:HG21	1.93	0.50
1:A:268:THR:HB	1:A:297:LYS:HE2	1.92	0.50
1:B:425:ASP:OD2	1:B:431:HIS:HE1	1.95	0.50
1:A:339:CYS:N	1:A:340:PRO:HA	2.27	0.50
1:B:51:MSE:HE2	1:B:55:GLU:HB3	1.94	0.50
1:B:453:GLU:O	1:B:457:MSE:HB2	2.11	0.50
1:B:51:MSE:CE	1:B:55:GLU:HB3	2.42	0.49
1:A:338:ALA:O	1:A:339:CYS:HB2	2.12	0.49
1:B:141:GLU:HG2	2:B:605:HOH:O	2.13	0.49
1:A:226:MSE:HE1	1:A:276:ALA:CB	2.43	0.49
1:A:426:GLU:HG2	2:A:577:HOH:O	2.13	0.49
1:B:271:TRP:HA	1:B:300:ALA:O	2.13	0.49
1:B:333:TRP:CH2	1:B:335:MSE:HE1	2.47	0.49
1:B:40:GLU:OE2	1:B:42:LYS:HE2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:GLU:OE1	1:B:513:ARG:NH1	2.45	0.48
1:B:342:VAL:HG12	1:B:343:THR:HG23	1.95	0.48
1:A:487:PRO:HA	1:A:490:ARG:HG3	1.94	0.48
1:A:506:ILE:HG13	1:A:507:SER:N	2.27	0.48
1:A:202:ASN:HB3	1:A:339:CYS:SG	2.54	0.48
1:A:302:GLY:O	1:A:303:ALA:HB3	2.14	0.48
1:A:52:ASN:OD1	1:A:55:GLU:HG3	2.14	0.48
1:A:41:PRO:HD3	1:A:257:MSE:SE	2.64	0.48
1:A:62:LYS:O	1:A:165:GLY:HA3	2.13	0.48
1:A:97:ARG:HG2	1:A:171:ASN:OD1	2.13	0.48
1:A:303:ALA:O	1:A:304:TRP:HB2	2.13	0.47
1:B:331:GLN:HE22	1:B:356:GLN:HE21	1.60	0.47
1:B:338:ALA:O	1:B:339:CYS:HB2	2.14	0.47
1:B:451:GLU:OE2	1:B:513:ARG:NH1	2.47	0.47
1:B:456:LEU:HD12	1:B:456:LEU:HA	1.67	0.47
1:A:67:ILE:HD11	1:A:98:VAL:HG21	1.96	0.47
1:A:205:ALA:O	1:A:209:GLN:HG3	2.14	0.47
1:B:54:LEU:O	1:B:58:GLU:HG2	2.15	0.47
1:A:197:MSE:HE2	1:A:395:TYR:C	2.40	0.47
1:B:137:LYS:HB3	1:B:138:PRO:HD3	1.97	0.47
1:B:316:LYS:HE2	1:B:320:GLU:OE1	2.15	0.47
1:A:237:VAL:HG12	1:A:247:TYR:CZ	2.49	0.47
1:A:264:LYS:HD3	1:A:265:TYR:CE1	2.50	0.47
1:A:370:LEU:HD22	1:A:382:GLY:HA2	1.94	0.47
1:B:154:GLU:N	1:B:154:GLU:OE2	2.47	0.47
1:B:199:THR:H	1:B:202:ASN:HD22	1.62	0.47
1:A:6:LYS:HD3	1:B:295:TYR:CD2	2.50	0.47
1:A:197:MSE:HE2	1:A:395:TYR:O	2.14	0.47
1:B:47:PHE:CE1	1:B:59:VAL:HG11	2.49	0.47
1:A:206:ASN:HD21	1:A:341:MSE:HG2	1.80	0.47
1:B:174:VAL:O	1:B:176:PRO:HD3	2.15	0.47
1:A:470:LYS:NZ	1:A:517:PHE:HD1	2.13	0.47
1:B:514:GLU:HB2	2:B:660:HOH:O	2.16	0.46
1:B:255:GLN:HG2	1:B:256:GLU:H	1.80	0.46
1:B:500:GLU:O	1:B:504:GLU:HG3	2.16	0.46
1:A:157:SER:O	1:A:161:VAL:HG23	2.16	0.46
1:B:304:TRP:HA	2:B:620:HOH:O	2.15	0.46
1:B:325:PRO:HG2	1:B:326:ARG:NH1	2.31	0.46
1:B:385:VAL:HA	1:B:416:PHE:O	2.15	0.46
1:A:137:LYS:HB3	1:A:138:PRO:CD	2.32	0.46
1:A:120:ASP:CG	1:A:398:ARG:HH22	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:PRO:HB2	1:A:230:HIS:CD2	2.51	0.46
1:B:478:VAL:HG13	1:B:516:GLU:CB	2.46	0.45
1:A:22:ARG:HG2	1:A:22:ARG:HH11	1.81	0.45
1:A:420:ASP:HB3	1:A:432:PHE:CE1	2.52	0.45
1:B:183:ILE:HG22	1:B:183:ILE:O	2.16	0.45
1:B:461:ALA:HB2	1:B:489:TYR:CD2	2.51	0.45
1:B:494:ASP:OD1	1:B:496:GLU:HB2	2.17	0.45
1:A:468:ILE:HG22	1:A:469:GLY:N	2.31	0.45
1:B:102:PRO:HG2	1:B:182:LEU:HD12	1.98	0.45
