



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 07:36 PM UTC

PDB ID : 8VDB / pdb_00008vdb
Title : Crystal structure of Bacillus subtilis FabHB, beta-ketoacyl carrier protein synthase III
Authors : Radka, C.D.; Rock, C.O.
Deposited on : 2023-12-14
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

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
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

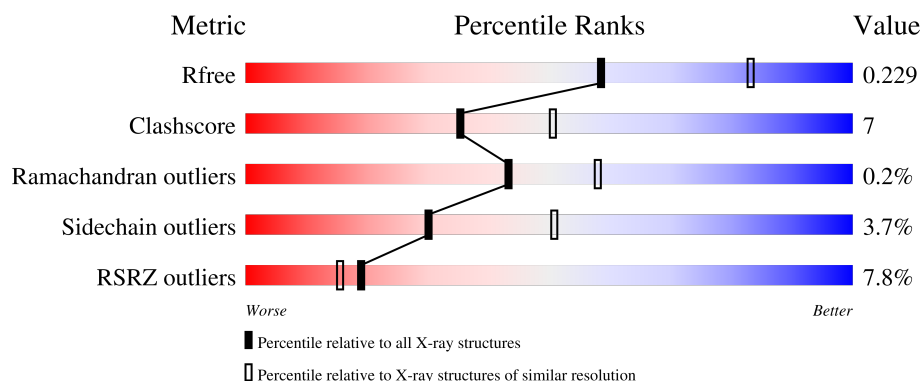
1 Overall quality at a glance

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 ≥ 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	345	9% 77% 17% • 6%
1	B	345	10% 75% 19% 6%
1	C	345	5% 77% 16% • 6%
1	D	345	6% 79% 15% • 6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10316 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 Beta-ketoacyl-[acyl-carrier-protein] synthase III 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	326	Total	C	N	O	S	0	0	0
			2475	1563	424	477	11			
1	B	326	Total	C	N	O	S	0	0	0
			2476	1564	425	476	11			
1	C	326	Total	C	N	O	S	0	0	0
			2496	1576	429	481	10			
1	D	325	Total	C	N	O	S	0	0	0
			2469	1558	423	477	11			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP O07600
A	-18	GLY	-	expression tag	UNP O07600
A	-17	SER	-	expression tag	UNP O07600
A	-16	SER	-	expression tag	UNP O07600
A	-15	HIS	-	expression tag	UNP O07600
A	-14	HIS	-	expression tag	UNP O07600
A	-13	HIS	-	expression tag	UNP O07600
A	-12	HIS	-	expression tag	UNP O07600
A	-11	HIS	-	expression tag	UNP O07600
A	-10	HIS	-	expression tag	UNP O07600
A	-9	SER	-	expression tag	UNP O07600
A	-8	SER	-	expression tag	UNP O07600
A	-7	GLY	-	expression tag	UNP O07600
A	-6	LEU	-	expression tag	UNP O07600
A	-5	VAL	-	expression tag	UNP O07600
A	-4	PRO	-	expression tag	UNP O07600
A	-3	ARG	-	expression tag	UNP O07600
A	-2	GLY	-	expression tag	UNP O07600
A	-1	SER	-	expression tag	UNP O07600
A	0	HIS	-	expression tag	UNP O07600
B	-19	MET	-	initiating methionine	UNP O07600

