



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:17 AM UTC

PDB ID : 1H4F / pdb_00001h4f
Title : E. COLI BETA-KETOACYL [ACYL CARRIER PROTEIN] SYNTHASE I
K328R
Authors : Olsen, J.G.; von Wettstein-Knowles, P.; Mcguire, K.A.; Henriksen, A.
Deposited on : 2003-02-26
Resolution : 2.00 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

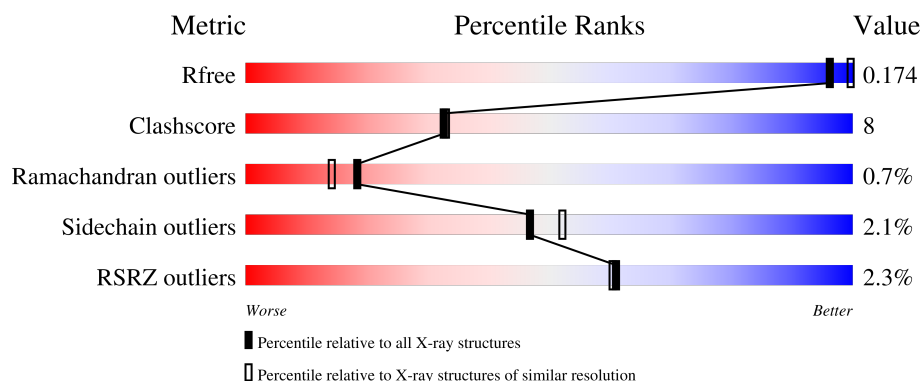
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	406	3% 80% 18% .
1	B	406	% 83% 14% .
1	C	406	2% 83% 15% .
1	D	406	2% 84% 13% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12848 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.

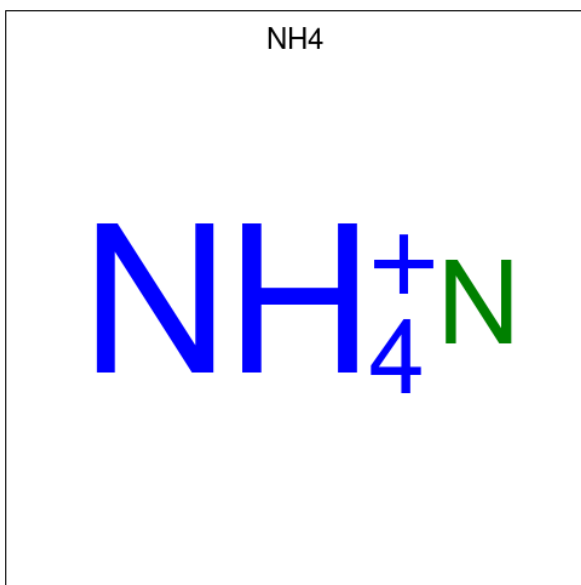
- Molecule 1 is a protein called 3-OXOACYL-[ACYL-CARRIER-PROTEIN] SYNTHASE I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	406	Total	C	N	O	S	0	0	1
			2975	1849	521	582	23			
1	B	406	Total	C	N	O	S	0	0	0
			2983	1853	521	586	23			
1	C	406	Total	C	N	O	S	0	0	0
			2983	1853	521	586	23			
1	D	406	Total	C	N	O	S	0	0	1
			2975	1849	521	582	23			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	328	ARG	LYS	engineered mutation	UNP P14926
B	328	ARG	LYS	engineered mutation	UNP P14926
C	328	ARG	LYS	engineered mutation	UNP P14926
D	328	ARG	LYS	engineered mutation	UNP P14926

- Molecule 2 is AMMONIUM ION (CCD ID: NH4) (formula: H₄N).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total N 1 1	0	0
2	B	1	Total N 1 1	0	0
2	C	1	Total N 1 1	0	0
2	D	1	Total N 1 1	0	0

