



# Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2020 – 07:44 pm BST

PDB ID : 1H4F  
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](mailto: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.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

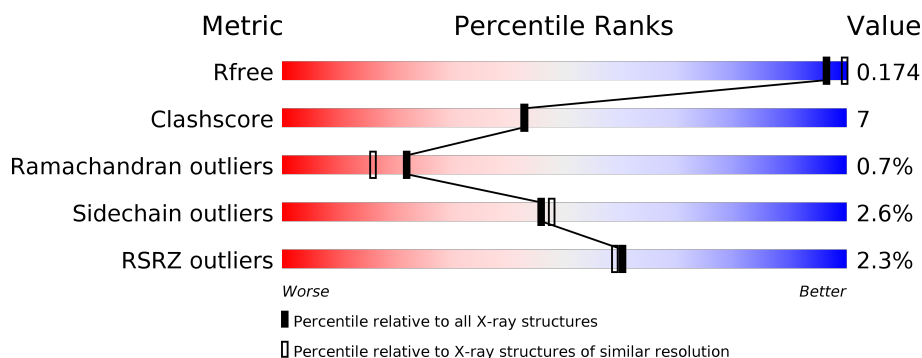
# 1 Overall quality at a glance

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))
$R_{free}$	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	<div> <div>4%</div> <div> <div></div> <div>85%</div> <div>13%</div> <div>•</div> </div> </div>
1	B	406	<div> <div></div> <div> <div>87%</div> <div>12%</div> <div>•</div> </div> </div>
1	C	406	<div> <div>2%</div> <div> <div></div> <div>88%</div> <div>11%</div> <div>•</div> </div> </div>
1	D	406	<div> <div>3%</div> <div> <div></div> <div>89%</div> <div>10%</div> <div>•</div> </div> </div>

## 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 (three-letter code: NH4) (formula: H<sub>4</sub>N).



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

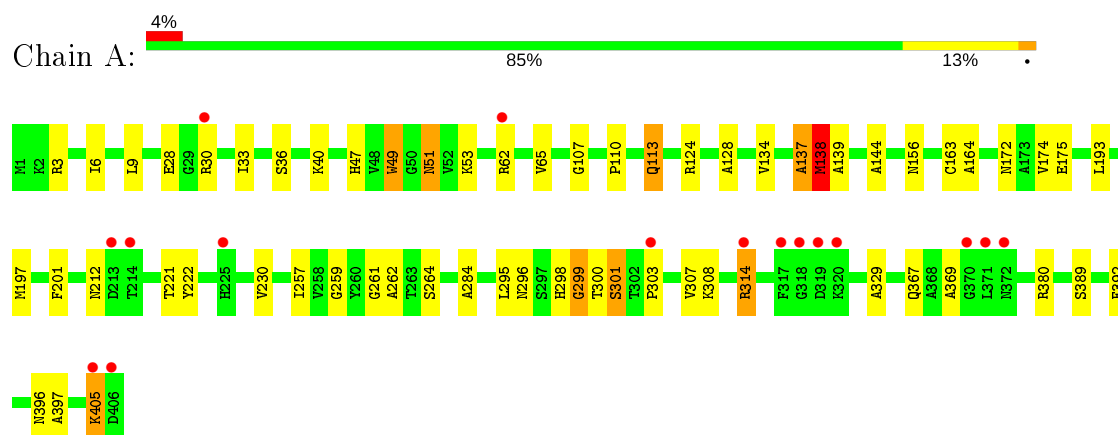
- Molecule 3 is water.

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

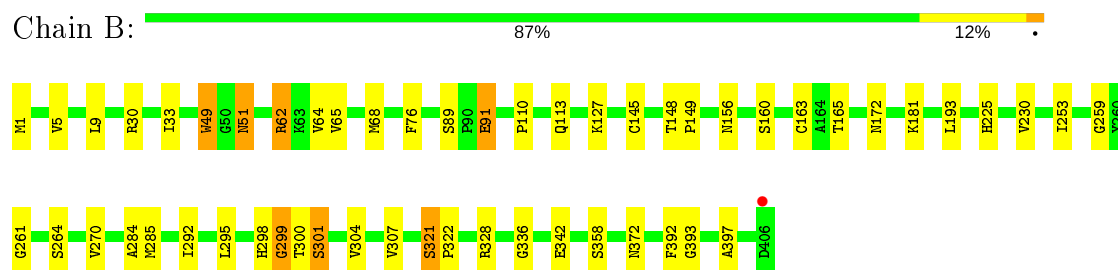
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

