



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:05 PM UTC

PDB ID : 2BUI / pdb\_00002bui  
Title : E. COLI BETA-KETOACYL (ACYL CARRIER PROTEIN) SYNTHASE I  
IN COMPLEX WITH OCTANOIC ACID, 120K  
Authors : Olsen, J.G.; Von Wettstein-Knowles, P.; Henriksen, A.  
Deposited on : 2005-06-13  
Resolution : 2.40 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.

The types of validation reports are described at

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

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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

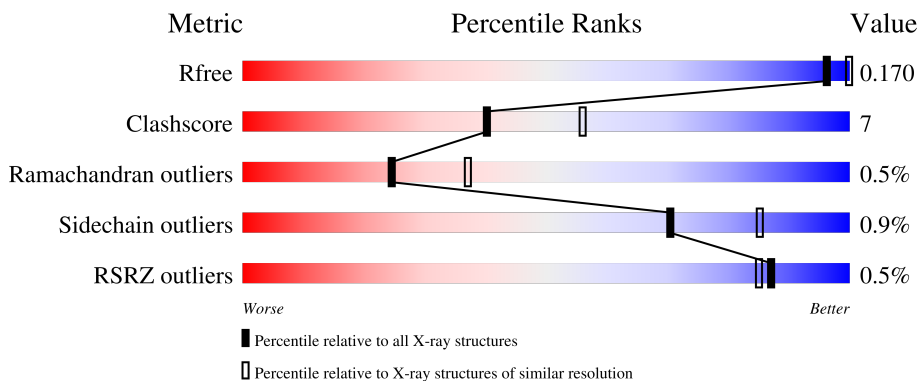
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


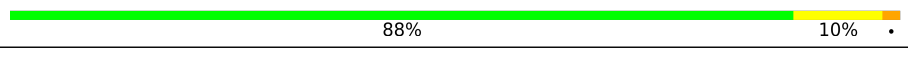
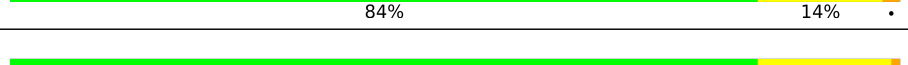

The reported resolution of this entry is 2.40 Å.

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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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  $\geq 3$ , 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	 86% 12%
1	B	406	 88% 10%
1	C	406	 84% 14%
1	D	406	 84% 15%

## 2 Entry composition [i](#)

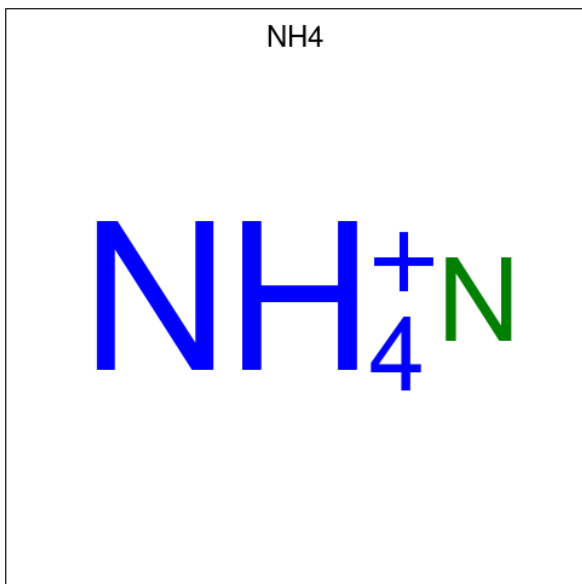
There are 4 unique types of molecules in this entry. The entry contains 12711 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	S			
1	A	406	Total 2981	C 1853	N 519	O 586	S 23	0	0	0
1	B	406	Total 2981	C 1853	N 519	O 586	S 23	0	0	0
1	C	406	Total 2981	C 1853	N 519	O 586	S 23	0	0	0
1	D	405	Total 2964	C 1843	N 517	O 581	S 23	0	0	1

- Molecule 2 is AMMONIUM ION (CCD ID: NH4) (formula: H<sub>4</sub>N).