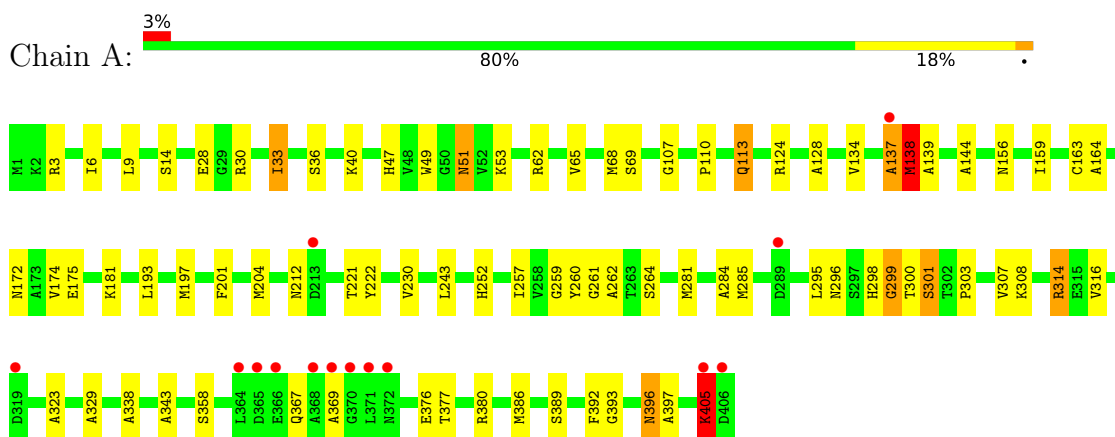
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	223	Total O 223 223	0	0
3	B	265	Total O 265 265	0	0
3	C	250	Total O 250 250	0	0
3	D	190	Total O 190 190	0	0

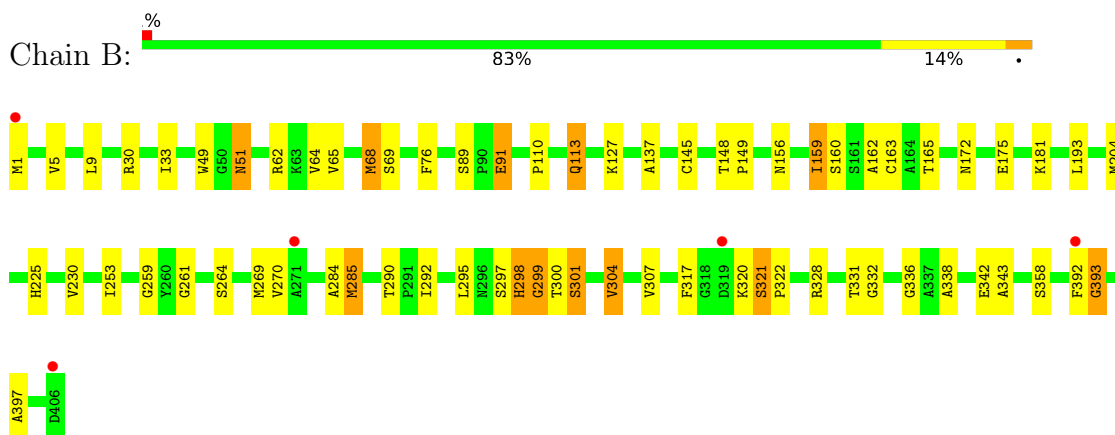
3 Residue-property plots [i](#)

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.

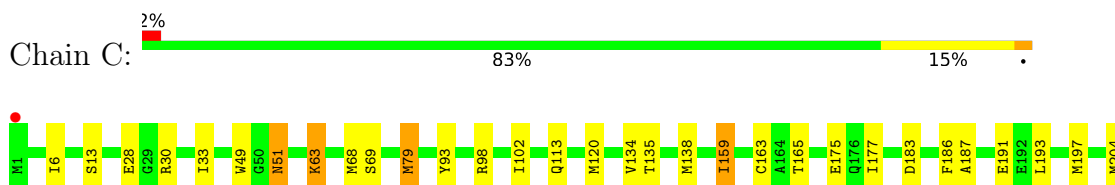
• Molecule 1: 3-OXOACYL-[ACYL-CARRIER-PROTEIN] SYNTHASE I

