



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 01:37 am BST

PDB ID : 2VB9  
Title : beta-ketoacyl-ACP synthase I (KAS) from E. coli, apo structure  
Authors : Pappenberger, G.; Schulz-Gasch, T.; Bailly, J.; Hennig, M.  
Deposited on : 2007-09-06  
Resolution : 1.50 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

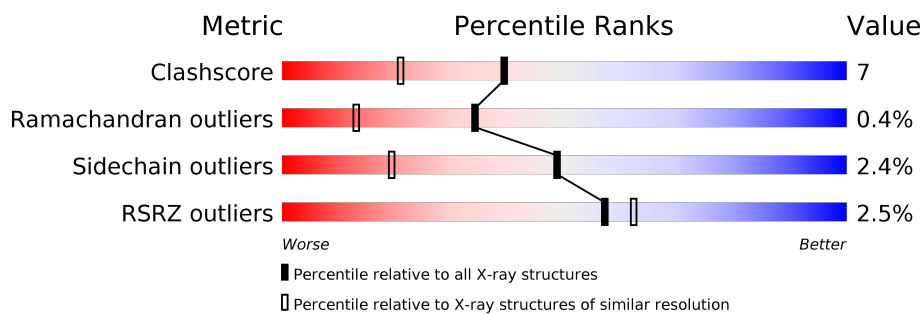
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.50 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))
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

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>2%</div> <div>85%</div> <div>11%</div> <div>..</div> </div>
1	B	406	<div> <div>%</div> <div>89%</div> <div>10%</div> <div>.</div> </div>
1	C	406	<div> <div>%</div> <div>89%</div> <div>10%</div> <div>.</div> </div>
1	D	406	<div> <div>6%</div> <div>81%</div> <div>17%</div> <div>.</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14389 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 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	404	Total	C	N	O	S	41	16	0
			3000	1864	519	591	26			
1	B	404	Total	C	N	O	S	24	18	0
			3001	1861	522	593	25			
1	C	406	Total	C	N	O	S	41	23	0
			3041	1893	525	595	28			
1	D	404	Total	C	N	O	S	44	19	0
			3011	1867	524	593	27			

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

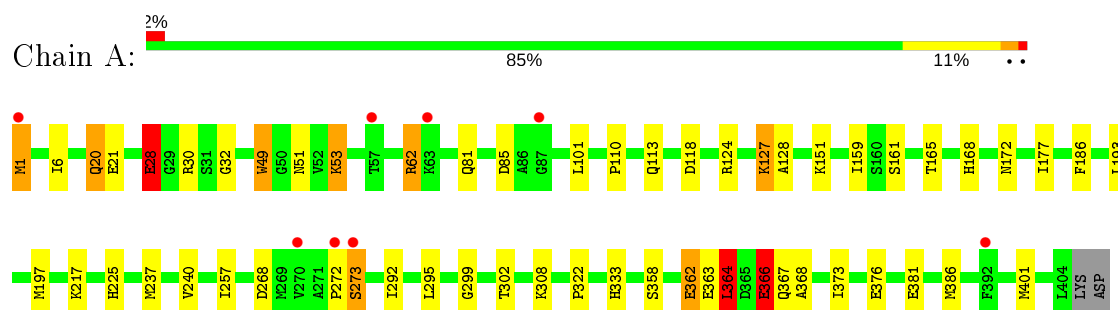
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	560	Total	O	0	0
			560	560		
3	B	605	Total	O	0	0
			605	605		
3	C	629	Total	O	0	0
			629	629		
3	D	540	Total	O	0	0
			540	540		

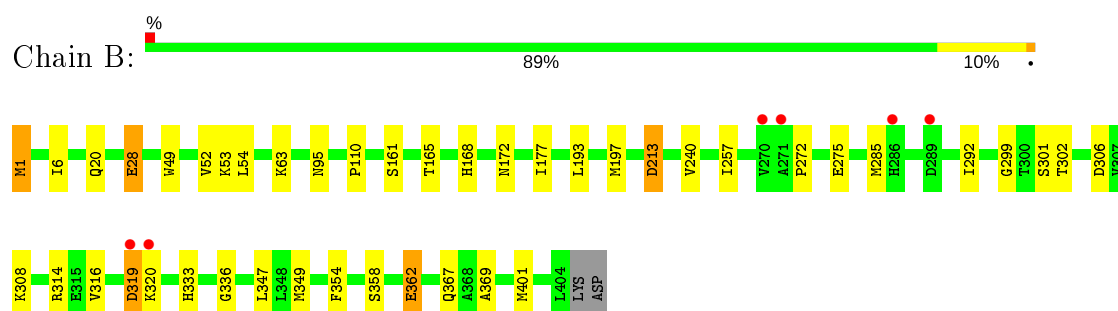
### 3 Residue-property plots [i](#)

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.