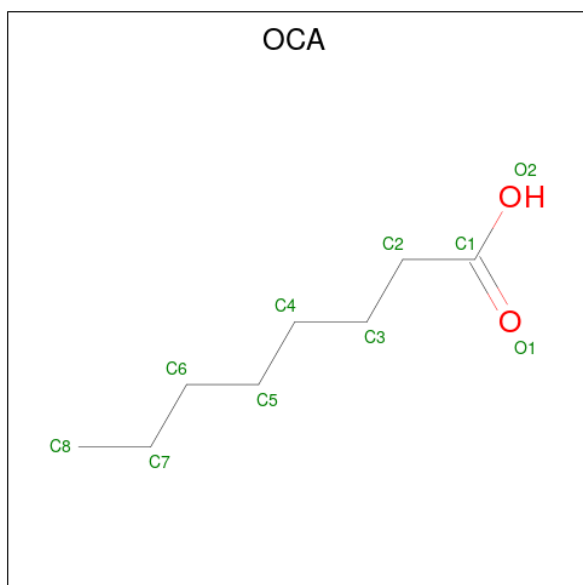
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	
2	A	1	Total 1	N 1	0	0
2	B	1	Total 1	N 1	0	0

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

- Molecule 3 is OCTANOIC ACID (CAPRYLIC ACID) (CCD ID: OCA) (formula: C<sub>8</sub>H<sub>16</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 9 8 1	0	0
3	B	1	Total C O 9 8 1	0	0
3	C	1	Total C O 9 8 1	0	0
3	D	1	Total C O 9 8 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	169	Total O 169 169	0	0
4	B	224	Total O 224 224	0	0
4	C	206	Total O 206 206	0	0

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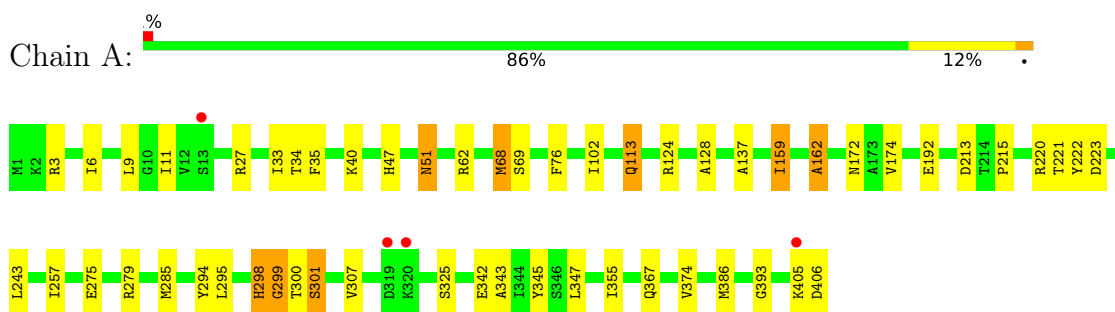
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
4	D	165	Total 165	O 165	0	0

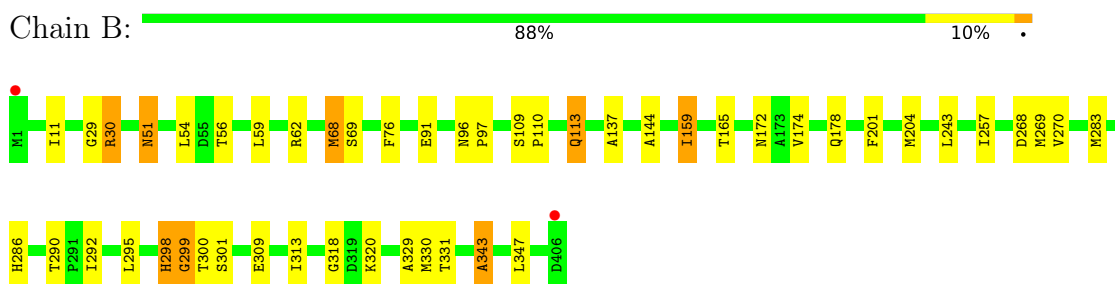
### 3 Residue-property plots [i](#)

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.