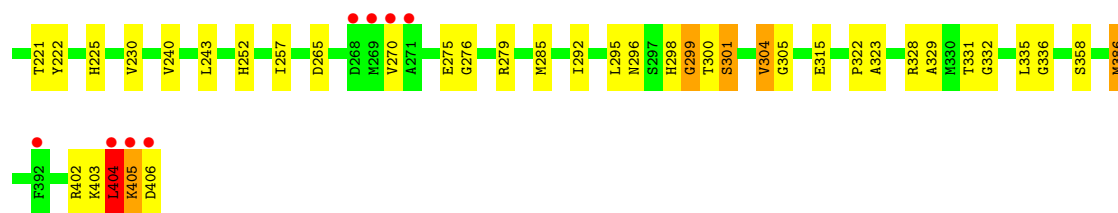


• Molecule 1: 3-OXOACYL-[ACYL-CARRIER-PROTEIN] SYNTHASE I

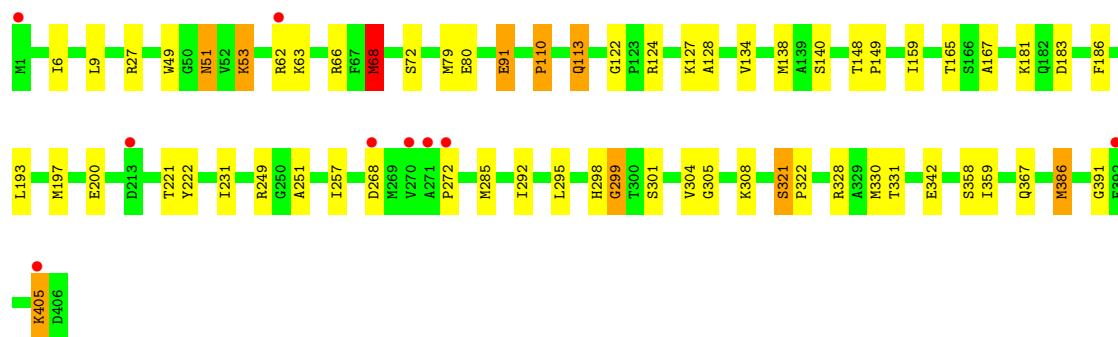
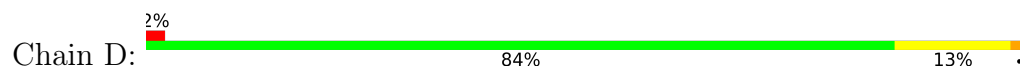


• Molecule 1: 3-OXOACYL-[ACYL-CARRIER-PROTEIN] SYNTHASE I





● Molecule 1: 3-OXOACYL-[ACYL-CARRIER-PROTEIN] SYNTHASE I



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	58.93Å 139.04Å 211.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.94 – 2.00 29.94 – 2.00	Depositor EDS
% Data completeness (in resolution range)	90.1 (29.94-2.00) 90.0 (29.94-2.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 1.82Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.178 , 0.227 0.175 , 0.174	Depositor DCC
R_{free} test set	6894 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	17.9	Xtriage
Anisotropy	0.431	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 51.4	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	0.95	EDS
Total number of atoms	12848	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 2.90% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NH4

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	0.83	1/3023 (0.0%)	1.11	15/4084 (0.4%)
1	B	0.83	1/3031 (0.0%)	1.12	18/4093 (0.4%)
1	C	0.86	4/3031 (0.1%)	1.11	13/4093 (0.3%)
1	D	0.83	2/3023 (0.1%)	1.08	11/4084 (0.3%)
All	All	0.84	8/12108 (0.1%)	1.11	57/16354 (0.3%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	120	MET	SD-CE	8.44	2.00	1.79
1	D	386	MET	SD-CE	-6.51	1.63	1.79
1	D	68	MET	SD-CE	-5.85	1.65	1.79
1	A	405	LYS	C-N	-5.31	1.25	1.33
1	B	285	MET	SD-CE	5.30	1.92	1.79
1	C	386	MET	SD-CE	-5.23	1.66	1.79
1	C	79	MET	SD-CE	5.17	1.92	1.79
1	C	197	MET	SD-CE	-5.16	1.66	1.79