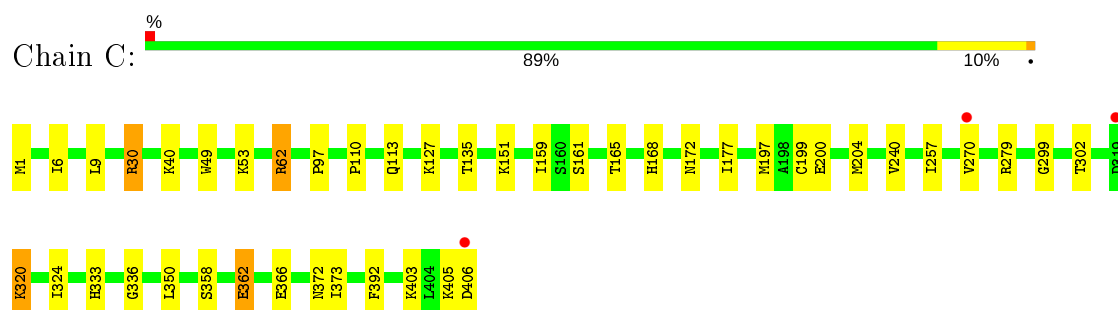
#### • Molecule 1: 3-OXOACYL-[ACYL-CARRIER-PROTEIN] SYNTHASE 1



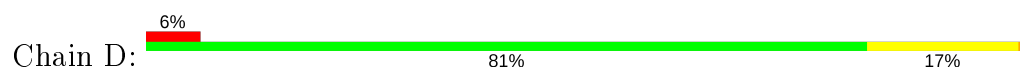
#### • Molecule 1: 3-OXOACYL-[ACYL-CARRIER-PROTEIN] SYNTHASE 1

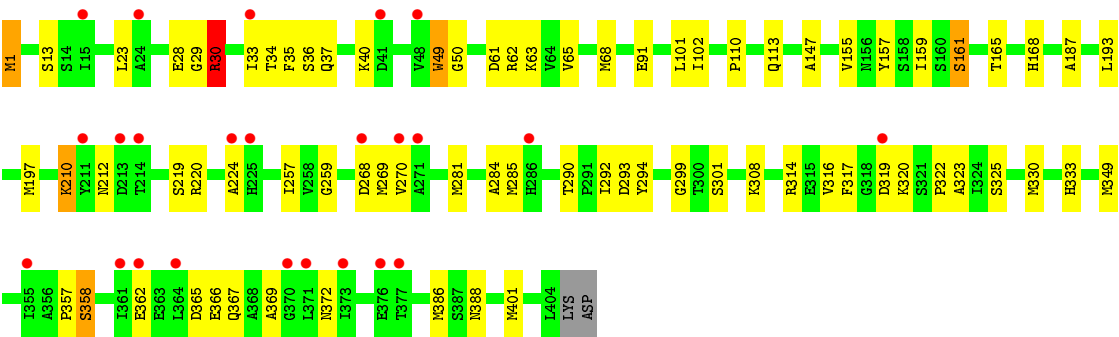


#### • Molecule 1: 3-OXOACYL-[ACYL-CARRIER-PROTEIN] SYNTHASE 1



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





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	58.91Å 138.35Å 211.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	115.47 – 1.50 19.90 – 1.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (115.47-1.50) 99.8 (19.90-1.50)	Depositor EDS
$R_{merge}$	0.01	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.38 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, $R_{free}$	0.197 , 0.238 0.199 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	13.6	Xtriage
Anisotropy	0.295	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 75.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	14389	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% 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

### 5.1 Standard geometry

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

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	0.91	8/3141 (0.3%)	0.94	17/4241 (0.4%)
1	B	0.80	3/3160 (0.1%)	0.83	9/4265 (0.2%)
1	C	1.03	9/3224 (0.3%)	0.87	10/4347 (0.2%)
1	D	0.92	8/3170 (0.3%)	0.96	13/4278 (0.3%)
All	All	0.92	28/12695 (0.2%)	0.90	49/17131 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
1	D	0	2
All	All	0	5