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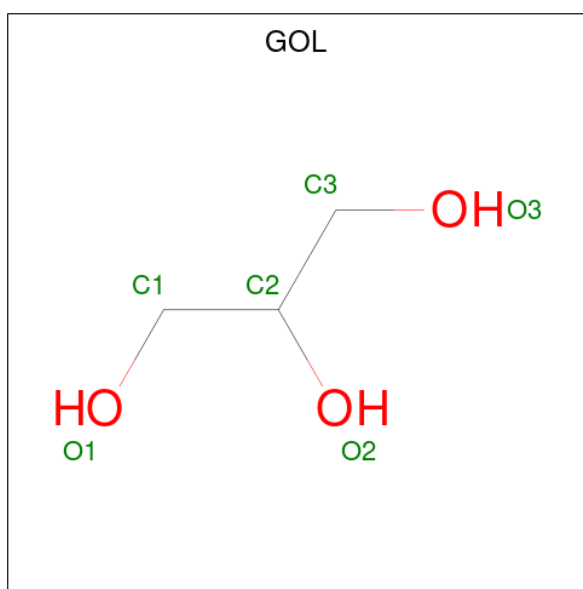
Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	expression tag	UNP O07600
B	-17	SER	-	expression tag	UNP O07600
B	-16	SER	-	expression tag	UNP O07600
B	-15	HIS	-	expression tag	UNP O07600
B	-14	HIS	-	expression tag	UNP O07600
B	-13	HIS	-	expression tag	UNP O07600
B	-12	HIS	-	expression tag	UNP O07600
B	-11	HIS	-	expression tag	UNP O07600
B	-10	HIS	-	expression tag	UNP O07600
B	-9	SER	-	expression tag	UNP O07600
B	-8	SER	-	expression tag	UNP O07600
B	-7	GLY	-	expression tag	UNP O07600
B	-6	LEU	-	expression tag	UNP O07600
B	-5	VAL	-	expression tag	UNP O07600
B	-4	PRO	-	expression tag	UNP O07600
B	-3	ARG	-	expression tag	UNP O07600
B	-2	GLY	-	expression tag	UNP O07600
B	-1	SER	-	expression tag	UNP O07600
B	0	HIS	-	expression tag	UNP O07600
C	-19	MET	-	initiating methionine	UNP O07600
C	-18	GLY	-	expression tag	UNP O07600
C	-17	SER	-	expression tag	UNP O07600
C	-16	SER	-	expression tag	UNP O07600
C	-15	HIS	-	expression tag	UNP O07600
C	-14	HIS	-	expression tag	UNP O07600
C	-13	HIS	-	expression tag	UNP O07600
C	-12	HIS	-	expression tag	UNP O07600
C	-11	HIS	-	expression tag	UNP O07600
C	-10	HIS	-	expression tag	UNP O07600
C	-9	SER	-	expression tag	UNP O07600
C	-8	SER	-	expression tag	UNP O07600
C	-7	GLY	-	expression tag	UNP O07600
C	-6	LEU	-	expression tag	UNP O07600
C	-5	VAL	-	expression tag	UNP O07600
C	-4	PRO	-	expression tag	UNP O07600
C	-3	ARG	-	expression tag	UNP O07600
C	-2	GLY	-	expression tag	UNP O07600
C	-1	SER	-	expression tag	UNP O07600
C	0	HIS	-	expression tag	UNP O07600
D	-19	MET	-	initiating methionine	UNP O07600
D	-18	GLY	-	expression tag	UNP O07600
D	-17	SER	-	expression tag	UNP O07600

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	expression tag	UNP O07600
D	-15	HIS	-	expression tag	UNP O07600
D	-14	HIS	-	expression tag	UNP O07600
D	-13	HIS	-	expression tag	UNP O07600
D	-12	HIS	-	expression tag	UNP O07600
D	-11	HIS	-	expression tag	UNP O07600
D	-10	HIS	-	expression tag	UNP O07600
D	-9	SER	-	expression tag	UNP O07600
D	-8	SER	-	expression tag	UNP O07600
D	-7	GLY	-	expression tag	UNP O07600
D	-6	LEU	-	expression tag	UNP O07600
D	-5	VAL	-	expression tag	UNP O07600
D	-4	PRO	-	expression tag	UNP O07600
D	-3	ARG	-	expression tag	UNP O07600
D	-2	GLY	-	expression tag	UNP O07600
D	-1	SER	-	expression tag	UNP O07600
D	0	HIS	-	expression tag	UNP O07600

