



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 01:23 AM UTC

PDB ID : 2VB9 / pdb_00002vb9
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

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
Xtrriage (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

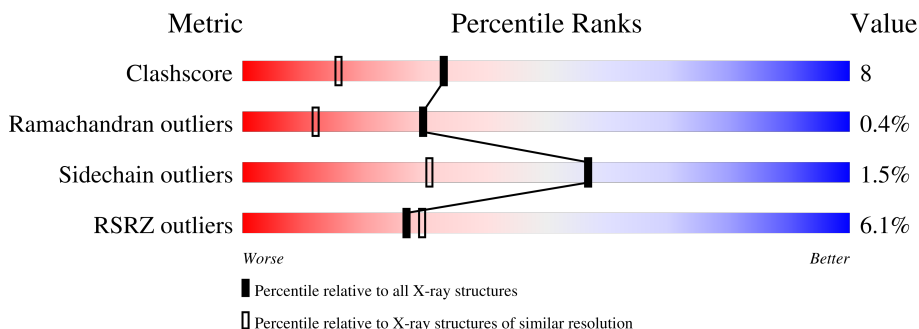
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)
RSRZ outliers	180081	4039 (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 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	 4% 86% 11% .
1	B	406	 3% 88% 10% .
1	C	406	 % 89% 10% .
1	D	406	 16% 81% 17% .

2 Entry composition [i](#)

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

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

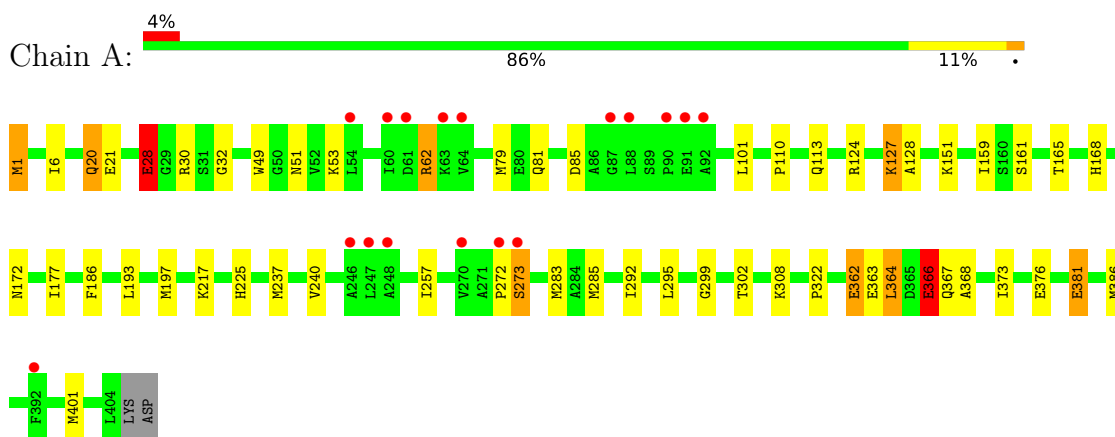
- Molecule 3 is water.

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

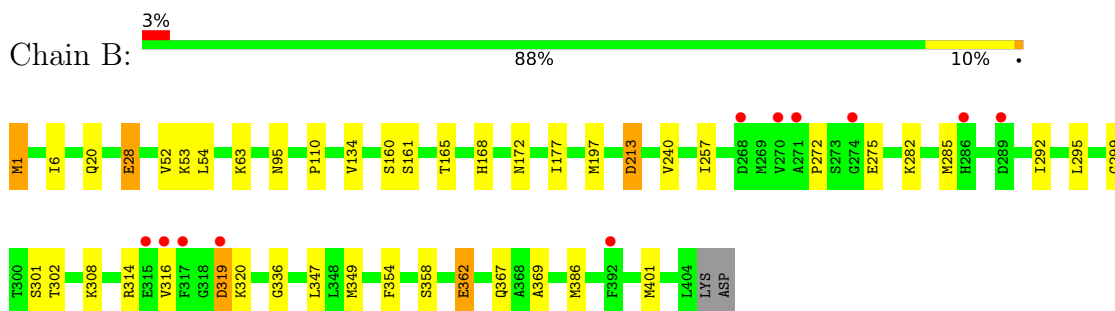
3 Residue-property plots [i](#)

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.