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	366	GLU	CG-CD	26.78	1.92	1.51
1	D	30	ARG	NE-CZ	21.41	1.60	1.33
1	C	62	ARG	CG-CD	-17.43	1.08	1.51
1	C	362	GLU	CG-CD	-15.39	1.28	1.51
1	B	319	ASP	CB-CG	15.05	1.83	1.51
1	A	28	GLU	CG-CD	-14.88	1.29	1.51
1	A	366	GLU	CG-CD	-14.15	1.30	1.51
1	D	63	LYS	CD-CE	13.09	1.83	1.51
1	A	362	GLU	CG-CD	12.46	1.70	1.51
1	B	63	LYS	CG-CD	11.41	1.91	1.52
1	A	381	GLU	CG-CD	11.14	1.68	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	28	GLU	CG-CD	10.82	1.68	1.51
1	A	151	LYS	CD-CE	10.44	1.77	1.51
1	D	366	GLU	CB-CG	10.01	1.71	1.52
1	C	62	ARG	CB-CG	-9.89	1.25	1.52
1	D	210	LYS	CD-CE	-9.21	1.28	1.51
1	A	217	LYS	CD-CE	8.89	1.73	1.51
1	C	127	LYS	CD-CE	8.73	1.73	1.51
1	C	320	LYS	CB-CG	8.18	1.74	1.52
1	B	28	GLU	CG-CD	-7.96	1.40	1.51
1	C	30	ARG	CD-NE	-7.63	1.33	1.46
1	D	308	LYS	CD-CE	-7.25	1.33	1.51
1	A	20	GLN	CG-CD	7.18	1.67	1.51
1	A	127	LYS	CG-CD	-6.33	1.30	1.52
1	D	62	ARG	CB-CG	-6.21	1.35	1.52
1	C	199	CYS	CB-SG	-6.11	1.71	1.82
1	D	91	GLU	CB-CG	5.46	1.62	1.52
1	C	406	ASP	CA-CB	-5.12	1.42	1.53

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	366	GLU	CG-CD-OE2	-18.66	80.98	118.30
1	D	30	ARG	CD-NE-CZ	-16.62	100.33	123.60
1	D	319	ASP	CB-CG-OD2	15.75	132.47	118.30
1	D	319	ASP	CB-CG-OD1	-15.44	104.40	118.30
1	D	30	ARG	NE-CZ-NH1	-14.56	113.02	120.30
1	A	366	GLU	CG-CD-OE1	14.32	146.94	118.30
1	A	1	MET	CA-C-O	-11.66	95.61	120.10
1	A	1	MET	CB-CA-C	-11.27	87.86	110.40
1	C	151[A]	LYS	CD-CE-NZ	10.05	134.81	111.70
1	C	151[B]	LYS	CD-CE-NZ	10.05	134.81	111.70
1	B	1	MET	CA-C-N	-9.64	95.99	117.20
1	D	320	LYS	CA-CB-CG	-9.46	92.59	113.40
1	A	28	GLU	CB-CG-CD	9.38	139.53	114.20
1	D	210	LYS	CG-CD-CE	8.91	138.64	111.90
1	D	1	MET	CB-CA-C	-8.53	93.35	110.40
1	A	381	GLU	CB-CG-CD	-8.49	91.28	114.20
1	D	28	GLU	CG-CD-OE1	7.87	134.04	118.30
1	C	1	MET	CA-C-N	-7.83	99.97	117.20
1	C	1	MET	CA-C-O	7.76	136.39	120.10
1	D	28	GLU	CG-CD-OE2	-7.67	102.96	118.30
1	C	366	GLU	CB-CG-CD	-7.65	93.56	114.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	362	GLU	CB-CG-CD	7.34	134.01	114.20
1	A	217	LYS	CD-CE-NZ	-7.09	95.39	111.70
1	B	1	MET	CA-C-O	6.62	134.01	120.10
1	B	63	LYS	CB-CG-CD	-6.53	94.63	111.60
1	A	151	LYS	CG-CD-CE	-6.37	92.78	111.90
1	B	362	GLU	CG-CD-OE2	6.15	130.59	118.30
1	A	28	GLU	CG-CD-OE1	-6.12	106.06	118.30
1	B	320	LYS	CG-CD-CE	6.08	130.14	111.90
1	A	376	GLU	CB-CG-CD	6.06	130.55	114.20
1	A	28	GLU	CG-CD-OE2	5.98	130.26	118.30
1	D	366	GLU	CA-CB-CG	5.95	126.48	113.40
1	A	268	ASP	CB-CG-OD1	-5.93	112.96	118.30
1	A	268	ASP	CB-CG-OD2	5.88	123.59	118.30
1	D	63	LYS	CG-CD-CE	-5.88	94.27	111.90
1	D	28	GLU	CB-CG-CD	-5.84	98.43	114.20
1	D	1	MET	CA-C-O	-5.74	108.04	120.10
1	C	279	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	C	362	GLU	CG-CD-OE2	5.54	129.37	118.30
1	A	118	ASP	CB-CG-OD1	5.45	123.21	118.30
1	A	362	GLU	CG-CD-OE1	-5.33	107.65	118.30
1	B	362	GLU	CG-CD-OE1	-5.29	107.73	118.30
1	A	364	LEU	CA-CB-CG	5.25	127.37	115.30
1	C	362	GLU	CB-CG-CD	5.22	128.30	114.20
1	C	62	ARG	CA-CB-CG	5.21	124.86	113.40
1	B	193	LEU	CB-CG-CD2	-5.18	102.19	111.00
1	C	366	GLU	CG-CD-OE1	5.17	128.64	118.30
1	A	381	GLU	CG-CD-OE2	-5.16	107.98	118.30
1	B	306	ASP	CB-CG-OD1	5.09	122.88	118.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	MET	Mainchain
1	A	366	GLU	Sidechain
1	B	1	MET	Mainchain
1	D	1	MET	Mainchain
1	D	30	ARG	Sidechain