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	6	0
			6	3	3		
2	C	1	Total	C	O	6	0
			6	3	3		
2	D	1	Total	C	O	6	0
			6	3	3		

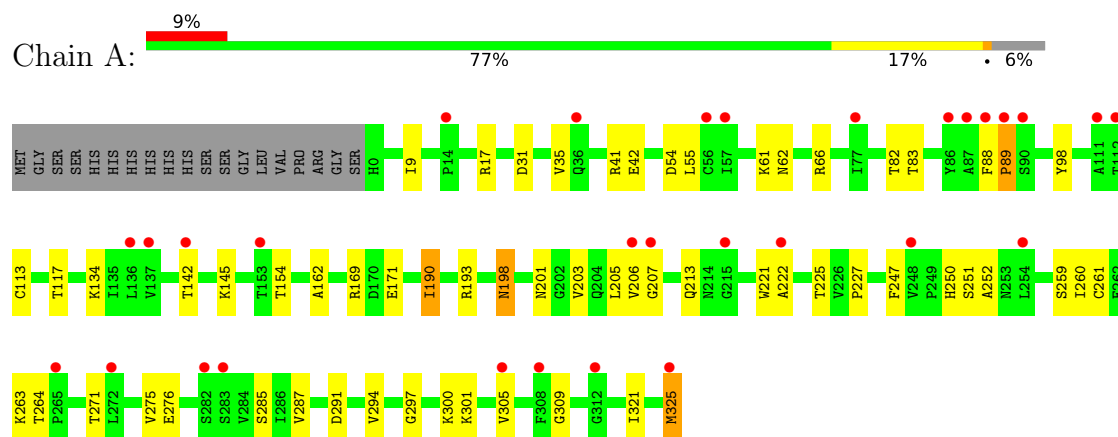
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	118	Total 118	O 118	0	0
3	B	81	Total 81	O 81	0	0
3	C	85	Total 85	O 85	0	0
3	D	98	Total 98	O 98	0	0

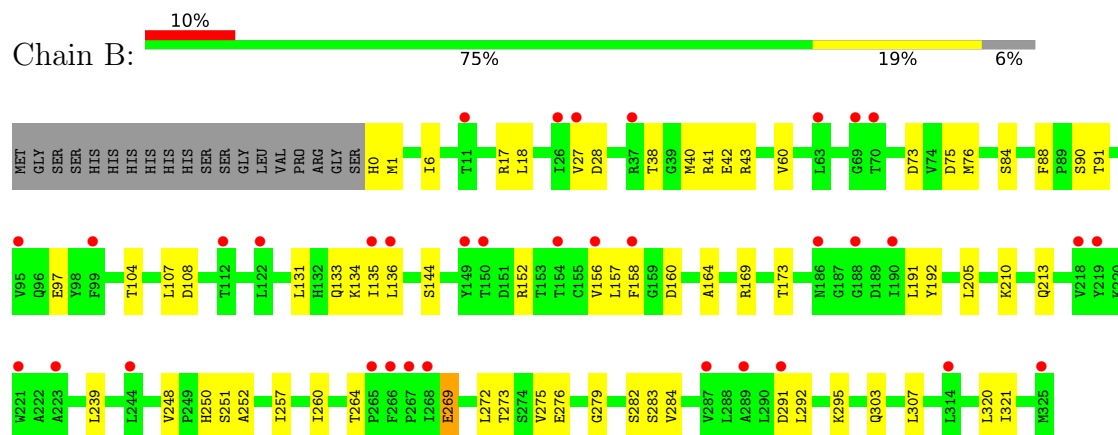
3 Residue-property plots

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.