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	137	ALA	N-CA-C	-8.85	96.14	109.86
1	D	68	MET	N-CA-C	8.76	123.88	109.95
1	A	68	MET	N-CA-C	8.31	123.39	109.76
1	B	68	MET	N-CA-C	8.23	123.25	109.76
1	C	68	MET	N-CA-C	7.11	121.62	110.17
1	A	252	HIS	N-CA-C	-7.08	97.69	108.96
1	C	243	LEU	N-CA-C	6.80	119.27	111.11
1	B	113	GLN	N-CA-C	-6.79	103.96	111.36
1	D	113	GLN	N-CA-C	-6.78	103.98	111.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	69	SER	N-CA-C	-6.74	100.49	110.46
1	A	343	ALA	N-CA-C	-6.60	104.17	111.36
1	C	159	ILE	N-CA-C	-6.54	98.84	108.97
1	B	332	GLY	N-CA-C	-6.46	101.84	112.83
1	A	243	LEU	N-CA-C	6.39	118.78	111.11
1	C	270	VAL	N-CA-C	6.35	117.04	111.90
1	B	297	SER	N-CA-C	6.17	118.67	110.53
1	D	391	GLY	N-CA-C	6.11	122.73	113.02
1	B	393	GLY	N-CA-C	-6.10	106.82	115.30
1	D	331	THR	N-CA-C	5.98	120.86	113.50
1	C	331	THR	N-CA-C	5.98	120.73	112.90
1	A	358	SER	N-CA-C	-5.95	98.83	108.41
1	C	332	GLY	N-CA-C	-5.95	102.72	112.83
1	C	134	VAL	N-CA-C	5.82	116.56	110.62
1	C	323	ALA	N-CA-C	-5.81	101.81	110.23
1	D	122	GLY	CA-C-N	5.75	125.42	119.56
1	D	122	GLY	C-N-CA	5.75	125.42	119.56
1	B	137	ALA	N-CA-C	5.74	119.46	112.23
1	B	331	THR	N-CA-C	5.70	120.51	113.50
1	B	338	ALA	N-CA-C	5.68	117.47	111.28
1	A	260	TYR	CA-C-N	-5.68	117.30	122.80
1	A	260	TYR	C-N-CA	-5.68	117.30	122.80
1	A	338	ALA	N-CA-C	5.64	117.43	111.28
1	B	304	VAL	N-CA-C	5.62	115.71	110.42
1	B	343	ALA	N-CA-C	-5.54	105.32	111.36
1	B	159	ILE	N-CA-C	-5.47	100.58	108.89
1	C	93	TYR	N-CA-C	5.46	120.21	113.50
1	D	183	ASP	N-CA-C	-5.38	106.85	113.41
1	A	69	SER	N-CA-C	-5.27	102.66	110.46
1	D	167	ALA	N-CA-C	-5.26	105.63	111.36
1	D	358	SER	N-CA-C	-5.25	98.75	107.99
1	B	298	HIS	N-CA-C	-5.21	105.28	111.69
1	C	304	VAL	N-CA-C	5.20	115.31	110.42
1	A	393	GLY	N-CA-C	-5.19	108.11	115.43
1	A	323	ALA	N-CA-C	-5.18	102.61	110.28
1	B	69	SER	N-CA-C	-5.17	102.35	110.36
1	A	396	ASN	N-CA-C	5.15	117.79	109.40
1	C	252	HIS	N-CA-C	-5.10	100.85	108.96
1	B	358	SER	N-CA-C	-5.09	99.03	107.99
1	B	317	PHE	N-CA-C	5.09	119.76	113.50
1	B	290	THR	CA-C-N	-5.09	115.33	120.31
1	B	290	THR	C-N-CA	-5.09	115.33	120.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	162	ALA	CB-CA-C	-5.08	110.70	116.54
1	A	33	ILE	N-CA-C	5.07	115.58	108.89
1	C	296	ASN	N-CA-C	-5.05	100.27	108.41
1	D	80	GLU	N-CA-C	-5.04	105.68	111.07
1	A	159	ILE	N-CA-C	-5.04	101.23	108.89
1	D	110	PRO	N-CA-C	-5.02	106.55	113.53

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	2975	0	2935	66	0
1	B	2983	0	2939	46	0
1	C	2983	0	2939	43	0
1	D	2975	0	2935	48	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	223	0	0	5	0
3	B	265	0	0	7	0
3	C	250	0	0	4	0
3	D	190	0	0	5	0
All	All	12848	0	11748	186	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 8.

All (186) 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:113:GLN:OE1	1:B:113:GLN:NE2	1.91	1.02
1:A:314:ARG:HH11	1:A:314:ARG:HB2	1.17	1.02