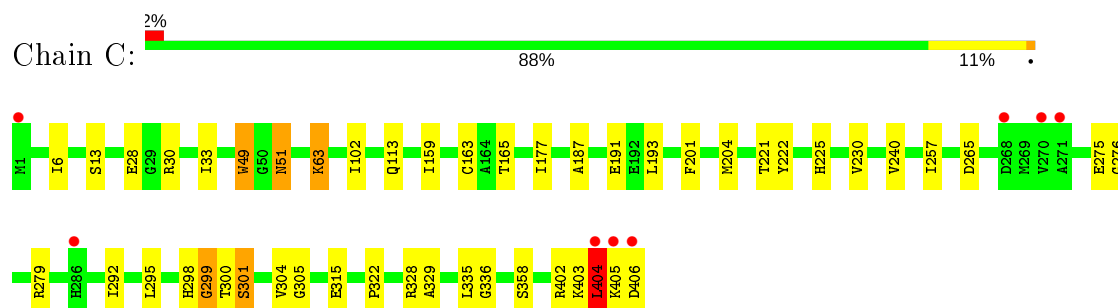
#### • Molecule 1: 3-OXOACYL-[ACYL-CARRIER-PROTEIN] SYNTHASE I



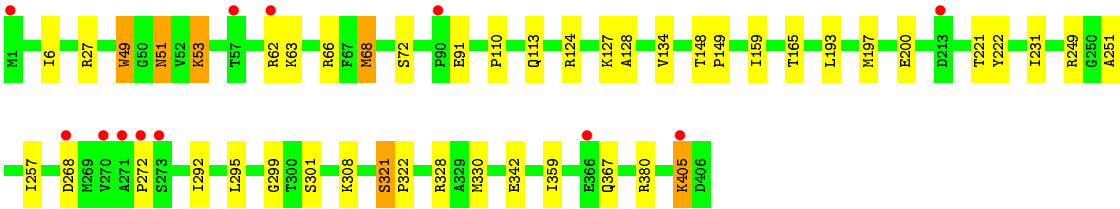
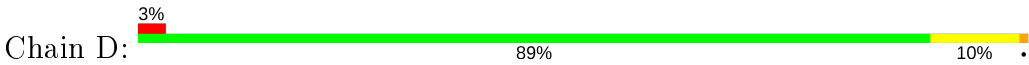
#### • Molecule 1: 3-OXOACYL-[ACYL-CARRIER-PROTEIN] SYNTHASE I



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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	58.93Å 139.04Å 211.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.94 – 2.00 29.94 – 1.82	Depositor EDS
% Data completeness (in resolution range)	90.1 (29.94-2.00) 87.4 (29.94-1.82)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 <sup>2</sup> )	17.9	Xtriage
Anisotropy	0.431	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 51.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.66	0/3023	0.79	1/4084 (0.0%)
1	B	0.69	0/3031	0.81	0/4093
1	C	0.69	0/3031	0.80	0/4093
1	D	0.65	0/3023	0.78	0/4084
All	All	0.67	0/12108	0.79	1/16354 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	137	ALA	N-CA-C	-5.50	96.14	111.00

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	2975	0	2935	58	0
1	B	2983	0	2939	40	0
1	C	2983	0	2939	38	0
1	D	2975	0	2935	40	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	6	0
3	C	250	0	0	4	0
3	D	190	0	0	5	0
All	All	12848	0	11748	162	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 7.