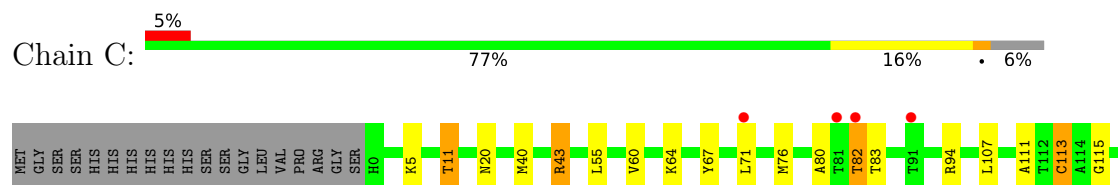
- Molecule 1: Beta-ketoacyl-[acyl-carrier-protein] synthase III 2

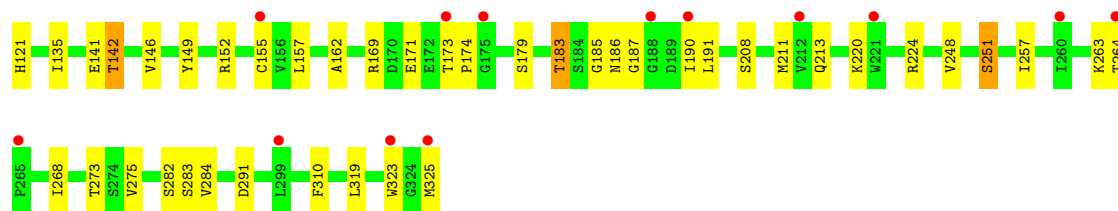


- Molecule 1: Beta-ketoacyl-[acyl-carrier-protein] synthase III 2

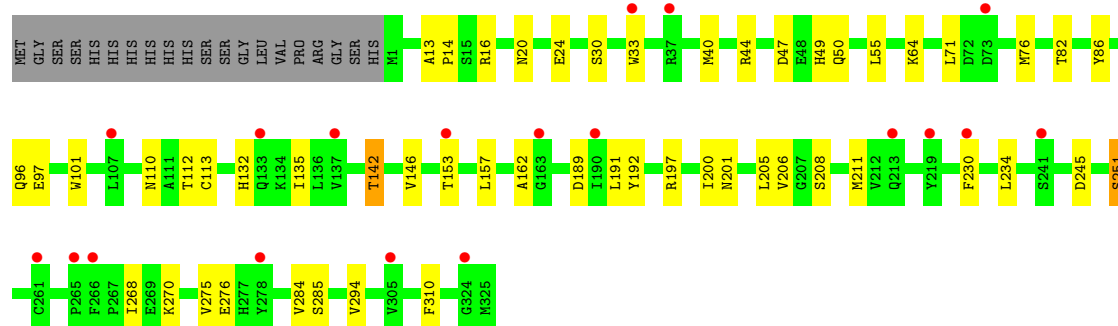
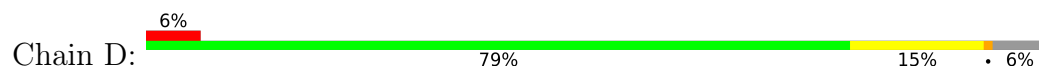


- Molecule 1: Beta-ketoacyl-[acyl-carrier-protein] synthase III 2





• Molecule 1: Beta-ketoacyl-[acyl-carrier-protein] synthase III 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	91.96Å 92.72Å 94.00Å 111.66° 110.13° 105.45°	Depositor
Resolution (Å)	45.20 – 2.40 45.20 – 2.40	Depositor EDS
% Data completeness (in resolution range)	93.1 (45.20-2.40) 93.1 (45.20-2.40)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, R_{free}	0.206 , 0.230 0.211 , 0.229	Depositor DCC
R_{free} test set	1995 reflections (2.11%)	wwPDB-VP
Wilson B-factor (Å ²)	46.5	Xtriage
Anisotropy	0.139	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 26.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.000 for -l,h+k+l,-k 0.000 for h+k+l,-l,-h 0.016 for k,h,-h-k-l 0.004 for -k,-h,-l 0.013 for l,-h-k-l,h 0.020 for -h-k-l,l,k 0.000 for -h,-k,h+k+l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10316	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.18% 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: GOL