## 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	3000	0	2956	39	0
1	B	3001	0	2946	36	0
1	C	3041	0	3011	35	0
1	D	3011	0	2963	75	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	560	0	0	13	0
3	B	605	0	0	15	1
3	C	629	0	0	17	3
3	D	540	0	0	37	2
All	All	14389	0	11876	176	3

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 (176) 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:D:49:TRP:O	3:D:2162:HOH:O	1.67	1.11
1:D:33:ILE:HA	3:D:2162:HOH:O	1.53	1.08
1:A:257[B]:ILE:HD13	1:A:401[B]:MET:HG2	1.37	1.06
1:D:322:PRO:HB2	3:D:2476:HOH:O	1.55	1.05
1:D:34:THR:HG23	3:D:2101:HOH:O	1.59	1.01
1:C:9:LEU:HB3	3:C:2022:HOH:O	1.61	1.00
1:D:323:ALA:O	3:D:2476:HOH:O	1.80	0.97
1:C:270:VAL:HG12	3:C:2464:HOH:O	1.65	0.97
1:D:49:TRP:C	3:D:2162:HOH:O	2.02	0.93
1:C:159[A]:ILE:HD13	1:D:159:ILE:HG12	1.52	0.92
1:D:37:GLN:NE2	3:D:2115:HOH:O	2.03	0.92
1:B:28:GLU:HG3	3:B:2117:HOH:O	1.71	0.90
1:D:358:SER:HA	3:D:2500:HOH:O	1.70	0.90
1:D:358:SER:CB	3:D:2502:HOH:O	2.20	0.89
1:D:358:SER:HB2	3:D:2502:HOH:O	1.71	0.89
1:A:172[B]:ASN:ND2	3:A:2333:HOH:O	2.05	0.89
1:D:61[A]:ASP:OD1	3:D:2186:HOH:O	1.88	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:281:MET:CE	1:D:388:ASN:HD21	1.86	0.88
1:D:35:PHE:HD1	3:D:2367:HOH:O	1.56	0.87
1:B:302:THR:CG2	3:B:2397:HOH:O	2.22	0.86
1:B:302:THR:HG22	3:B:2397:HOH:O	1.77	0.85
1:C:392[A]:PHE:HD2	3:C:2464:HOH:O	1.58	0.85
1:D:325:SER:HA	3:D:2502:HOH:O	1.76	0.84
1:D:314[B]:ARG:NH2	1:D:369:ALA:O	2.11	0.83
1:D:281:MET:HE1	1:D:388:ASN:HD21	1.44	0.82
1:C:392[A]:PHE:CD2	3:C:2464:HOH:O	2.34	0.81
1:A:273:SER:O	3:A:2426:HOH:O	2.00	0.80
1:C:159[A]:ILE:CD1	1:D:159:ILE:HG12	2.12	0.79
1:C:9:LEU:HD23	3:C:2022:HOH:O	1.83	0.79
1:B:285[B]:MET:CE	1:B:316:VAL:HG11	2.14	0.77
1:C:172:ASN:HB3	3:C:2367:HOH:O	1.83	0.76
1:C:97[A]:PRO:HG2	3:C:2118:HOH:O	1.87	0.74
1:D:23:LEU:HD23	3:D:2059:HOH:O	1.87	0.73
1:D:285:MET:HE1	1:D:316:VAL:HG11	1.70	0.73
1:C:113:GLN:HE21	1:D:113:GLN:HG2	1.52	0.72
1:D:224:ALA:N	3:D:2379:HOH:O	2.22	0.72
1:B:285[B]:MET:HE1	1:B:316:VAL:HG11	1.72	0.72
1:C:200:GLU:OE2	1:D:113:GLN:NE2	2.22	0.71