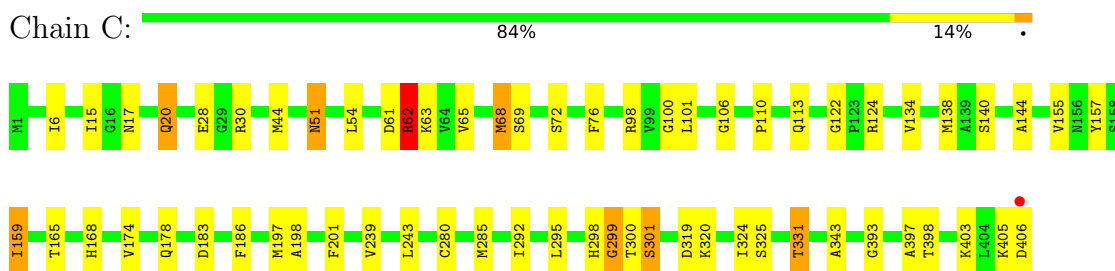
- Molecule 1: 3-OXOACYL-[ACYL-CARRIER-PROTEIN] SYNTHASE I



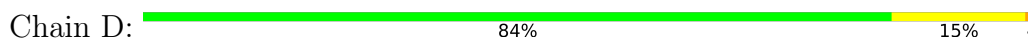
- Molecule 1: 3-OXOACYL-[ACYL-CARRIER-PROTEIN] SYNTHASE I

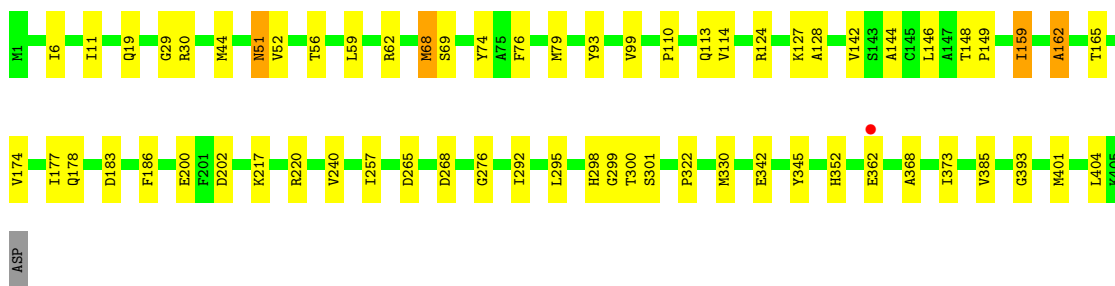


- Molecule 1: 3-OXOACYL-[ACYL-CARRIER-PROTEIN] SYNTHASE I



- 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, $\alpha$ , $\beta$ , $\gamma$	59.04Å 138.66Å 212.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.98 – 2.40 14.98 – 2.40	Depositor EDS
% Data completeness (in resolution range)	90.4 (14.98-2.40) 90.0 (14.98-2.40)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.81 (at 2.29Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.175 , 0.222 0.169 , 0.170	Depositor DCC
$R_{free}$ test set	3411 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.9	Xtrriage
Anisotropy	0.467	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 48.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	12711	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% 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, OCA

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	0.38	0/3029	0.90	9/4090 (0.2%)
1	B	0.39	0/3029	0.91	11/4090 (0.3%)
1	C	0.39	0/3029	0.90	10/4090 (0.2%)
1	D	0.38	1/3012 (0.0%)	0.91	7/4070 (0.2%)
All	All	0.39	1/12099 (0.0%)	0.90	37/16340 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	404	LEU	C-N	-5.43	1.25	1.33