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	0.23	0/2517	0.48	1/3411 (0.0%)
1	B	0.26	0/2519	0.47	0/3413
1	C	0.24	0/2539	0.47	0/3438
1	D	0.24	0/2511	0.43	0/3405
All	All	0.24	0/10086	0.46	1/13667 (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	89	PRO	N-CA-C	-6.01	100.10	112.47

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	2475	0	2464	41	0
1	B	2476	0	2467	46	0
1	C	2496	0	2498	36	0
1	D	2469	0	2458	35	0
2	A	6	0	8	0	0
2	C	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	6	0	8	0	0
3	A	118	0	0	8	0
3	B	81	0	0	6	0
3	C	85	0	0	4	0
3	D	98	0	0	4	0
All	All	10316	0	9911	146	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 (146) 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:40:MET:HE1	1:B:157:LEU:HA	1.49	0.94
1:B:251:SER:HA	1:B:257:ILE:HD11	1.62	0.81
1:B:136:LEU:HD11	1:B:164:ALA:HB1	1.67	0.77
1:C:76:MET:HB3	1:C:135:ILE:HG12	1.68	0.75
1:B:295:LYS:NZ	3:B:403:HOH:O	2.22	0.70
1:B:276:GLU:HG3	3:B:444:HOH:O	1.92	0.69
1:C:263:LYS:NZ	3:C:501:HOH:O	2.27	0.68
1:B:269:GLU:HG2	1:D:33:TRP:HZ2	1.60	0.66
1:B:191:LEU:HD13	1:B:213:GLN:HB2	1.77	0.65
1:B:133:GLN:HE22	1:B:169:ARG:HD2	1.62	0.64
1:D:64:LYS:HZ1	1:D:71:LEU:H	1.45	0.64
1:B:248:VAL:HG22	1:B:272:LEU:HB2	1.81	0.62
1:A:260:ILE:O	1:A:264:THR:HG22	2.01	0.61
1:D:47:ASP:H	1:D:50:GLN:HE21	1.49	0.60
1:D:24:GLU:HG2	1:D:30:SER:HA	1.83	0.60
1:C:191:LEU:HD13	1:C:213:GLN:HB3	1.83	0.59
1:A:251:SER:HB2	1:A:285:SER:HB2	1.83	0.59
1:C:220:LYS:O	1:C:224:ARG:HG3	2.02	0.59
1:B:144:SER:OG	1:B:160:ASP:OD2	2.20	0.59
1:C:149:TYR:HD1	1:C:155:CYS:HG	1.51	0.59
1:A:261:CYS:SG	1:A:271:THR:HG21	2.43	0.58
1:A:41:ARG:HG3	1:A:276:GLU:HG3	1.85	0.57
1:B:303:GLN:NE2	3:B:404:HOH:O	2.23	0.57
1:B:60:VAL:HG22	1:B:136:LEU:HD21	1.86	0.56
1:B:260:ILE:O	1:B:264:THR:HG22	2.06	0.56
1:D:76:MET:HB3	1:D:135:ILE:HG12	1.88	0.55
1:A:190:ILE:HD11	3:A:590:HOH:O	2.07	0.55
1:C:179:SER:HB2	1:C:319:LEU:HD23	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:142:THR:HG22	1:D:142:THR:O	2.07	0.54
1:A:83:THR:HB	1:A:142:THR:HG22	1.89	0.54
1:B:84:SER:HG	1:B:91:THR:HG1	1.54	0.54
1:C:113:CYS:HB2	1:C:310:PHE:O	2.07	0.54
1:C:94:ARG:HD2	3:C:547:HOH:O	2.07	0.54
1:C:83:THR:HB	1:C:142:THR:HG22	1.89	0.54
1:B:107:LEU:HD12	1:C:111:ALA:HB2	1.89	0.54
1:D:76:MET:HB2	1:D:132:HIS:CE1	2.43	0.53
1:C:169:ARG:NH1	1:C:171:GLU:OE2	2.40	0.53
1:C:20:ASN:OD1	1:C:43:ARG:NH2	2.35	0.52
1:C:107:LEU:HA	3:C:521:HOH:O	2.10	0.52