1:D:29:GLY:N	3:D:2086:HOH:O	2.25	0.70
1:D:281:MET:CE	1:D:388:ASN:ND2	2.53	0.70
1:C:177[A]:ILE:HD12	1:C:240:VAL:HG12	1.73	0.69
1:D:357:PRO:O	3:D:2500:HOH:O	2.08	0.69
1:B:6[A]:ILE:HD12	1:B:347:LEU:HD11	1.76	0.68
1:A:364:LEU:HD21	1:A:373[B]:ILE:HD12	1.75	0.68
1:C:9:LEU:CD2	3:C:2022:HOH:O	2.38	0.68
1:A:113:GLN:OE1	3:A:2282:HOH:O	2.11	0.67
1:D:281:MET:HE2	1:D:388:ASN:ND2	2.09	0.67
1:A:161:SER:OG	1:A:168:HIS:HD2	1.78	0.67
1:B:213:ASP:CB	3:B:2409:HOH:O	2.43	0.67
1:B:161:SER:OG	1:B:168:HIS:HD2	1.77	0.67
1:C:113:GLN:OE1	3:C:2307:HOH:O	2.13	0.67
1:A:21:GLU:HG3	3:A:2052:HOH:O	1.94	0.66
1:D:35:PHE:CD1	3:D:2367:HOH:O	2.40	0.66
1:B:285[A]:MET:SD	1:B:292:ILE:HD11	2.35	0.65
1:C:405:LYS:HG2	3:C:2625:HOH:O	1.97	0.65
1:C:6:ILE:HD11	1:C:257[A]:ILE:HD11	1.79	0.64
1:B:275:GLU:HG2	3:B:2466:HOH:O	1.98	0.64
1:C:161:SER:OG	1:C:168:HIS:HD2	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:281:MET:HE2	1:D:388:ASN:HD21	1.63	0.64
1:B:28:GLU:HG2	3:B:2100:HOH:O	1.97	0.64
1:B:362:GLU:HG3	3:B:2540:HOH:O	2.00	0.62
1:D:285:MET:HE3	1:D:386:MET:HE1	1.81	0.62
1:B:272:PRO:O	1:B:308:LYS:HE2	2.00	0.61
1:A:302[A]:THR:HG23	3:A:2363:HOH:O	2.01	0.60
1:D:285:MET:CE	1:D:386:MET:CE	2.79	0.60
1:A:101:LEU:HD21	1:A:237[B]:MET:HE1	1.82	0.60
1:D:110:PRO:HG2	1:D:197:MET:HB2	1.83	0.60
1:D:212:ASN:O	3:D:2367:HOH:O	2.17	0.60
1:A:257[B]:ILE:HD13	1:A:401[B]:MET:CG	2.22	0.59
1:D:323:ALA:N	3:D:2476:HOH:O	2.35	0.59
1:A:32:GLY:O	1:A:53[B]:LYS:NZ	2.36	0.59
1:A:124:ARG:HB2	1:A:128:ALA:HB2	1.84	0.59
1:B:285[B]:MET:CE	1:B:316:VAL:CG1	2.80	0.59
1:A:364:LEU:HD13	1:A:368:ALA:HB3	1.84	0.59
1:A:295[B]:LEU:HD23	1:A:386[B]:MET:HG2	1.85	0.58
1:B:213:ASP:HB2	3:B:2409:HOH:O	2.03	0.58
1:C:177[A]:ILE:CD1	1:C:240:VAL:HG12	2.33	0.58
1:D:285:MET:HE2	1:D:386:MET:HE3	1.84	0.58
1:C:302[B]:THR:HG22	3:C:2507:HOH:O	2.03	0.58
1:D:34:THR:CG2	3:D:2101:HOH:O	2.31	0.58
1:B:285[B]:MET:HE3	1:B:316:VAL:HG11	1.85	0.58
1:B:302:THR:HG21	3:B:2397:HOH:O	1.94	0.58
1:D:290:THR:HB	3:D:2444:HOH:O	2.04	0.58
1:D:293:ASP:OD2	3:D:2450:HOH:O	2.17	0.57
1:C:324:ILE:HB	1:C:373[B]:ILE:HD13	1.87	0.57
1:B:53:LYS:HE2	3:B:2123:HOH:O	2.05	0.57