All (162) 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:HB2	1:A:314:ARG:HH11	1.17	1.02
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:H	1:C:51:ASN:HD22	1.26	0.83
1:B:51:ASN:HD22	1:B:51:ASN:H	1.26	0.81
1:A:51:ASN:H	1:A:51:ASN:HD22	1.30	0.79
1:D:51:ASN:HD22	1:D:51:ASN:H	1.30	0.78
1:A:137:ALA:O	1:A:138:MET:HB3	1.83	0.78
1:D:124:ARG:HH21	1:D:127:LYS:HZ3	1.35	0.74
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: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: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:N	1:D:51:ASN:HD22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:63:LYS:NZ	3:D:2049:HOH:O	2.34	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:A:295:LEU:C	1:A:295:LEU:HD23	2.22	0.60
1:B:49:TRP:CE3	1:B:193:LEU:HG	2.36	0.60
1:D:91:GLU:H	1:D:91:GLU:CD	2.05	0.59
1:B:1:MET:HB3	3:B:2002:HOH:O	2.01	0.59
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:ND2	1:B:51:ASN:H	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:295:LEU:HD23	1:D:295:LEU:C	2.25	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:N	1:A:51:ASN:HD22	1.99	0.56
1:A:51:ASN:ND2	1:A:53:LYS:HE3	2.21	0.56
1:B:62:ARG:HD3	1:B:62:ARG:C	2.26	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:124:ARG:HH21	1:D:127:LYS:NZ	2.03	0.55
1:B:91:GLU:CD	1:B:91:GLU:H	2.10	0.54
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:C:204:MET:CE	1:D:134:VAL:HG21	2.38	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: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:C:329:ALA:HB3	3:C:2207:HOH:O	2.09	0.52
1:C:51:ASN:N	1:C:51:ASN:HD22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:292:ILE:O	1:C:322:PRO:HB3	2.10	0.51
1:C:201:PHE:HA	1:C:204:MET:HE2	1.93	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:204:MET:HE2	1:D:134:VAL:HG21	1.93	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
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:9:LEU:HD12	1:A:9:LEU:C	2.34	0.48
1:A:172:ASN:HD21	1:B:172:ASN:HD21	1.59	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:B:298:HIS:O	1:B:299:GLY:C	2.52	0.48
1:B:9:LEU:C	1:B:9:LEU:HD12	2.35	0.48
1:C:295:LEU:C	1:C:295:LEU:HD23	2.34	0.47
1:A:156:ASN:HB2	1:B:264:SER:HB2	1.96	0.47
1:A:51:ASN:H	1:A:51:ASN:ND2	2.05	0.47
1:C:328:ARG:HG3	1:C:328:ARG:HH11	1.80	0.47
1:D:51:ASN:N	1:D:51:ASN:ND2	2.61	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:D:51:ASN:HA	1:D:193:LEU:HD23	1.97	0.46
1:D:221:THR:O	1:D:222:TYR:HB2	2.16	0.46
1:D:193:LEU:HD11	1:D:231:ILE:HG23	1.97	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:D:53:LYS:HD3	1:D:53:LYS:N	2.30	0.46
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N	1:C:406:ASP:OD2	2.49	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
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: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: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:B:68:MET:HE1	1:B:76:PHE:HB2	2.00	0.43
1:D:159:ILE:O	1:D:165:THR:HG23	2.19	0.43
1:A:124:ARG:NH2	3:A:2112:HOH:O	2.49	0.43
1:A:298:HIS:O	1:A:299:GLY:C	2.57	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: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: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:295:LEU:C	1:B:295:LEU:HD23	2.41	0.41
1:B:328:ARG:NH1	1:B:342:GLU:OE2	2.53	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:300:THR:O	1:B:301:SER:CB	2.69	0.41
1:C:298:HIS:O	1:C:299:GLY:C	2.59	0.41
1:A:295:LEU:C	1:A:295:LEU:CD2	2.90	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:308:LYS:HD3	1:A:308:LYS:HA	1.85	0.40
1:A:156:ASN:CB	1:B:264:SER:HB2	2.51	0.40
1:B:62:ARG:HG2	1:B:62:ARG:HH11	1.87	0.40
1:C:102:ILE:O	1:C:187:ALA:HA	2.20	0.40
1:A:295:LEU:HD23	1:A:296:ASN:N	2.37	0.40
1:A:36:SER:HB2	1:A:49:TRP:CE2	2.57	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 ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	404/406 (100%)	384 (95%)	15 (4%)	5 (1%)	13	7
1	B	404/406 (100%)	386 (96%)	16 (4%)	2 (0%)	29	23
1	C	404/406 (100%)	390 (96%)	11 (3%)	3 (1%)	22	16
1	D	404/406 (100%)	388 (96%)	14 (4%)	2 (0%)	29	23
All	All	1616/1624 (100%)	1548 (96%)	56 (4%)	12 (1%)	22	16