1:C:40:MET:HE2	1:C:275:VAL:HG22	1.91	0.52
1:D:146:VAL:HG23	1:D:211:MET:HE2	1.92	0.52
1:B:6:ILE:HD12	1:B:321:ILE:HD12	1.90	0.51
1:A:291:ASP:HA	1:A:294:VAL:HG12	1.93	0.51
1:B:104:THR:O	1:C:183:THR:HG22	2.10	0.51
1:C:11:THR:HB	1:C:291:ASP:OD2	2.11	0.51
1:A:82:THR:HB	3:A:520:HOH:O	2.10	0.51
1:A:55:LEU:HB3	1:A:162:ALA:HB2	1.93	0.51
1:A:142:THR:OG1	1:A:145:LYS:HE2	2.10	0.51
1:B:73:ASP:HB2	1:B:134:LYS:HD2	1.93	0.51
1:C:64:LYS:HG2	1:C:71:LEU:HD12	1.93	0.51
1:B:28:ASP:O	1:B:152:ARG:HD2	2.11	0.50
1:B:307:LEU:HD11	1:B:321:ILE:HD13	1.93	0.50
1:C:146:VAL:HG23	1:C:211:MET:HE2	1.93	0.50
1:C:5:LYS:NZ	1:C:173:THR:OG1	2.44	0.50
1:B:40:MET:HG2	1:B:275:VAL:HG22	1.92	0.50
1:D:13:ALA:HB1	1:D:44:ARG:HG3	1.94	0.49
1:A:251:SER:HB3	1:A:275:VAL:HG13	1.94	0.49
1:A:9:ILE:HG22	1:A:325:MET:HE1	1.95	0.49
1:A:221:TRP:O	1:A:222:ALA:HB3	2.12	0.49
1:B:41:ARG:HG3	1:B:41:ARG:HH11	1.78	0.49
1:A:193:ARG:NH2	3:A:506:HOH:O	2.30	0.49
1:D:200:ILE:HG22	1:D:201:ASN:CG	2.38	0.49
1:A:206:VAL:HG22	1:A:207:GLY:H	1.78	0.48
1:C:67:TYR:HA	3:C:506:HOH:O	2.13	0.48
1:C:251:SER:HA	1:C:257:ILE:HD11	1.96	0.48
1:B:131:LEU:HD13	1:C:121:HIS:CE1	2.47	0.48
1:D:64:LYS:HD2	1:D:71:LEU:HD12	1.95	0.48
1:D:113:CYS:HB2	1:D:310:PHE:O	2.13	0.48
1:A:142:THR:HG23	1:A:142:THR:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:PRO:HA	1:A:264:THR:HB	1.95	0.48
1:A:169:ARG:NH1	1:A:171:GLU:OE1	2.42	0.48
1:C:142:THR:O	1:C:142:THR:HG23	2.13	0.48
1:B:279:GLY:O	3:B:401:HOH:O	2.20	0.47
1:A:169:ARG:NE	3:A:515:HOH:O	2.46	0.47
1:D:294:VAL:O	3:D:501:HOH:O	2.20	0.47
1:A:88:PHE:HA	1:D:110:ASN:HD21	1.79	0.47
1:D:40:MET:HE2	1:D:275:VAL:HG22	1.96	0.47
1:B:76:MET:HB3	1:B:135:ILE:HG12	1.95	0.47
1:B:88:PHE:CD1	1:C:82:THR:HG21	2.50	0.47
1:D:192:TYR:CZ	1:D:205:LEU:HD22	2.49	0.47
1:D:40:MET:HB3	1:D:275:VAL:O	2.16	0.46
1:C:187:GLY:HA2	1:C:190:ILE:HD13	1.98	0.46
1:A:62:ASN:OD1	1:A:66:ARG:NH1	2.48	0.46
1:D:200:ILE:HG12	1:D:205:LEU:HD21	1.97	0.45
1:B:282:SER:OG	1:B:283:SER:N	2.48	0.45
1:B:43:ARG:HG3	1:B:158:PHE:O	2.16	0.45
1:D:16:ARG:NH1	3:D:512:HOH:O	2.49	0.45
1:A:54:ASP:OD2	1:D:197:ARG:NH2	2.49	0.45
1:A:297:GLY:O	1:A:300:LYS:HE2	2.17	0.45
1:D:14:PRO:HB3	1:D:50:GLN:NE2	2.31	0.45
1:D:97:GLU:HB3	3:D:524:HOH:O	2.16	0.45
1:A:17:ARG:HD3	1:A:42:GLU:OE1	2.17	0.45
1:A:250:HIS:CD2	1:A:252:ALA:HB2	2.51	0.45
1:B:0:HIS:CG	1:B:1:MET:H	2.35	0.45
1:D:40:MET:SD	1:D:157:LEU:HA	2.57	0.45
1:D:96:GLN:NE2	1:D:101:TRP:O	2.44	0.45