1:C:302[B]:THR:CG2	3:C:2507:HOH:O	2.54	0.56
1:D:281:MET:HE1	1:D:388:ASN:ND2	2.16	0.56
1:D:50:GLY:HA2	3:D:2162:HOH:O	2.04	0.56
1:A:257[B]:ILE:CD1	1:A:401[B]:MET:HG2	2.23	0.55
1:D:365:ASP:N	3:D:2379:HOH:O	2.39	0.55
1:C:362:GLU:HG3	3:C:2567:HOH:O	2.05	0.55
1:D:50:GLY:N	3:D:2162:HOH:O	2.33	0.55
1:B:285[B]:MET:HE1	1:B:316:VAL:CG1	2.35	0.55
1:D:161:SER:OG	1:D:168:HIS:HD2	1.89	0.55
1:D:65:VAL:HA	1:D:68[B]:MET:SD	2.47	0.55
1:A:62:ARG:O	3:A:2192:HOH:O	2.18	0.55
1:D:285:MET:HE2	1:D:386:MET:CE	2.37	0.55
1:B:177[B]:ILE:HD12	1:B:240:VAL:HG12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:210:LYS:HB3	3:D:2363:HOH:O	2.07	0.55
1:D:314[A]:ARG:NH1	3:D:2467:HOH:O	2.39	0.54
1:D:268:ASP:HB2	3:D:2423:HOH:O	2.07	0.54
1:A:177[A]:ILE:CD1	1:A:240:VAL:HG12	2.38	0.54
1:D:210:LYS:C	3:D:2363:HOH:O	2.46	0.53
1:D:294:TYR:HA	3:D:2476:HOH:O	2.07	0.53
1:D:50:GLY:CA	3:D:2162:HOH:O	2.57	0.53
1:D:285:MET:CE	1:D:386:MET:HE3	2.39	0.52
1:A:177[A]:ILE:HD12	1:A:240:VAL:HG12	1.91	0.52
1:A:30:ARG:NH1	3:A:2098:HOH:O	2.42	0.52
1:B:362:GLU:CG	3:B:2540:HOH:O	2.57	0.52
1:A:363[B]:GLU:HG3	3:A:2511:HOH:O	2.09	0.51
1:C:113:GLN:HE21	1:D:113:GLN:CG	2.21	0.51
1:B:177[B]:ILE:CD1	1:B:240:VAL:HG12	2.41	0.51
1:D:330:MET:HG3	3:D:2501:HOH:O	2.09	0.51
1:D:220:ARG:HH22	1:D:362:GLU:CD	2.15	0.50
1:A:113:GLN:HE21	1:B:110:PRO:HA	1.75	0.50
1:A:101:LEU:HD23	1:A:186:PHE:HB2	1.94	0.49
1:D:259:GLY:HA3	1:D:284:ALA:O	2.12	0.49
1:A:272:PRO:HB2	3:A:2427:HOH:O	2.11	0.49
1:C:372:ASN:ND2	3:C:2585:HOH:O	2.36	0.49
1:A:49:TRP:CE3	1:A:193:LEU:HG	2.48	0.49
1:B:285[B]:MET:HE3	1:B:316:VAL:CG1	2.41	0.49
1:A:6:ILE:HD11	1:A:257[A]:ILE:HD11	1.94	0.48
1:C:204[B]:MET:HE1	1:C:270:VAL:HG11	1.94	0.48
1:A:101:LEU:HD21	1:A:237[B]:MET:CE	2.43	0.48
1:D:40:LYS:HB3	3:D:2115:HOH:O	2.12	0.48
1:A:292:ILE:O	1:A:322:PRO:HB3	2.13	0.47
1:D:292:ILE:O	1:D:322:PRO:HB3	2.14	0.47
1:B:165:THR:HB	1:B:336:GLY:HA2	1.97	0.47
1:B:95[A]:ASN:ND2	3:B:2287:HOH:O	2.48	0.47
1:A:110:PRO:HG2	1:A:197:MET:HB2	1.97	0.47
1:D:281:MET:HB3	1:D:285:MET:CE	2.45	0.46
1:D:294:TYR:CE2	1:D:349[A]:MET:CE	2.98	0.46