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	68	MET	N-CA-C	7.38	122.05	110.17
1	A	343	ALA	N-CA-C	-7.08	103.65	111.36
1	D	68	MET	N-CA-C	6.97	121.40	110.17
1	D	69	SER	N-CA-C	-6.71	100.27	110.14
1	C	68	MET	N-CA-C	6.62	120.83	110.17
1	A	68	MET	N-CA-C	6.50	120.66	110.32
1	B	343	ALA	N-CA-C	-6.48	104.30	111.36
1	B	269	MET	N-CA-C	6.37	118.31	111.36
1	D	159	ILE	N-CA-C	-6.33	99.16	108.97
1	B	243	LEU	N-CA-C	6.30	118.67	111.11
1	C	343	ALA	N-CA-C	-6.08	104.73	111.36
1	A	159	ILE	N-CA-C	-5.97	99.82	108.36
1	A	243	LEU	N-CA-C	5.96	118.29	111.02
1	C	122	GLY	CA-C-N	5.95	125.49	119.19
1	C	122	GLY	C-N-CA	5.95	125.49	119.19
1	A	11	ILE	N-CA-C	5.84	115.53	108.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	298	HIS	N-CA-C	-5.76	105.13	111.82
1	B	113	GLN	N-CA-C	-5.75	105.09	111.36
1	A	69	SER	N-CA-C	-5.68	101.78	110.14
1	C	134	VAL	N-CA-C	5.68	115.87	110.42
1	B	11	ILE	N-CA-C	5.65	115.81	108.35
1	B	69	SER	N-CA-C	-5.52	102.03	110.14
1	C	62	ARG	N-CA-C	5.45	117.22	111.28
1	D	113	GLN	N-CA-C	-5.42	105.46	111.36
1	C	69	SER	N-CA-C	-5.40	102.21	110.14
1	C	159	ILE	N-CA-C	-5.40	100.67	108.71
1	D	162	ALA	CB-CA-C	-5.32	110.42	116.54
1	C	331	THR	N-CA-C	5.30	119.46	112.89
1	D	183	ASP	N-CA-C	-5.30	106.94	113.41
1	A	113	GLN	N-CA-C	-5.29	105.59	111.36
1	D	11	ILE	N-CA-C	5.20	115.06	107.88
1	B	290	THR	N-CA-C	-5.20	103.64	110.39
1	C	243	LEU	N-CA-C	5.19	117.35	111.02
1	A	298	HIS	N-CA-C	-5.11	105.79	111.36
1	B	159	ILE	N-CA-C	-5.07	101.15	108.71
1	A	162	ALA	CB-CA-C	-5.05	110.73	116.54
1	B	331	THR	N-CA-C	5.03	119.47	113.23