1:A:31:ASP:OD1	3:A:501:HOH:O	2.21	0.45
1:A:134:LYS:HE3	1:A:134:LYS:HB2	1.80	0.45
1:D:189:ASP:HB3	1:D:200:ILE:HG21	1.99	0.45
1:A:198:ASN:C	1:A:205:LEU:HG	2.42	0.45
1:B:133:GLN:NE2	1:B:169:ARG:HD2	2.30	0.45
1:A:88:PHE:O	1:A:89:PRO:C	2.59	0.44
1:C:40:MET:SD	1:C:157:LEU:HA	2.58	0.44
1:C:55:LEU:HB3	1:C:162:ALA:HB2	1.99	0.44
1:B:97:GLU:HB2	1:C:185:GLY:HA3	2.00	0.44
1:C:80:ALA:HB1	1:C:115:GLY:HA3	1.98	0.44
1:D:251:SER:HB2	1:D:285:SER:HB2	2.00	0.44
1:A:61:LYS:HE2	1:A:98:TYR:OH	2.18	0.44
1:B:43:ARG:NH2	1:B:156:VAL:O	2.41	0.44
1:D:55:LEU:HB3	1:D:162:ALA:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:323:TRP:CZ2	1:C:325:MET:HE3	2.53	0.43
1:B:60:VAL:CG2	1:B:136:LEU:HD21	2.48	0.43
1:B:90:SER:HB2	1:B:108:ASP:CG	2.44	0.43
1:A:31:ASP:O	1:A:35:VAL:HG13	2.17	0.43
1:A:222:ALA:HA	1:A:225:THR:HB	2.00	0.43
1:C:186:ASN:OD1	1:C:186:ASN:N	2.50	0.43
1:B:88:PHE:HD1	1:C:82:THR:HG21	1.84	0.43
1:B:192:TYR:CE1	1:B:205:LEU:HD22	2.54	0.43
1:D:40:MET:HA	1:D:276:GLU:HA	2.00	0.43
1:A:259:SER:O	1:A:263:LYS:HG2	2.19	0.42
1:B:273:THR:HG22	3:B:410:HOH:O	2.18	0.42
1:C:5:LYS:HE2	1:C:5:LYS:HB2	1.68	0.42
1:A:247:PHE:HB3	1:A:271:THR:HG22	2.00	0.42
1:B:18:LEU:HD23	1:B:43:ARG:HD3	2.02	0.42
1:A:301:LYS:HE3	1:A:301:LYS:HB2	1.90	0.42
1:A:213:GLN:NE2	3:A:521:HOH:O	2.51	0.42
1:B:97:GLU:HG3	1:C:186:ASN:HA	2.02	0.42
1:A:41:ARG:NH2	3:A:503:HOH:O	2.47	0.42
1:D:245:ASP:O	1:D:270:LYS:HD2	2.20	0.42
1:A:193:ARG:NH1	3:A:520:HOH:O	2.52	0.41
1:A:193:ARG:O	1:D:86:TYR:HB3	2.20	0.41
1:C:141:GLU:HG3	1:C:282:SER:HB3	2.03	0.41
1:D:20:ASN:O	1:D:24:GLU:HG3	2.21	0.41
1:B:291:ASP:O	1:B:292:LEU:C	2.64	0.41
1:B:250:HIS:CD2	1:B:252:ALA:HB2	2.56	0.41
1:A:117:THR:HG21	1:A:309:GLY:H	1.86	0.41
1:B:75:ASP:HA	1:B:104:THR:HA	2.03	0.41
1:B:210:LYS:NZ	3:B:417:HOH:O	2.52	0.41
1:D:49:HIS:O	3:D:502:HOH:O	2.22	0.41
1:B:38:THR:CB	1:B:40:MET:HE2	2.51	0.40
1:A:88:PHE:H	1:A:89:PRO:CD	2.34	0.40
1:B:269:GLU:HG2	1:D:33:TRP:CZ2	2.49	0.40
1:D:200:ILE:CG1	1:D:205:LEU:HD21	2.51	0.40
1:D:230:PHE:HE1	1:D:234:LEU:HD11	1.87	0.40
1:B:17:ARG:HD3	1:B:42:GLU:OE1	2.21	0.40
1:C:60:VAL:O	1:C:64:LYS:HG3	2.22	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	324/345 (94%)	307 (95%)	16 (5%)	1 (0%)	36	50
1	B	324/345 (94%)	313 (97%)	11 (3%)	0	100	100
1	C	324/345 (94%)	309 (95%)	13 (4%)	2 (1%)	21	32
1	D	323/345 (94%)	307 (95%)	16 (5%)	0	100	100
All	All	1295/1380 (94%)	1236 (95%)	56 (4%)	3 (0%)	43	58