1:B:362:GLU:HB3	3:B:2541:HOH:O	2.14	0.46
1:D:219:SER:HB3	3:D:2378:HOH:O	2.15	0.46
1:D:159:ILE:O	1:D:165:THR:HG23	2.16	0.46
1:C:110:PRO:HG2	1:C:197:MET:HB2	1.98	0.45
1:A:295[B]:LEU:HD23	1:A:386[B]:MET:CG	2.46	0.45
1:A:272:PRO:HG2	1:A:308:LYS:HG3	1.99	0.45
1:B:367:GLN:HB3	3:B:2557:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172[B]:ASN:HD21	1:B:172[B]:ASN:HD21	1.65	0.44
1:B:314:ARG:NH2	1:B:369:ALA:O	2.35	0.44
1:C:204[A]:MET:SD	1:C:392[A]:PHE:HE2	2.41	0.44
1:D:257:ILE:HD13	1:D:401[A]:MET:HG2	2.00	0.44
1:D:155[B]:VAL:CG2	1:D:157:TYR:CE2	3.01	0.44
1:B:257[B]:ILE:HD13	1:B:401[B]:MET:HG2	1.99	0.44
1:D:33:ILE:HG13	3:D:2373:HOH:O	2.17	0.44
1:D:49:TRP:CE3	1:D:193:LEU:HG	2.53	0.44
1:A:81:GLN:HG3	3:A:2224:HOH:O	2.17	0.43
1:B:349:MET:HB3	1:B:354:PHE:O	2.17	0.43
1:C:40[B]:LYS:NZ	3:C:2138:HOH:O	2.50	0.43
1:D:285:MET:HE2	1:D:317:PHE:CZ	2.52	0.43
1:B:110:PRO:HG2	1:B:197:MET:HB2	2.00	0.43
1:D:285:MET:HE3	1:D:386:MET:CE	2.42	0.43
1:D:314[A]:ARG:NH2	1:D:367:GLN:O	2.51	0.43
1:C:113:GLN:NE2	1:D:113:GLN:OE1	2.52	0.42
1:A:28:GLU:HG2	3:A:2086:HOH:O	2.19	0.42
1:D:101[A]:LEU:HD23	1:D:147:ALA:HB2	2.01	0.42
1:C:53:LYS:HE2	3:C:2105:HOH:O	2.19	0.42
1:D:270:VAL:HG22	3:D:2422:HOH:O	2.18	0.42
1:C:165:THR:HB	1:C:336:GLY:HA2	2.00	0.42
1:C:350:LEU:HD11	1:C:403:LYS:HG3	2.02	0.42
1:C:135:THR:HG21	1:D:269[B]:MET:HG3	2.01	0.42
1:A:366:GLU:HG3	1:A:367:GLN:N	2.35	0.41
1:A:85:ASP:HB2	3:A:2019:HOH:O	2.18	0.41
1:B:213:ASP:HB3	3:B:2409:HOH:O	2.18	0.41
1:A:302[A]:THR:HG22	3:A:2459:HOH:O	2.20	0.41
1:D:102:ILE:O	1:D:187:ALA:HA	2.21	0.41
1:C:204[B]:MET:HE1	1:C:270:VAL:CG1	2.50	0.41
1:B:257[B]:ILE:CD1	1:B:401[B]:MET:HG2	2.51	0.41
1:C:30:ARG:HD3	3:C:2100:HOH:O	2.20	0.40
1:A:51:ASN:HA	1:A:193:LEU:CD2	2.50	0.40
1:A:225:HIS:HE1	1:A:363[B]:GLU:OE2	2.04	0.40
1:D:36:SER:HB2	1:D:49:TRP:CE2	2.56	0.40
1:B:52:VAL:HG12	1:B:54:LEU:H	1.86	0.40
1:A:159:ILE:O	1:A:165:THR:HG23	2.21	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:2188:HOH:O	3:D:2060:HOH:O[1_455]	2.03	0.17
3:C:2236:HOH:O	3:D:2496:HOH:O[1_455]	2.07	0.13
3:B:2270:HOH:O	3:C:2249:HOH:O[2_664]	2.19	0.01