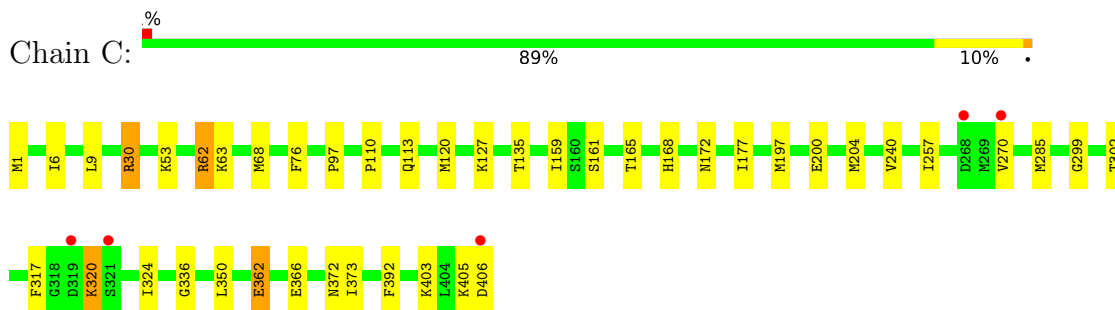
- Molecule 1: 3-OXOACYL-[ACYL-CARRIER-PROTEIN] SYNTHASE 1




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

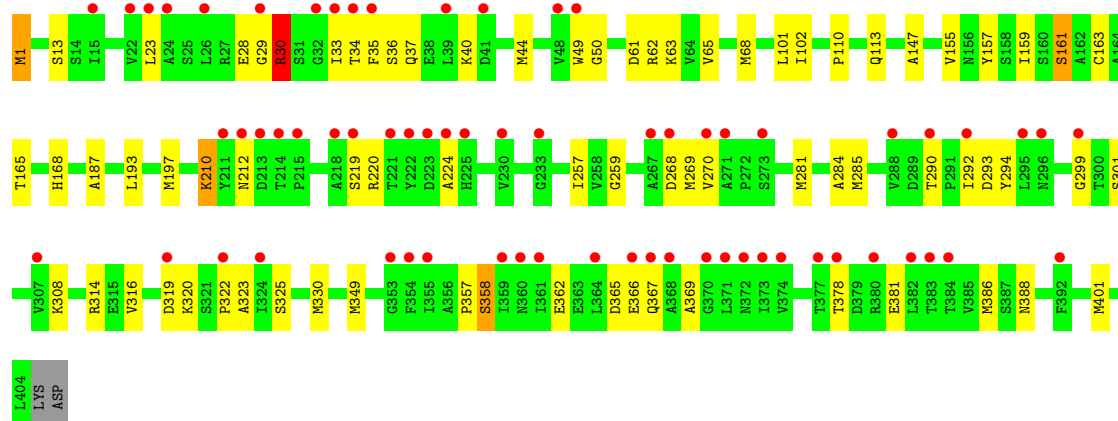


- Molecule 1: 3-OXOACYL-[ACYL-CARRIER-PROTEIN] SYNTHASE 1



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

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	58.91Å 138.35Å 211.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	115.47 – 1.50 115.47 – 1.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (115.47-1.50) 99.8 (115.47-1.50)	Depositor EDS
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.38 (at 1.50Å)	Xtrriage
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 ²)	13.6	Xtrriage
Anisotropy	0.295	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 77.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14389	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtrriage'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.*

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:
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	0.97	8/3141 (0.3%)	1.15	12/4241 (0.3%)
1	B	0.92	3/3160 (0.1%)	0.97	7/4265 (0.2%)
1	C	1.03	8/3224 (0.2%)	1.00	6/4347 (0.1%)
1	D	1.06	8/3170 (0.3%)	1.09	17/4278 (0.4%)
All	All	1.00	27/12695 (0.2%)	1.06	42/17131 (0.2%)