1:B:493:VAL:HG23	1:B:493:VAL:O	2.17	0.45
1:A:233:GLU:O	1:A:237:VAL:HG13	2.17	0.45
1:A:459:HIS:C	1:A:461:ALA:H	2.24	0.45
1:B:336:THR:HA	1:B:340:PRO:HB3	1.99	0.45
1:B:350:LEU:O	1:B:353:SER:HB3	2.17	0.45
1:A:85:SER:HA	1:A:249:VAL:HG11	1.99	0.45
1:A:365:LEU:C	1:A:365:LEU:HD23	2.42	0.45
1:A:67:ILE:CG2	1:A:161:VAL:HG11	2.47	0.44
1:A:44:PRO:O	1:A:129:HIS:HE1	2.00	0.44
1:A:306:VAL:HG22	1:A:307:ALA:N	2.32	0.44
1:B:275:PRO:HG3	1:B:304:TRP:HZ2	1.83	0.44
1:A:468:ILE:HD12	1:A:482:PHE:HE1	1.81	0.44
1:B:364:GLU:HG2	1:B:415:PHE:HE1	1.83	0.44
1:A:277:LEU:HD11	1:A:314:LEU:HD22	1.99	0.44
1:A:337:GLU:N	1:A:337:GLU:OE1	2.48	0.44
1:B:468:ILE:HG22	1:B:469:GLY:N	2.32	0.43
1:A:365:LEU:HD23	1:A:366:LYS:N	2.33	0.43
1:B:255:GLN:HG2	1:B:256:GLU:N	2.33	0.43
1:B:303:ALA:HB1	1:B:304:TRP:CE3	2.53	0.43
1:B:486:LYS:O	1:B:487:PRO:C	2.61	0.43
1:B:67:ILE:HG12	1:B:72:VAL:HG21	2.00	0.43
1:A:273:VAL:HG23	1:A:275:PRO:HD2	1.99	0.43
1:A:288:ASN:HD22	1:A:288:ASN:HA	1.65	0.43
1:A:333:TRP:CH2	1:A:335:MSE:HE1	2.53	0.43
1:A:459:HIS:HB3	1:A:462:VAL:HG23	2.01	0.43
1:A:506:ILE:HG13	1:A:507:SER:H	1.84	0.43
1:B:468:ILE:HG22	1:B:469:GLY:H	1.84	0.43
1:A:453:GLU:CG	1:A:467:VAL:HG12	2.49	0.42
1:B:478:VAL:HG13	1:B:516:GLU:HB2	2.00	0.42
1:B:503:ARG:HG2	2:B:660:HOH:O	2.19	0.42
1:A:274:PRO:HB2	1:A:275:PRO:HD3	2.01	0.42
1:A:187:GLY:O	1:A:188:GLY:C	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:VAL:O	1:A:157:SER:HA	2.20	0.42
1:B:339:CYS:N	1:B:340:PRO:CA	2.77	0.42
1:A:230:HIS:HB2	2:A:604:HOH:O	2.20	0.42
1:B:318:ALA:HA	1:B:322:CYS:HB2	2.00	0.42
1:B:281:VAL:HG13	1:B:317:LEU:CD1	2.50	0.42
1:B:302:GLY:O	1:B:303:ALA:HB3	2.20	0.42
1:B:269:PHE:CD2	1:B:269:PHE:C	2.98	0.42
1:A:59:VAL:HG23	1:A:60:THR:N	2.35	0.41
1:A:420:ASP:HB3	1:A:432:PHE:HE1	1.84	0.41
1:A:504:GLU:C	1:A:505:ARG:HG3	2.46	0.41
1:A:458:LYS:HE2	2:A:624:HOH:O	2.21	0.41
1:B:43:PHE:HZ	1:B:252:MSE:HE3	1.85	0.41
1:B:66:GLY:O	1:B:70:LYS:HG2	2.21	0.41
1:B:486:LYS:HE2	1:B:488:GLU:OE1	2.20	0.41
1:A:83:PRO:O	1:A:84:ASN:C	2.63	0.41
1:B:22:ARG:HH22	1:B:208:LEU:CD1	2.33	0.41
1:B:239:LEU:O	1:B:240:MSE:C	2.64	0.41
1:A:102:PRO:HD2	1:A:181:ALA:O	2.21	0.41
1:A:484:VAL:HG13	1:A:522:PRO:HA	2.03	0.41
1:B:281:VAL:HG13	1:B:317:LEU:HD12	2.02	0.41
1:B:206:ASN:HA	1:B:209:GLN:OE1	2.21	0.41
1:A:115:GLU:HB2	1:A:139:VAL:CG2	2.51	0.40
1:B:51:MSE:HA	1:B:55:GLU:OE1	2.20	0.40
1:B:348:LEU:HB2	2:B:587:HOH:O	2.21	0.40
1:A:226:MSE:HE3	1:A:272:ALA:HB1	2.03	0.40
1:B:255:GLN:HG3	1:B:283:THR:OG1	2.22	0.40
1:A:37:ILE:HG21	1:A:265:TYR:CE2	2.56	0.40
1:A:433:GLN:O	1:A:434:ASP:HB2	2.22	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	487/549 (89%)	462 (95%)	21 (4%)	4 (1%)	16	10
1	B	486/549 (88%)	470 (97%)	15 (3%)	1 (0%)	43	44
All	All	973/1098 (89%)	932 (96%)	36 (4%)	5 (0%)	24	20