## 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	419/406 (103%)	401 (96%)	17 (4%)	1 (0%)	47	23
1	B	421/406 (104%)	408 (97%)	11 (3%)	2 (0%)	29	9
1	C	428/406 (105%)	414 (97%)	13 (3%)	1 (0%)	47	23
1	D	422/406 (104%)	407 (96%)	12 (3%)	3 (1%)	22	6
All	All	1690/1624 (104%)	1630 (96%)	53 (3%)	7 (0%)	34	13

All (7) 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	B	301	SER
1	D	301	SER
1	D	161	SER

### 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	324/309 (105%)	311 (96%)	13 (4%)	31 6
1	B	326/309 (106%)	320 (98%)	6 (2%)	59 30
1	C	333/309 (108%)	328 (98%)	5 (2%)	65 39
1	D	327/309 (106%)	319 (98%)	8 (2%)	49 19
All	All	1310/1236 (106%)	1278 (98%)	32 (2%)	49 19

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

Mol	Chain	Res	Type
1	A	20	GLN
1	A	28	GLU
1	A	49	TRP
1	A	53[A]	LYS
1	A	53[B]	LYS
1	A	62	ARG
1	A	127	LYS
1	A	273	SER
1	A	333	HIS
1	A	358	SER
1	A	362	GLU
1	A	364	LEU
1	A	366	GLU
1	B	20	GLN
1	B	49	TRP
1	B	213	ASP
1	B	319	ASP
1	B	333	HIS
1	B	358	SER
1	C	49	TRP
1	C	62	ARG
1	C	320	LYS
1	C	333	HIS
1	C	358	SER
1	D	13[A]	SER
1	D	13[B]	SER
1	D	30	ARG
1	D	49	TRP
1	D	333	HIS
1	D	358	SER
1	D	372[A]	ASN
1	D	372[B]	ASN



Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	113	GLN
1	A	168	HIS
1	B	20	GLN
1	B	168	HIS
1	C	113	GLN
1	C	168	HIS
1	D	113	GLN
1	D	168	HIS
1	D	388	ASN

### 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 2 ligands modelled in this entry, 2 are monoatomic - 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

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	404/406 (99%)	0.05	8 (1%) 65 70	8, 18, 29, 39	12 (2%)
1	B	404/406 (99%)	-0.35	6 (1%) 73 78	6, 14, 27, 46	7 (1%)
1	C	406/406 (100%)	-0.42	3 (0%) 87 90	6, 12, 24, 37	11 (2%)
1	D	404/406 (99%)	0.33	24 (5%) 22 24	8, 19, 36, 50	13 (3%)
All	All	1618/1624 (99%)	-0.10	41 (2%) 57 62	6, 16, 30, 50	43 (2%)

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	270	VAL	5.7
1	B	270	VAL	5.3
1	D	270	VAL	4.6
1	D	271	ALA	4.3
1	D	319	ASP	4.1
1	C	319	ASP	3.7
1	A	272	PRO	3.6
1	D	213	ASP	3.4
1	C	406	ASP	3.2
1	D	370	GLY	2.9
1	D	361	ILE	2.8
1	D	364	LEU	2.7
1	A	392	PHE	2.7
1	B	319	ASP	2.7
1	A	63	LYS	2.6
1	B	286	HIS	2.6
1	B	271	ALA	2.6
1	D	376[A]	GLU	2.6
1	A	273	SER	2.6
1	D	286	HIS	2.5
1	B	289	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	270	VAL	2.4
1	D	268	ASP	2.4
1	A	1	MET	2.4
1	A	57	THR	2.3
1	D	33	ILE	2.3
1	D	24	ALA	2.3
1	D	48	VAL	2.2
1	D	355	ILE	2.2
1	A	87	GLY	2.2
1	D	371	LEU	2.2
1	D	225	HIS	2.2
1	D	377	THR	2.1
1	B	320	LYS	2.1
1	D	15	ILE	2.1
1	D	211	TYR	2.1
1	D	362	GLU	2.1
1	D	41	ASP	2.1
1	D	214	THR	2.1
1	D	224	ALA	2.1
1	D	373[A]	ILE	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	CL	A	1405	1/1	0.86	0.05	68,68,68,68	0
2	CL	B	1405	1/1	0.98	0.04	40,40,40,40	0

## 6.5 Other polymers

There are no such residues in this entry.