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	404	LEU
1	A	299	GLY
1	B	299	GLY

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Mol	Chain	Res	Type
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%)	301 (98%)	7 (2%)	50	53
1	B	309/309 (100%)	299 (97%)	10 (3%)	39	38
1	C	309/309 (100%)	301 (97%)	8 (3%)	46	48
1	D	308/309 (100%)	301 (98%)	7 (2%)	50	53
All	All	1234/1236 (100%)	1202 (97%)	32 (3%)	46	48

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	TRP
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	49	TRP
1	B	51	ASN
1	B	62	ARG
1	B	65	VAL
1	B	91	GLU

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Mol	Chain	Res	Type
1	B	127	LYS
1	B	163	CYS
1	B	321	SER
1	B	358	SER
1	B	372	ASN
1	C	13	SER
1	C	49	TRP
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	D	49	TRP
1	D	51	ASN
1	D	53	LYS
1	D	68	MET
1	D	321	SER
1	D	380	ARG
1	D	405	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	113	GLN
1	A	212	ASN
1	A	225	HIS
1	A	360	ASN
1	B	51	ASN
1	B	94	GLN
1	B	113	GLN
1	B	172	ASN
1	B	225	HIS
1	B	367	GLN
1	B	372	ASN
1	C	51	ASN
1	C	94	GLN
1	C	178	GLN
1	C	225	HIS
1	C	372	ASN
1	D	20	GLN

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Mol	Chain	Res	Type
1	D	51	ASN
1	D	94	GLN
1	D	113	GLN
1	D	341	GLN
1	D	367	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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	406/406 (100%)	-0.03	16 (3%) 39 38	6, 19, 39, 55	0
1	B	406/406 (100%)	-0.44	1 (0%) 95 94	4, 13, 30, 55	0
1	C	406/406 (100%)	-0.29	8 (1%) 65 63	6, 15, 30, 70	0
1	D	406/406 (100%)	-0.11	12 (2%) 50 49	8, 18, 34, 54	0
All	All	1624/1624 (100%)	-0.22	37 (2%) 60 59	4, 16, 35, 70	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	406	ASP	9.5
1	A	406	ASP	9.4
1	C	404	LEU	8.4
1	C	405	LYS	5.5
1	D	271	ALA	5.5
1	B	406	ASP	5.4
1	D	270	VAL	5.1
1	A	319	ASP	4.8
1	D	1	MET	4.8
1	A	370	GLY	4.4
1	C	1	MET	3.9
1	C	270	VAL	3.7
1	D	213	ASP	3.6
1	C	271	ALA	3.6
1	A	213	ASP	3.2
1	D	62	ARG	3.2
1	A	320	LYS	3.2
1	D	268	ASP	3.0
1	D	366	GLU	2.9
1	A	303	PRO	2.7
1	A	318	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	405	LYS	2.5
1	A	371	LEU	2.4
1	C	286	HIS	2.4
1	C	268	ASP	2.4
1	A	62	ARG	2.3
1	D	273	SER	2.3
1	A	405	LYS	2.2
1	A	214	THR	2.2
1	D	272	PRO	2.2
1	D	57	THR	2.1
1	A	225	HIS	2.1
1	A	372	ASN	2.1
1	A	314	ARG	2.1
1	A	317	PHE	2.0
1	D	90	PRO	2.0
1	A	30	ARG	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 carbohydrates 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, 95<sup>th</sup> 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	0.95	0.30	17,17,17,17	0
2	NH4	C	1407	1/1	0.97	0.27	10,10,10,10	0
2	NH4	D	1406	1/1	0.98	0.36	12,12,12,12	0
2	NH4	B	1407	1/1	0.99	0.27	9,9,9,9	0

## 6.5 Other polymers

There are no such residues in this entry.