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:204:MET:HE2	1:D:134:VAL:HG21	1.46	0.96
1:C:402:ARG:HE	1:C:404:LEU:HD12	1.36	0.87
1:A:314:ARG:HB2	1:A:314:ARG:NH1	1.90	0.86
1:C:51:ASN:HD22	1:C:51:ASN:H	1.26	0.83
1:D:124:ARG:HH21	1:D:127:LYS:HZ3	1.27	0.82
1:B:51:ASN:H	1:B:51:ASN:HD22	1.26	0.81
1:A:51:ASN:H	1:A:51:ASN:HD22	1.30	0.79
1:D:51:ASN:H	1:D:51:ASN:HD22	1.30	0.78
1:A:137:ALA:O	1:A:138:MET:HB3	1.83	0.78
1:C:177:ILE:HD12	1:C:240:VAL:HG12	1.72	0.71
1:C:6:ILE:HD11	1:C:257:ILE:HD11	1.72	0.71
1:C:28:GLU:OE2	1:C:30:ARG:NH1	2.25	0.70
1:A:134:VAL:O	1:A:138:MET:HB3	1.91	0.69
1:B:30:ARG:NH1	3:B:2049:HOH:O	2.25	0.69
1:B:321:SER:HB3	3:B:2233:HOH:O	1.93	0.68
1:C:63:LYS:H	1:C:63:LYS:HD3	1.59	0.68
1:D:268:ASP:HB3	3:D:2137:HOH:O	1.93	0.67
1:A:307:VAL:HG22	1:A:367:GLN:HG3	1.78	0.65
1:A:281:MET:HE3	1:A:316:VAL:HG21	1.77	0.65
1:A:295:LEU:C	1:A:295:LEU:HD23	2.22	0.65
1:A:172:ASN:HD21	1:B:172:ASN:ND2	1.95	0.64
1:B:285:MET:SD	1:B:292:ILE:HD11	2.36	0.64
1:B:148:THR:HB	1:B:149:PRO:HD3	1.79	0.64
1:D:91:GLU:H	1:D:91:GLU:CD	2.05	0.64
1:B:68:MET:HE1	1:B:76:PHE:HB2	1.78	0.64
1:A:6:ILE:HD11	1:A:257:ILE:HD11	1.78	0.63
1:D:68:MET:HB3	1:D:72:SER:HB2	1.80	0.63
1:D:51:ASN:HD22	1:D:51:ASN:N	1.90	0.63
1:C:403:LYS:O	1:C:404:LEU:HD22	1.99	0.62
1:D:405:LYS:HD3	1:D:405:LYS:H	1.65	0.62
1:D:295:LEU:C	1:D:295:LEU:HD23	2.25	0.61
1:D:63:LYS:NZ	3:D:2049:HOH:O	2.34	0.61
1:A:204:MET:HE1	1:A:392:PHE:CZ	2.36	0.61
1:A:137:ALA:O	1:A:138:MET:CB	2.48	0.61
1:C:30:ARG:NH2	3:C:2049:HOH:O	2.32	0.61
1:D:292:ILE:O	1:D:322:PRO:HB3	2.01	0.61
1:B:62:ARG:HD3	1:B:62:ARG:C	2.26	0.60
1:B:49:TRP:CE3	1:B:193:LEU:HG	2.36	0.60
1:A:285:MET:SD	1:A:386:MET:HE1	2.42	0.59
1:B:1:MET:HB3	3:B:2002:HOH:O	2.01	0.59
1:B:91:GLU:H	1:B:91:GLU:CD	2.10	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:148:THR:HB	1:D:149:PRO:HD3	1.84	0.59
1:A:307:VAL:HG13	1:A:367:GLN:HG3	1.86	0.58
1:B:51:ASN:H	1:B:51:ASN:ND2	2.00	0.57
1:A:40:LYS:HE2	1:A:47:HIS:CE1	2.39	0.57
1:C:300:THR:O	1:C:301:SER:CB	2.52	0.57
1:B:225:HIS:HD2	3:B:2177:HOH:O	1.87	0.57
1:D:51:ASN:H	1:D:51:ASN:ND2	2.00	0.57
1:A:175:GLU:OE1	1:B:181:LYS:NZ	2.27	0.57
1:C:33:ILE:HD12	1:C:230:VAL:HG11	1.87	0.57
1:A:51:ASN:HD22	1:A:51:ASN:N	1.99	0.56
1:A:51:ASN:ND2	1:A:53:LYS:HE3	2.21	0.56
1:D:49:TRP:CE3	1:D:193:LEU:HG	2.41	0.56
1:A:110:PRO:HG3	3:B:2132:HOH:O	2.06	0.55
1:A:307:VAL:CG2	1:A:367:GLN:HG3	2.36	0.55
1:B:89:SER:OG	1:B:91:GLU:HG2	2.06	0.55
1:D:272:PRO:HG2	1:D:308:LYS:HG3	1.87	0.55
1:D:330:MET:HG2	1:D:359:ILE:HD13	1.88	0.54
1:A:124:ARG:HB2	1:A:128:ALA:HB2	1.88	0.53
1:A:9:LEU:C	1:A:9:LEU:HD12	2.34	0.53
1:A:28:GLU:HG3	1:A:30:ARG:HB2	1.91	0.53
1:C:405:LYS:HB3	1:C:405:LYS:NZ	2.24	0.53
1:A:3:ARG:HH22	1:A:405:LYS:HE2	1.74	0.53