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	2981	0	2938	42	0
1	B	2981	0	2938	36	0
1	C	2981	0	2938	48	0
1	D	2964	0	2921	41	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	9	0	15	1	0
3	B	9	0	15	1	0
3	C	9	0	15	2	0
3	D	9	0	15	2	0
4	A	169	0	0	1	0
4	B	224	0	0	5	0
4	C	206	0	0	3	0
4	D	165	0	0	4	0
All	All	12711	0	11795	157	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 (157) 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:B:51:ASN:H	1:B:51:ASN:HD22	1.16	0.90
1:A:51:ASN:H	1:A:51:ASN:HD22	1.17	0.90
1:C:62:ARG:HB2	1:C:62:ARG:HH11	1.35	0.89
1:C:51:ASN:HD22	1:C:51:ASN:H	1.21	0.85
1:C:280:CYS:SG	1:C:398:THR:HG23	2.19	0.82
1:A:102:ILE:HD13	1:A:172:ASN:HD22	1.45	0.81
1:C:62:ARG:HB2	1:C:62:ARG:NH1	1.99	0.78
1:B:292:ILE:H	1:B:320:LYS:HZ3	1.35	0.75
1:D:51:ASN:H	1:D:51:ASN:HD22	1.35	0.74
1:D:6:ILE:HD11	1:D:257:ILE:HD11	1.69	0.73
1:D:177:ILE:HD12	1:D:240:VAL:HG12	1.71	0.73
1:B:30:ARG:HH11	1:B:30:ARG:HB2	1.55	0.70
1:A:51:ASN:HD22	1:A:51:ASN:N	1.89	0.68
1:C:61:ASP:OD2	1:C:63:LYS:HG2	1.96	0.65
1:C:51:ASN:HD22	1:C:51:ASN:N	1.95	0.65
1:A:220:ARG:HD3	1:A:223:ASP:OD2	1.98	0.64
1:D:51:ASN:HD22	1:D:51:ASN:N	1.96	0.64
1:C:28:GLU:CD	1:C:30:ARG:HH21	2.05	0.64
1:D:268:ASP:HB3	4:D:2107:HOH:O	1.99	0.62
1:C:100:GLY:HA3	1:C:155:VAL:HG12	1.82	0.61
1:B:68:MET:HE1	1:B:76:PHE:HB2	1.83	0.61
1:D:19:GLN:HG2	4:D:2006:HOH:O	2.01	0.60
1:C:68:MET:HE1	1:C:76:PHE:HB2	1.82	0.60
1:C:174:VAL:O	1:C:178:GLN:HG3	2.02	0.60
1:B:113:GLN:HG3	1:B:137:ALA:HB1	1.82	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:GLU:HG2	4:A:2087:HOH:O	2.03	0.59
1:C:15:ILE:HD13	1:C:331:THR:HG22	1.85	0.58
1:A:34:THR:HG22	1:A:35:PHE:N	2.18	0.58
1:D:300:THR:O	1:D:301:SER:HB3	2.04	0.58
1:C:113:GLN:NE2	1:D:110:PRO:HB3	2.18	0.57
1:B:91:GLU:H	1:B:91:GLU:CD	2.13	0.57
1:A:33:ILE:HD12	1:A:33:ILE:N	2.20	0.56
1:A:113:GLN:HG3	1:B:113:GLN:OE1	2.05	0.56
1:A:174:VAL:HG21	1:A:257:ILE:HG21	1.87	0.56
1:B:268:ASP:HB3	4:B:2159:HOH:O	2.04	0.56
1:B:201:PHE:HZ	3:B:905:OCA:H42	1.72	0.55
1:A:68:MET:HE1	1:A:76:PHE:HB2	1.89	0.55
1:C:20:GLN:NE2	1:C:20:GLN:H	2.05	0.55
1:C:110:PRO:HG2	1:C:197:MET:HE3	1.88	0.54
1:C:300:THR:O	1:C:301:SER:HB3	2.07	0.54
1:A:124:ARG:HB2	1:A:128:ALA:HB2	1.88	0.54
1:C:44:MET:HE1	1:C:198:ALA:HB1	1.90	0.54
1:D:342:GLU:HA	1:D:345:TYR:CD2	2.43	0.54
1:D:385:VAL:HG23	1:D:401:MET:HE3	1.88	0.54
1:B:298:HIS:ND1	4:B:2172:HOH:O	2.33	0.54
1:D:217:LYS:O	1:D:220:ARG:HD2	2.07	0.54
1:C:138:MET:HB3	3:D:905:OCA:H83	1.90	0.53
1:A:113:GLN:HE21	1:A:137:ALA:HB1	1.73	0.53