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 (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	30	ARG	NE-CZ	25.30	1.60	1.33
1	C	366	GLU	CG-CD	16.03	1.92	1.52
1	C	62	ARG	CG-CD	-14.69	1.08	1.52
1	B	63	LYS	CG-CD	12.93	1.91	1.52
1	B	319	ASP	CB-CG	12.52	1.83	1.52
1	D	63	LYS	CD-CE	10.51	1.83	1.52
1	C	362	GLU	CG-CD	-9.27	1.28	1.52
1	C	30	ARG	CD-NE	-9.13	1.33	1.46
1	A	28	GLU	CG-CD	-8.97	1.29	1.52
1	C	62	ARG	CB-CG	-8.87	1.25	1.52
1	A	366	GLU	CG-CD	-8.53	1.30	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	151	LYS	CD-CE	8.30	1.77	1.52
1	D	210	LYS	CD-CE	-8.08	1.28	1.52
1	A	362	GLU	CG-CD	7.44	1.70	1.52
1	C	320	LYS	CB-CG	7.40	1.74	1.52
1	A	127	LYS	CG-CD	-7.17	1.30	1.52
1	A	217	LYS	CD-CE	7.01	1.73	1.52
1	C	127	LYS	CD-CE	6.88	1.73	1.52
1	A	381	GLU	CG-CD	6.65	1.68	1.52
1	D	28	GLU	CG-CD	6.45	1.68	1.52
1	D	308	LYS	CD-CE	-6.44	1.33	1.52
1	D	366	GLU	CB-CG	6.24	1.71	1.52
1	A	20	GLN	CG-CD	6.20	1.67	1.52
1	D	1	MET	CA-C	5.78	1.65	1.52
1	D	62	ARG	CB-CG	-5.55	1.35	1.52
1	C	406	ASP	CA-CB	-5.39	1.42	1.53
1	B	1	MET	CA-C	5.21	1.63	1.52

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	30	ARG	CD-NE-CZ	-17.20	100.33	124.40
1	A	366	GLU	CG-CD-OE2	-16.27	80.98	118.40
1	A	28	GLU	CB-CG-CD	15.84	139.53	112.60
1	A	1	MET	CA-C-O	-14.82	95.61	120.80
1	B	362	GLU	CB-CG-CD	12.59	134.01	112.60
1	A	381	GLU	CB-CG-CD	-12.54	91.28	112.60
1	A	366	GLU	CG-CD-OE1	12.41	146.94	118.40
1	D	210	LYS	CG-CD-CE	11.88	138.64	111.30
1	A	1	MET	CB-CA-C	-11.70	87.86	110.10
1	C	366	GLU	CB-CG-CD	-11.20	93.56	112.60
1	D	320	LYS	CA-CB-CG	-10.75	92.59	114.10
1	A	376	GLU	CB-CG-CD	10.56	130.55	112.60
1	C	362	GLU	CB-CG-CD	9.24	128.30	112.60
1	C	1	MET	CA-C-O	9.17	136.39	120.80
1	D	1	MET	CB-CA-C	-8.82	93.35	110.10
1	A	362	GLU	CB-CG-CD	8.81	127.57	112.60
1	D	30	ARG	NE-CZ-NH1	-8.48	113.02	121.50
1	D	28	GLU	CB-CG-CD	-8.34	98.43	112.60
1	B	320	LYS	CG-CD-CE	8.19	130.14	111.30
1	A	151	LYS	CG-CD-CE	-8.05	92.78	111.30
1	B	1	MET	CA-C-O	7.77	134.01	120.80
1	D	1	MET	CA-C-O	-7.51	108.04	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	63	LYS	CG-CD-CE	-7.40	94.27	111.30
1	B	63	LYS	CB-CG-CD	-7.25	94.63	111.30
1	B	28	GLU	CB-CG-CD	6.87	124.27	112.60
1	D	28	GLU	CG-CD-OE1	6.80	134.04	118.40
1	D	28	GLU	CG-CD-OE2	-6.71	102.96	118.40
1	D	308	LYS	CG-CD-CE	6.20	125.56	111.30
1	D	366	GLU	CA-CB-CG	6.19	126.48	114.10
1	D	319	ASP	CB-CG-OD2	6.12	132.47	118.40
1	D	319	ASP	CB-CG-OD1	-6.09	104.40	118.40
1	C	63	LYS	CG-CD-CE	6.04	125.19	111.30
1	D	381	GLU	CB-CG-CD	-5.76	102.80	112.60
1	D	366	GLU	CB-CG-CD	5.68	122.25	112.60
1	C	62	ARG	CB-CG-CD	5.49	123.92	111.30
1	D	319	ASP	CA-CB-CG	-5.48	107.12	112.60
1	C	62	ARG	CA-CB-CG	5.38	124.86	114.10
1	A	28	GLU	CG-CD-OE1	-5.37	106.06	118.40
1	B	362	GLU	CG-CD-OE2	5.30	130.59	118.40
1	B	134	VAL	N-CA-C	5.20	115.82	110.36
1	A	217	LYS	CD-CE-NZ	-5.16	95.39	111.90
1	A	28	GLU	CG-CD-OE2	5.16	130.26	118.40