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	139	VAL
1	A	339	CYS
1	B	339	CYS
1	A	460	GLU
1	A	188	GLY

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	430/453 (95%)	420 (98%)	10 (2%)	44	49
1	B	430/453 (95%)	418 (97%)	12 (3%)	38	40
All	All	860/906 (95%)	838 (97%)	22 (3%)	40	43

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	130	SER
1	A	162	MSE
1	A	237	VAL
1	A	316	LYS
1	A	340	PRO
1	A	354	THR
1	A	392	PHE
1	A	460	GLU
1	A	517	PHE
1	B	2	GLU

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Mol	Chain	Res	Type
1	B	131	MSE
1	B	192	MSE
1	B	252	MSE
1	B	340	PRO
1	B	348	LEU
1	B	368	ILE
1	B	392	PHE
1	B	410	GLU
1	B	456	LEU
1	B	458	LYS
1	B	496	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	129	HIS
1	A	200	HIS
1	A	202	ASN
1	A	206	ASN
1	A	230	HIS
1	A	238	ASN
1	A	282	ASN
1	A	288	ASN
1	B	116	HIS
1	B	119	ASN
1	B	156	ASN
1	B	200	HIS
1	B	238	ASN
1	B	329	HIS
1	B	331	GLN
1	B	345	ASN
1	B	402	ASN
1	B	431	HIS

5.3.3 RNA ⓘ

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	479/549 (87%)	0.68	60 (12%) 8 8	14, 33, 64, 77	0
1	B	477/549 (86%)	0.23	21 (4%) 39 44	13, 25, 61, 72	0
All	All	956/1098 (87%)	0.45	81 (8%) 16 18	13, 29, 63, 77	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	449	PRO	6.2
1	A	522	PRO	6.2
1	B	522	PRO	5.8
1	B	517	PHE	5.0
1	A	191	GLY	4.8
1	B	304	TRP	4.7
1	A	517	PHE	4.4
1	A	450	PHE	4.2
1	A	136	PHE	4.0
1	A	513	ARG	4.0
1	A	521	LEU	3.9
1	B	288	ASN	3.8
1	A	138	PRO	3.6
1	B	449	PRO	3.6
1	B	478	VAL	3.5
1	B	471	PRO	3.5
1	A	141	GLU	3.5
1	B	521	LEU	3.5
1	A	116	HIS	3.5
1	A	468	ILE	3.4
1	A	469	GLY	3.4
1	A	462	VAL	3.4
1	A	466	ALA	3.3
1	A	190	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	518	VAL	3.2
1	A	470	LYS	3.2
1	A	188	GLY	3.2
1	A	155	VAL	3.1
1	A	189	THR	3.1
1	B	437	LYS	3.1
1	A	187	GLY	3.1
1	A	493	VAL	3.1
1	A	471	PRO	3.0
1	A	487	PRO	3.0
1	A	455	LEU	3.0
1	A	114	LEU	3.0
1	A	373	GLY	3.0
1	A	467	VAL	2.8
1	B	436	VAL	2.8
1	B	487	PRO	2.8
1	A	402	ASN	2.8
1	A	193	PRO	2.8
1	B	515	VAL	2.7
1	A	399	GLU	2.6
1	A	459	HIS	2.6
1	B	513	ARG	2.6
1	A	472	ASP	2.6
1	A	139	VAL	2.6
1	A	515	VAL	2.5
1	A	71	GLY	2.5
1	A	454	ALA	2.5
1	A	479	PRO	2.5
1	B	187	GLY	2.5
1	A	465	VAL	2.4
1	A	451	GLU	2.4
1	B	507	SER	2.4
1	A	491	GLY	2.4
1	A	460	GLU	2.4
1	A	489	TYR	2.4
1	B	499	ILE	2.3
1	B	479	PRO	2.3
1	A	452	LEU	2.2
1	B	13	TYR	2.2
1	A	483	ILE	2.2
1	B	191	GLY	2.2
1	A	514	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	488	GLU	2.2
1	A	140	LEU	2.2
1	A	161	VAL	2.2
1	A	110	LYS	2.2
1	A	403	GLN	2.1
1	A	370	LEU	2.1
1	A	461	ALA	2.1
1	A	167	GLU	2.1
1	B	489	TYR	2.1
1	A	164	SER	2.1
1	A	502	VAL	2.1
1	A	134	GLU	2.0
1	A	133	TYR	2.0
1	A	137	LYS	2.0
1	A	377	GLY	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.