1:B:298:HIS:CE1	4:B:2172:HOH:O	2.61	0.53
1:A:51:ASN:H	1:A:51:ASN:ND2	1.94	0.53
1:C:62:ARG:HH11	1:C:62:ARG:CB	2.15	0.52
1:B:51:ASN:HD22	1:B:51:ASN:N	1.93	0.52
1:A:405:LYS:HG3	1:A:405:LYS:O	2.09	0.52
1:D:124:ARG:HH21	1:D:127:LYS:HE2	1.74	0.52
1:C:113:GLN:CD	1:D:110:PRO:HB3	2.35	0.51
1:A:300:THR:O	1:A:301:SER:HB3	2.10	0.51
1:D:51:ASN:H	1:D:51:ASN:ND2	2.06	0.51
1:D:52:VAL:HG23	1:D:52:VAL:O	2.11	0.51
1:A:113:GLN:OE1	1:B:110:PRO:HB3	2.11	0.51
1:D:30:ARG:N	1:D:330:MET:HE3	2.25	0.51
1:C:124:ARG:HH11	1:C:124:ARG:HG2	1.76	0.50
1:D:292:ILE:O	1:D:322:PRO:HB3	2.11	0.50
1:A:355:ILE:CG2	1:A:374:VAL:HG21	2.42	0.50
1:B:51:ASN:H	1:B:51:ASN:ND2	1.95	0.50
1:A:342:GLU:HA	1:A:345:TYR:CD2	2.46	0.50
1:B:62:ARG:HD3	1:B:62:ARG:C	2.37	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:101:LEU:HD23	1:C:186:PHE:HB2	1.94	0.49
1:C:68:MET:HE2	1:C:72:SER:HB3	1.94	0.49
1:B:298:HIS:O	1:B:299:GLY:C	2.56	0.48
1:A:393:GLY:HA3	1:B:144:ALA:HB1	1.95	0.48
1:A:159:ILE:HD13	1:B:159:ILE:HG12	1.96	0.48
1:C:110:PRO:CD	1:C:197:MET:HE3	2.44	0.48
1:D:352:HIS:HE1	4:D:2007:HOH:O	1.96	0.48
1:A:285:MET:SD	1:A:386:MET:HE1	2.54	0.48
1:A:355:ILE:HG22	1:A:374:VAL:HG21	1.95	0.47
1:B:29:GLY:HA2	1:B:330:MET:SD	2.54	0.47
1:A:295:LEU:C	1:A:295:LEU:HD23	2.39	0.47
1:C:300:THR:O	1:C:301:SER:CB	2.62	0.47
1:C:110:PRO:CG	1:C:197:MET:HE3	2.45	0.47
1:C:319:ASP:HB2	4:C:2161:HOH:O	2.14	0.47
1:A:51:ASN:N	1:A:51:ASN:ND2	2.60	0.46
1:D:124:ARG:HB2	1:D:128:ALA:HB2	1.97	0.46
1:A:6:ILE:HD13	1:A:347:LEU:HD11	1.97	0.46
1:A:62:ARG:HH11	1:A:62:ARG:HG3	1.79	0.46
1:C:17:ASN:CG	1:C:54:LEU:HB2	2.40	0.46
1:D:174:VAL:HG21	1:D:257:ILE:HG21	1.96	0.46
1:D:368:ALA:HB1	1:D:373:ILE:HD12	1.97	0.46
1:C:393:GLY:HA3	1:D:144:ALA:HB1	1.96	0.46
1:A:298:HIS:O	1:A:299:GLY:C	2.59	0.46
1:D:162:ALA:HB1	3:D:905:OCA:O1	2.15	0.46
1:A:40:LYS:HG3	1:A:47:HIS:CE1	2.51	0.45
1:D:79:MET:HE3	1:D:186:PHE:CG	2.50	0.45
1:A:307:VAL:HG11	1:A:367:GLN:CD	2.41	0.45
1:C:138:MET:HE3	1:C:140:SER:OG	2.17	0.45
1:B:54:LEU:HD12	4:B:2058:HOH:O	2.16	0.45
1:B:56:THR:HA	1:B:59:LEU:HD12	1.98	0.45
1:B:159:ILE:O	1:B:165:THR:HG23	2.16	0.45
1:A:3:ARG:HH12	1:A:406:ASP:HA	1.81	0.45
1:A:27:ARG:NH1	1:A:27:ARG:HB3	2.32	0.45
1:C:155:VAL:CG2	1:C:157:TYR:CE1	3.00	0.44
1:B:329:ALA:HB3	4:B:2185:HOH:O	2.18	0.44
1:A:213:ASP:C	1:A:215:PRO:HD3	2.43	0.44
1:A:62:ARG:HD3	1:A:62:ARG:C	2.42	0.44
1:D:142:VAL:O	1:D:146:LEU:HD13	2.18	0.44
1:D:298:HIS:CE1	4:D:2123:HOH:O	2.71	0.44
1:C:113:GLN:NE2	1:D:200:GLU:OE1	2.50	0.44