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 [\(i\)](#)

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	3000	0	2956	44	0
1	B	3001	0	2946	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3041	0	3011	38	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	14	0
3	B	605	0	0	18	1
3	C	629	0	0	18	3
3	D	540	0	0	37	2
All	All	14389	0	11876	186	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 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:D:281:MET:HE2	1:D:388:ASN:HD21	1.02	1.17
1:D:49:TRP:O	3:D:2162:HOH:O	1.67	1.11
1:D:281:MET:HE2	1:D:388:ASN:ND2	1.67	1.10
1:D:285:MET:HE2	1:D:386:MET:HE1	1.13	1.10
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:285:MET:CE	1:D:386:MET:HE1	1.85	1.05
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:49:TRP:C	3:D:2162:HOH:O	2.02	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:B:285[B]:MET:HE1	1:B:316:VAL:HG11	1.46	0.96
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:B:285[B]:MET:HE1	1:B:316:VAL:CG1	2.02	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
1:D:281:MET:CE	1:D:388:ASN:HD21	1.86	0.88
1:D:285:MET:HE2	1:D:386:MET:CE	2.00	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:101:LEU:HD21	1:A:237[B]:MET:HE1	1.59	0.85
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: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:HE2	1:B:386:MET:HE1	1.67	0.77
1:C:172:ASN:HB3	3:C:2367:HOH:O	1.83	0.76
1:B:285[B]:MET:CE	1:B:316:VAL:HG11	2.14	0.75
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: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:C:200:GLU:OE2	1:D:113:GLN:NE2	2.22	0.71
1:D:294:TYR:CE2	1:D:349[A]:MET:HE1	2.27	0.70
1:D:29:GLY:N	3:D:2086:HOH:O	2.25	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: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:A:101:LEU:CD2	1:A:237[B]:MET:HE1	2.24	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
1:B:28:GLU:HG2	3:B:2100:HOH:O	1.97	0.64
1:D:281:MET:HB3	1:D:285:MET:HE3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:362:GLU:HG3	3:B:2540:HOH:O	2.00	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:281:MET:CE	1:D:388:ASN:ND2	2.53	0.60
1:D:285:MET:HE1	1:D:316:VAL:HG11	1.81	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: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: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:302:THR:HG21	3:B:2397:HOH:O	1.94	0.58
1:D:210:LYS:C	3:D:2363:HOH:O	2.46	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:B:285[B]:MET:CE	1:B:316:VAL:CG1	2.80	0.56