1:D:124:ARG:HH21	1:D:127:LYS:NZ	2.03	0.53
1:A:110:PRO:HG2	1:A:197:MET:HB2	1.91	0.53
1:A:174:VAL:HG21	1:A:257:ILE:HG21	1.91	0.53
1:D:367:GLN:O	1:D:367:GLN:HG3	2.08	0.52
1:B:9:LEU:C	1:B:9:LEU:HD12	2.35	0.52
1:B:298:HIS:O	1:B:299:GLY:C	2.52	0.52
1:C:295:LEU:HD23	1:C:295:LEU:C	2.34	0.52
1:C:329:ALA:HB3	3:C:2207:HOH:O	2.09	0.52
1:C:51:ASN:HD22	1:C:51:ASN:N	2.02	0.52
1:C:113:GLN:NE2	1:D:200:GLU:OE2	2.43	0.52
1:A:49:TRP:CE3	1:A:193:LEU:HG	2.45	0.52
1:C:292:ILE:O	1:C:322:PRO:HB3	2.10	0.51
1:D:328:ARG:NH1	1:D:342:GLU:OE2	2.44	0.51
1:C:159:ILE:CD1	1:D:159:ILE:HG12	2.41	0.51
1:C:51:ASN:H	1:C:51:ASN:ND2	2.04	0.51
1:C:165:THR:HB	1:C:336:GLY:HA2	1.92	0.50
1:A:201:PHE:HE1	1:A:392:PHE:HE2	1.59	0.50
1:A:221:THR:O	1:A:222:TYR:HB2	2.11	0.50
1:A:262:ALA:HA	1:A:396:ASN:O	2.11	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:175:GLU:OE1	1:D:181:LYS:NZ	2.45	0.49
1:D:124:ARG:HB2	1:D:128:ALA:HB2	1.94	0.49
1:C:225:HIS:CD2	3:C:2165:HOH:O	2.65	0.49
1:D:6:ILE:HD11	1:D:257:ILE:HD11	1.95	0.49
1:C:265:ASP:OD1	1:C:276:GLY:HA3	2.13	0.49
1:A:300:THR:O	1:A:301:SER:CB	2.61	0.49
1:A:307:VAL:CG1	1:A:367:GLN:HG3	2.43	0.49
1:C:177:ILE:CD1	1:C:240:VAL:HG12	2.41	0.48
1:D:51:ASN:HA	1:D:193:LEU:CD2	2.44	0.48
1:A:139:ALA:HB3	1:B:160:SER:OG	2.13	0.48
1:A:172:ASN:HD21	1:B:172:ASN:HD21	1.59	0.48
1:B:68:MET:HE1	1:B:76:PHE:CB	2.43	0.48
1:B:261:GLY:O	1:B:397:ALA:HA	2.14	0.48
1:A:113:GLN:NE2	1:B:110:PRO:HG3	2.29	0.48
1:D:285:MET:SD	1:D:386:MET:HE1	2.54	0.47
1:A:298:HIS:O	1:A:299:GLY:C	2.57	0.47
1:A:156:ASN:HB2	1:B:264:SER:HB2	1.96	0.47
1:C:328:ARG:HH11	1:C:328:ARG:HG3	1.80	0.47
1:A:33:ILE:HD12	1:A:230:VAL:HG11	1.96	0.47
1:D:328:ARG:HG2	1:D:328:ARG:HH11	1.80	0.46
1:A:181:LYS:NZ	1:B:175:GLU:OE1	2.47	0.46
1:D:51:ASN:HA	1:D:193:LEU:HD23	1.97	0.46
1:D:193:LEU:HD11	1:D:231:ILE:HG23	1.97	0.46
1:D:221:THR:O	1:D:222:TYR:HB2	2.16	0.46
1:A:47:HIS:H	1:A:212:ASN:ND2	2.13	0.46
1:C:402:ARG:NE	1:C:404:LEU:HD12	2.16	0.46
1:B:270:VAL:HG12	1:B:392:PHE:HD2	1.80	0.46
1:B:295:LEU:C	1:B:295:LEU:HD23	2.41	0.46
1:C:79:MET:HE3	1:C:186:PHE:CD1	2.51	0.46
1:D:53:LYS:N	1:D:53:LYS:HD3	2.30	0.46
1:C:298:HIS:O	1:C:299:GLY:C	2.59	0.45
1:B:33:ILE:HD12	1:B:230:VAL:HG11	1.99	0.45
1:A:300:THR:O	1:A:301:SER:HB3	2.15	0.45
1:A:314:ARG:HH11	1:A:314:ARG:CB	2.07	0.45
1:B:5:VAL:HB	1:B:253:ILE:HG23	1.97	0.45
1:C:221:THR:O	1:C:222:TYR:HB2	2.17	0.45
1:C:406:ASP:OD2	1:C:406:ASP:N	2.49	0.45
1:A:14:SER:O	1:A:53:LYS:NZ	2.47	0.45
1:B:259:GLY:HA3	1:B:284:ALA:O	2.16	0.45
1:C:191:GLU:HG2	1:C:335:LEU:HB2	1.99	0.45
1:C:404:LEU:O	1:C:405:LYS:HB3	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:ALA:C	1:B:269:MET:HE1	2.42	0.44
1:D:110:PRO:HA	1:D:113:GLN:NE2	2.32	0.44
1:A:62:ARG:HA	1:A:65:VAL:HG12	2.00	0.44
1:B:68:MET:HG2	1:B:145:CYS:HB3	1.99	0.44