1:C:144:ALA:HB1	1:D:393:GLY:HA3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:51:ASN:H	1:C:51:ASN:ND2	1.99	0.44
1:B:159:ILE:HD11	1:B:172:ASN:CG	2.43	0.44
1:B:318:GLY:C	1:B:320:LYS:H	2.25	0.44
1:C:106:GLY:C	3:C:905:OCA:H61	2.43	0.44
1:B:283:MET:HA	1:B:286:HIS:CD2	2.53	0.43
1:B:174:VAL:HG21	1:B:257:ILE:HG21	2.00	0.43
1:C:159:ILE:CD1	1:D:159:ILE:HD13	2.48	0.43
1:D:68:MET:HE1	1:D:76:PHE:HB2	2.01	0.43
1:A:300:THR:O	1:A:301:SER:CB	2.67	0.43
1:A:221:THR:O	1:A:222:TYR:HB2	2.17	0.43
1:C:319:ASP:C	1:C:320:LYS:HG3	2.43	0.43
1:D:265:ASP:OD1	1:D:276:GLY:HA3	2.18	0.43
1:C:298:HIS:CE1	4:C:2150:HOH:O	2.72	0.43
1:C:298:HIS:O	1:C:299:GLY:C	2.62	0.43
1:A:307:VAL:HG11	1:A:367:GLN:OE1	2.19	0.43
1:C:98:ARG:HE	1:C:183:ASP:CG	2.27	0.43
1:C:405:LYS:O	1:C:406:ASP:HB2	2.19	0.43
1:D:52:VAL:HG21	1:D:74:TYR:CE1	2.54	0.43
1:B:174:VAL:O	1:B:178:GLN:HG3	2.18	0.42
1:D:93:TYR:HA	1:D:99:VAL:HG21	2.01	0.42
1:C:285:MET:SD	1:C:292:ILE:HD11	2.58	0.42
1:B:62:ARG:HD3	1:B:62:ARG:O	2.20	0.42
1:D:300:THR:O	1:D:301:SER:CB	2.66	0.42
1:A:34:THR:CG2	1:A:35:PHE:N	2.82	0.42
1:C:201:PHE:HZ	3:C:905:OCA:H42	1.85	0.42
1:A:162:ALA:HB1	3:A:905:OCA:O1	2.19	0.42
1:D:56:THR:HA	1:D:59:LEU:CD1	2.50	0.42
1:A:275:GLU:CD	1:A:279:ARG:HE	2.27	0.41
1:C:6:ILE:HA	1:C:239:VAL:O	2.20	0.41
1:D:29:GLY:C	1:D:330:MET:HE3	2.45	0.41
1:B:295:LEU:C	1:B:295:LEU:HD23	2.46	0.41
1:B:300:THR:O	1:B:301:SER:HB3	2.20	0.41
1:C:17:ASN:OD1	1:C:54:LEU:HB2	2.20	0.41
1:C:320:LYS:HG3	4:C:2161:HOH:O	2.19	0.41
1:D:295:LEU:C	1:D:295:LEU:HD23	2.44	0.41
1:A:9:LEU:C	1:A:9:LEU:HD12	2.46	0.41
1:B:96:ASN:HA	1:B:97:PRO:HD2	1.97	0.41
1:D:174:VAL:O	1:D:178:GLN:HG3	2.20	0.41
1:B:343:ALA:O	1:B:347:LEU:HG	2.21	0.41
1:C:62:ARG:HA	1:C:65:VAL:HG12	2.01	0.41
1:C:324:ILE:HG22	1:C:325:SER:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:MET:HE1	1:B:270:VAL:HG11	2.02	0.41
1:B:309:GLU:O	1:B:313:ILE:HG13	2.21	0.41
1:D:148:THR:HB	1:D:149:PRO:CD	2.51	0.41
1:D:110:PRO:O	1:D:114:VAL:HG23	2.21	0.41
1:B:109:SER:HB3	1:B:137:ALA:HA	2.03	0.41
1:A:27:ARG:HB3	1:A:27:ARG:HH11	1.86	0.40
1:A:294:TYR:OH	1:A:325:SER:HB3	2.20	0.40
1:C:168:HIS:CD2	1:C:397:ALA:HB2	2.57	0.40
1:D:44:MET:HE3	1:D:202:ASP:HB2	2.04	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%)	380 (94%)	22 (5%)	2 (0%)	24 37
1	B	404/406 (100%)	387 (96%)	16 (4%)	1 (0%)	43 58
1	C	404/406 (100%)	385 (95%)	16 (4%)	3 (1%)	18 28
1	D	403/406 (99%)	382 (95%)	19 (5%)	2 (0%)	24 37
All	All	1615/1624 (99%)	1534 (95%)	73 (4%)	8 (0%)	24 37