1:C:302[B]:THR:CG2	3:C:2507:HOH:O	2.54	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: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:B:177[B]:ILE:HD12	1:B:240:VAL:HG12	1.88	0.55
1:D:220:ARG:HH22	1:D:362:GLU:CD	2.15	0.55
1:D:294:TYR:CD2	1:D:349[A]:MET:HE1	2.42	0.55
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:50:GLY:CA	3:D:2162:HOH:O	2.57	0.53
1:D:294:TYR:HA	3:D:2476:HOH:O	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:ARG:NH1	3:A:2098:HOH:O	2.42	0.52
1:A:177[A]:ILE:HD12	1:A:240:VAL:HG12	1.91	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:A:113:GLN:HE21	1:B:110:PRO:HA	1.75	0.50
1:B:285[B]:MET:HE1	1:B:316:VAL:HG12	1.90	0.49
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:A:79:MET:SD	1:A:237[B]:MET:HE3	2.52	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:A:6:ILE:HD11	1:A:257[A]:ILE:HD11	1.94	0.48
1:D:40:LYS:HB3	3:D:2115:HOH:O	2.12	0.48
1:B:282:LYS:NZ	3:B:2470:HOH:O	2.45	0.48
1:A:292:ILE:O	1:A:322:PRO:HB3	2.13	0.47
1:A:285:MET:SD	1:A:386[B]:MET:HE1	2.54	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:C:68[B]:MET:HE1	1:C:76:PHE:CD2	2.49	0.46
1:D:281:MET:HB3	1:D:285:MET:CE	2.45	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:A:283:MET:HE1	3:B:2295: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:B:160[C]:SER:OG	3:B:2363:HOH:O	2.20	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:D:294:TYR:CE2	1:D:349[A]:MET:CE	2.98	0.45
1:B:367:GLN:HB3	3:B:2557:HOH:O	2.16	0.45
1:A:172[B]:ASN:HD21	1:B:172[B]:ASN:HD21	1.65	0.44
1:C:285[B]:MET:HE1	1:C:317:PHE:CE1	2.52	0.44
1:B:314:ARG:NH2	1:B:369:ALA:O	2.35	0.44
1:D:50:GLY:N	3:D:2162:HOH:O	2.33	0.44
1:D:294:TYR:CZ	1:D:349[A]:MET:HE1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:120:MET:HE2	1:D:44:MET:HG3	1.98	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:85:ASP:CG	3:A:2019:HOH:O	2.61	0.43
1:A:81:GLN:HG3	3:A:2224:HOH:O	2.17	0.43
1:C:285[B]:MET:HE2	3:C:2286:HOH:O	2.18	0.43
1:B:349:MET:HB3	1:B:354:PHE:O	2.17	0.43
1:B:110:PRO:HG2	1:B:197:MET:HB2	2.00	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:B:295:LEU:HD23	1:B:295:LEU:C	2.45	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:85:ASP:HB2	3:A:2019:HOH:O	2.18	0.41
1:A:366:GLU:HG3	1:A:367:GLN:N	2.35	0.41
1:C:403:LYS:NZ	3:C:2621:HOH:O	2.53	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:B:257[B]:ILE:CD1	1:B:401[B]:MET:HG2	2.51	0.41
1:C:204[B]:MET:HE1	1:C:270:VAL:HG11	2.02	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%)	43 22
1	B	421/406 (104%)	408 (97%)	11 (3%)	2 (0%)	24 8
1	C	428/406 (105%)	414 (97%)	13 (3%)	1 (0%)	43 22
1	D	422/406 (104%)	407 (96%)	12 (3%)	3 (1%)	18 5
All	All	1690/1624 (104%)	1630 (96%)	53 (3%)	7 (0%)	30 12