1:A:295:LEU:C	1:A:295:LEU:CD2	2.90	0.44
1:B:204:MET:HE1	1:B:270:VAL:HG11	1.99	0.44
1:C:33:ILE:HG13	3:C:2161:HOH:O	2.18	0.44
1:A:51:ASN:HD21	1:A:53:LYS:HE3	1.81	0.44
1:A:124:ARG:NH1	3:A:2111:HOH:O	2.50	0.43
1:C:204:MET:HE2	1:D:134:VAL:CG2	2.32	0.43
1:D:308:LYS:HD3	1:D:308:LYS:HA	1.82	0.43
1:A:164:ALA:HA	1:A:389:SER:HB3	2.01	0.43
1:B:292:ILE:O	1:B:322:PRO:HB3	2.18	0.43
1:B:64:VAL:HG13	1:B:149:PRO:HG3	1.99	0.43
1:D:62:ARG:O	1:D:66:ARG:HB2	2.18	0.43
1:D:159:ILE:O	1:D:165:THR:HG23	2.19	0.43
1:D:79:MET:HE3	1:D:186:PHE:CG	2.54	0.43
1:C:135:THR:HA	1:C:138:MET:HE2	2.01	0.43
1:D:298:HIS:O	1:D:299:GLY:C	2.60	0.43
1:A:124:ARG:NH2	3:A:2112:HOH:O	2.49	0.43
1:C:328:ARG:HG3	1:C:328:ARG:NH1	2.34	0.43
1:D:27:ARG:HD2	3:D:2020:HOH:O	2.19	0.43
1:A:329:ALA:HB3	3:A:2201:HOH:O	2.19	0.42
1:C:304:VAL:HG23	1:C:305:GLY:H	1.84	0.42
1:A:113:GLN:NE2	1:A:137:ALA:HB1	2.34	0.42
1:C:49:TRP:CE3	1:C:193:LEU:HG	2.55	0.42
1:D:9:LEU:C	1:D:9:LEU:HD12	2.45	0.42
1:A:144:ALA:HB1	1:B:393:GLY:HA3	2.01	0.42
1:D:321:SER:HB3	3:D:2176:HOH:O	2.19	0.42
1:C:275:GLU:OE2	1:C:279:ARG:NE	2.42	0.42
1:A:261:GLY:O	1:A:397:ALA:HA	2.19	0.42
1:B:304:VAL:O	1:B:307:VAL:HG22	2.19	0.41
1:C:403:LYS:O	1:C:404:LEU:C	2.63	0.41
1:D:138:MET:HE3	1:D:140:SER:OG	2.19	0.41
1:D:249:ARG:CZ	1:D:251:ALA:HB2	2.50	0.41
1:A:380:ARG:NH1	3:A:2209:HOH:O	2.53	0.41
1:B:165:THR:HB	1:B:336:GLY:HA2	2.02	0.41
1:B:320:LYS:NZ	3:B:2232:HOH:O	2.54	0.41
1:B:328:ARG:NH1	1:B:342:GLU:OE2	2.53	0.41
1:D:51:ASN:N	1:D:51:ASN:ND2	2.61	0.41
1:D:304:VAL:O	1:D:305:GLY:C	2.64	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:GLU:O	1:A:377:THR:C	2.63	0.41
1:A:107:GLY:HA2	3:B:2143:HOH:O	2.20	0.41
1:A:259:GLY:HA3	1:A:284:ALA:O	2.19	0.41
1:A:264:SER:HB2	1:B:156:ASN:HB2	2.02	0.41
1:B:300:THR:O	1:B:301:SER:CB	2.69	0.41
1:A:281:MET:HE3	1:A:316:VAL:CG2	2.49	0.41
1:D:79:MET:HE3	1:D:186:PHE:CD1	2.56	0.41
1:C:98:ARG:HE	1:C:183:ASP:CG	2.29	0.40
3:A:2132:HOH:O	1:B:160:SER:HB2	2.21	0.40
1:D:110:PRO:HG2	1:D:197:MET:HB2	2.03	0.40
1:A:51:ASN:H	1:A:51:ASN:ND2	2.05	0.40
1:A:156:ASN:CB	1:B:264:SER:HB2	2.51	0.40
1:A:308:LYS:HA	1:A:308:LYS:HD3	1.85	0.40
1:B:62:ARG:HH11	1:B:62:ARG:HG2	1.87	0.40
1:C:102:ILE:O	1:C:187:ALA:HA	2.20	0.40
1:A:36:SER:HB2	1:A:49:TRP:CE2	2.57	0.40
1:A:295:LEU:HD23	1:A:296:ASN:N	2.37	0.40
1:B:159:ILE:HD11	1:B:172:ASN:CG	2.47	0.40
1:C:285:MET:SD	1:C:386:MET:HE1	2.62	0.40
1:D:251:ALA:HB1	3:D:2005:HOH:O	2.20	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	404/406 (100%)	384 (95%)	15 (4%)	5 (1%)	10	6
1	B	404/406 (100%)	386 (96%)	16 (4%)	2 (0%)	24	21
1	C	404/406 (100%)	390 (96%)	11 (3%)	3 (1%)	18	14
1	D	404/406 (100%)	388 (96%)	14 (4%)	2 (0%)	24	21
All	All	1616/1624 (100%)	1548 (96%)	56 (4%)	12 (1%)	18	14