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	299	GLY
1	B	299	GLY
1	C	299	GLY
1	D	299	GLY
1	A	301	SER
1	C	301	SER

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Mol	Chain	Res	Type
1	C	165	THR
1	D	165	THR

### 5.3.2 Protein sidechains [i](#)

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	309/309 (100%)	308 (100%)	1 (0%)	86	93
1	B	309/309 (100%)	307 (99%)	2 (1%)	78	89
1	C	309/309 (100%)	304 (98%)	5 (2%)	55	76
1	D	307/309 (99%)	304 (99%)	3 (1%)	68	84
All	All	1234/1236 (100%)	1223 (99%)	11 (1%)	70	85

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	B	30	ARG
1	B	51	ASN
1	C	20	GLN
1	C	51	ASN
1	C	62	ARG
1	C	295	LEU
1	C	403	LYS
1	D	51	ASN
1	D	62	ARG
1	D	362	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	51	ASN
1	A	95	ASN
1	A	172	ASN

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Mol	Chain	Res	Type
1	A	225	HIS
1	A	252	HIS
1	B	51	ASN
1	B	94	GLN
1	B	176	GLN
1	B	178	GLN
1	B	252	HIS
1	B	372	ASN
1	C	20	GLN
1	C	51	ASN
1	C	94	GLN
1	C	95	ASN
1	D	51	ASN
1	D	94	GLN
1	D	352	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

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

Of 8 ligands modelled in this entry, 4 are modelled with single atom - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	OCA	A	905	1	7,8,9	0.41	0	6,7,9	0.62	0
3	OCA	B	905	1	7,8,9	0.40	0	6,7,9	0.63	0
3	OCA	C	905	1	7,8,9	0.43	0	6,7,9	0.62	0
3	OCA	D	905	1	7,8,9	0.45	0	6,7,9	0.63	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OCA	A	905	1	-	1/6/6/7	-
3	OCA	B	905	1	-	2/6/6/7	-
3	OCA	C	905	1	-	2/6/6/7	-
3	OCA	D	905	1	-	2/6/6/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	905	OCA	O1-C1-C2-C3
3	B	905	OCA	O1-C1-C2-C3
3	C	905	OCA	O1-C1-C2-C3
3	D	905	OCA	O1-C1-C2-C3
3	D	905	OCA	C3-C4-C5-C6
3	C	905	OCA	C4-C5-C6-C7
3	B	905	OCA	C4-C5-C6-C7

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	905	OCA	1	0
3	B	905	OCA	1	0
3	C	905	OCA	2	0
3	D	905	OCA	2	0

## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.41	4 (0%) 79 76	8, 19, 40, 67	0
1	B	406/406 (100%)	-0.76	2 (0%) 87 85	7, 14, 25, 49	0
1	C	406/406 (100%)	-0.75	1 (0%) 91 89	7, 14, 26, 60	0
1	D	405/406 (99%)	-0.59	1 (0%) 91 89	8, 18, 31, 43	0
All	All	1623/1624 (99%)	-0.63	8 (0%) 87 85	7, 16, 32, 67	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	405	LYS	3.1
1	B	406	ASP	3.0
1	C	406	ASP	2.7
1	D	362	GLU	2.6
1	A	320	LYS	2.1
1	A	13	SER	2.1
1	A	319	ASP	2.0
1	B	1	MET	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, 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(Å <sup>2</sup> )	Q<0.9
3	OCA	D	905	9/10	0.91	0.09	26,27,28,29	0
3	OCA	A	905	9/10	0.92	0.09	23,23,25,26	0
3	OCA	C	905	9/10	0.93	0.09	24,26,27,28	0
3	OCA	B	905	9/10	0.94	0.07	14,21,24,25	0
2	NH4	D	902	1/1	0.95	0.05	8,8,8,8	0
2	NH4	B	902	1/1	0.96	0.08	7,7,7,7	0
2	NH4	C	902	1/1	0.97	0.06	2,2,2,2	0
2	NH4	A	902	1/1	0.97	0.07	6,6,6,6	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.