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%)	315 (97%)	9 (3%)	38	11
1	B	326/309 (106%)	322 (99%)	4 (1%)	63	38
1	C	333/309 (108%)	331 (99%)	2 (1%)	78	62
1	D	327/309 (106%)	322 (98%)	5 (2%)	57	31
All	All	1310/1236 (106%)	1290 (98%)	20 (2%)	57	31

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	28	GLU
1	A	62	ARG
1	A	127	LYS
1	A	273	SER
1	A	362	GLU
1	A	364	LEU
1	A	366	GLU
1	A	381	GLU
1	B	20	GLN
1	B	213	ASP
1	B	319	ASP
1	B	358	SER
1	C	62	ARG
1	C	320	LYS
1	D	13[A]	SER
1	D	13[B]	SER
1	D	30	ARG
1	D	163	CYS
1	D	358	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	113	GLN
1	A	168	HIS
1	A	176	GLN
1	A	367	GLN
1	A	396	ASN
1	B	20	GLN
1	B	168	HIS

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Mol	Chain	Res	Type
1	B	396	ASN
1	C	95	ASN
1	C	113	GLN
1	C	168	HIS
1	C	176	GLN
1	C	372	ASN
1	C	396	ASN
1	D	19	GLN
1	D	37	GLN
1	D	113	GLN
1	D	168	HIS
1	D	178	GLN
1	D	286	HIS
1	D	388	ASN
1	D	396	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 oligosaccharides 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 [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, 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	404/406 (99%)	0.44	17 (4%) 40 44	7, 18, 29, 39	27 (6%)
1	B	404/406 (99%)	-0.14	11 (2%) 56 60	6, 13, 26, 46	23 (5%)
1	C	406/406 (100%)	-0.26	5 (1%) 76 80	5, 12, 23, 37	32 (7%)
1	D	404/406 (99%)	0.78	65 (16%) 4 4	7, 19, 35, 50	32 (7%)
All	All	1618/1624 (99%)	0.20	98 (6%) 27 29	5, 15, 29, 50	114 (7%)

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	270	VAL	6.0
1	D	364	LEU	5.0
1	A	270	VAL	4.4
1	D	271	ALA	4.1
1	D	270	VAL	4.1
1	D	361	ILE	4.0
1	A	392	PHE	3.7
1	C	319	ASP	3.5
1	A	272	PRO	3.4
1	D	224	ALA	3.4
1	D	33	ILE	3.3
1	D	48	VAL	3.3
1	D	211	TYR	3.2
1	D	322	PRO	3.1
1	D	355	ILE	3.1
1	D	214	THR	3.1
1	D	377	THR	3.0
1	D	35	PHE	3.0
1	D	49	TRP	3.0
1	D	374	VAL	2.9
1	D	354	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	292	ILE	2.9
1	D	324	ILE	2.9
1	C	406	ASP	2.9
1	B	392	PHE	2.8
1	C	270	VAL	2.8
1	A	63	LYS	2.8
1	D	290	THR	2.8
1	A	92	ALA	2.7
1	D	24	ALA	2.7
1	A	273	SER	2.7
1	D	213	ASP	2.7
1	D	26	LEU	2.6
1	D	307	VAL	2.6
1	B	271	ALA	2.6
1	D	378	THR	2.6
1	A	60	ILE	2.5
1	B	286	HIS	2.5
1	D	22	VAL	2.5
1	A	54	LEU	2.5
1	D	360	ASN	2.5
1	D	29	GLY	2.5
1	D	32	GLY	2.5
1	D	371	LEU	2.5
1	D	267	ALA	2.4
1	D	380	ARG	2.4
1	D	215	PRO	2.4
1	D	222	TYR	2.4
1	D	373[A]	ILE	2.4
1	D	366	GLU	2.4
1	D	382	LEU	2.4
1	B	317	PHE	2.4
1	C	321	SER	2.4
1	D	219	SER	2.4
1	D	392	PHE	2.4
1	A	248	ALA	2.4
1	D	15	ILE	2.4
1	D	384	THR	2.4
1	D	370	GLY	2.4
1	D	368	ALA	2.3
1	B	316	VAL	2.3
1	A	88	LEU	2.3
1	D	34	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	223	ASP	2.3
1	A	247	LEU	2.3
1	D	295	LEU	2.3
1	D	212	ASN	2.3
1	D	230	VAL	2.3
1	A	87	GLY	2.2
1	D	225	HIS	2.2
1	B	319	ASP	2.2
1	D	41	ASP	2.2
1	D	221	THR	2.2
1	A	64	VAL	2.2
1	D	39	LEU	2.2
1	D	23	LEU	2.1
1	A	90	PRO	2.1
1	A	246	ALA	2.1
1	B	274	GLY	2.1
1	D	353	GLY	2.1
1	D	383	THR	2.1
1	A	91	GLU	2.1
1	D	372[A]	ASN	2.1
1	B	268[A]	ASP	2.1
1	D	218	ALA	2.1
1	D	359	ILE	2.1
1	B	315	GLU	2.1
1	A	61[A]	ASP	2.1
1	D	233	GLY	2.1
1	D	268	ASP	2.1
1	D	319	ASP	2.1
1	D	288	VAL	2.0
1	D	367	GLN	2.0
1	D	299	GLY	2.0
1	D	273	SER	2.0
1	B	289	ASP	2.0
1	C	268[A]	ASP	2.0
1	D	296	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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(\AA^2)	Q<0.9
2	CL	A	1405	1/1	0.81	0.17	68,68,68,68	0
2	CL	B	1405	1/1	0.97	0.05	40,40,40,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.