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	404	LEU
1	A	299	GLY
1	B	299	GLY
1	C	299	GLY
1	C	301	SER
1	D	299	GLY
1	A	301	SER
1	A	369	ALA
1	D	301	SER
1	B	301	SER
1	A	138	MET
1	A	303	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	308/309 (100%)	302 (98%)	6 (2%)	50	56
1	B	309/309 (100%)	303 (98%)	6 (2%)	50	56
1	C	309/309 (100%)	301 (97%)	8 (3%)	40	44
1	D	308/309 (100%)	302 (98%)	6 (2%)	50	56
All	All	1234/1236 (100%)	1208 (98%)	26 (2%)	47	52

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	113	GLN
1	A	138	MET
1	A	163	CYS
1	A	314	ARG
1	A	405	LYS
1	B	51	ASN
1	B	65	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	91	GLU
1	B	127	LYS
1	B	163	CYS
1	B	321	SER
1	C	13	SER
1	C	51	ASN
1	C	63	LYS
1	C	163	CYS
1	C	315	GLU
1	C	358	SER
1	C	404	LEU
1	C	405	LYS
1	D	51	ASN
1	D	53	LYS
1	D	68	MET
1	D	91	GLU
1	D	321	SER
1	D	405	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	ASN
1	A	51	ASN
1	A	95	ASN
1	A	113	GLN
1	A	176	GLN
1	A	212	ASN
1	A	225	HIS
1	A	360	ASN
1	A	367	GLN
1	A	396	ASN
1	B	19	GLN
1	B	37	GLN
1	B	51	ASN
1	B	94	GLN
1	B	113	GLN
1	B	172	ASN
1	B	176	GLN
1	B	225	HIS
1	B	372	ASN
1	B	396	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	51	ASN
1	C	94	GLN
1	C	225	HIS
1	C	252	HIS
1	C	372	ASN
1	C	396	ASN
1	D	20	GLN
1	D	51	ASN
1	D	94	GLN
1	D	113	GLN
1	D	341	GLN
1	D	367	GLN
1	D	396	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 4 are modelled with single atom - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	406/406 (100%)	-0.16	14 (3%) 48 47	6, 19, 39, 55	0
1	B	406/406 (100%)	-0.64	5 (1%) 76 76	4, 13, 30, 55	0
1	C	406/406 (100%)	-0.55	9 (2%) 62 61	6, 15, 30, 70	0
1	D	406/406 (100%)	-0.22	9 (2%) 62 61	8, 18, 34, 54	0
All	All	1624/1624 (100%)	-0.39	37 (2%) 61 60	4, 16, 35, 70	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	404	LEU	7.0
1	C	406	ASP	5.5
1	D	271	ALA	5.3
1	D	270	VAL	4.7
1	C	270	VAL	4.3
1	A	406	ASP	3.9
1	B	406	ASP	3.7
1	A	319	ASP	3.3
1	C	405	LYS	3.2
1	D	213	ASP	3.2
1	D	268	ASP	3.2
1	D	405	LYS	3.0
1	C	271	ALA	2.9
1	A	371	LEU	2.8
1	D	392	PHE	2.7
1	A	370	GLY	2.7
1	C	392	PHE	2.7
1	C	1	MET	2.7
1	A	372	ASN	2.6
1	A	405	LYS	2.5
1	A	365	ASP	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	369	ALA	2.4
1	D	1	MET	2.4
1	C	269	MET	2.4
1	A	368	ALA	2.3
1	B	392	PHE	2.3
1	B	319	ASP	2.2
1	D	62	ARG	2.2
1	C	268	ASP	2.2
1	A	289	ASP	2.2
1	B	271	ALA	2.1
1	A	364	LEU	2.0
1	D	272	PRO	2.0
1	A	366	GLU	2.0
1	B	1	MET	2.0
1	A	137	ALA	2.0
1	A	213	ASP	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NH4	A	1406	1/1	0.94	0.10	17,17,17,17	0
2	NH4	C	1407	1/1	0.96	0.05	10,10,10,10	0
2	NH4	D	1406	1/1	0.97	0.09	12,12,12,12	0
2	NH4	B	1407	1/1	0.98	0.05	9,9,9,9	0

6.5 Other polymers [i](#)

There are no such residues in this entry.