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	201	ASN
1	C	174	PRO
1	C	152	ARG

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	262/284 (92%)	253 (97%)	9 (3%)	32	54
1	B	262/284 (92%)	256 (98%)	6 (2%)	44	66
1	C	266/284 (94%)	252 (95%)	14 (5%)	20	36
1	D	262/284 (92%)	252 (96%)	10 (4%)	29	49
All	All	1052/1136 (93%)	1013 (96%)	39 (4%)	30	51

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	113	CYS
1	A	154	THR
1	A	190	ILE
1	A	198	ASN
1	A	203	VAL
1	A	287	VAL
1	A	305	VAL
1	A	321	ILE
1	A	325	MET
1	B	27	VAL
1	B	173	THR
1	B	239	LEU
1	B	269	GLU
1	B	284	VAL
1	B	320	LEU
1	C	11	THR
1	C	43	ARG
1	C	82	THR
1	C	113	CYS
1	C	142	THR
1	C	183	THR
1	C	208	SER
1	C	248	VAL
1	C	251	SER
1	C	264	THR
1	C	268	ILE
1	C	273	THR
1	C	283	SER
1	C	284	VAL
1	D	82	THR
1	D	112	THR
1	D	142	THR
1	D	153	THR
1	D	191	LEU
1	D	206	VAL
1	D	208	SER
1	D	251	SER
1	D	268	ILE
1	D	284	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	213	GLN
1	B	133	GLN
1	B	198	ASN
1	B	201	ASN
1	C	36	GLN
1	C	133	GLN
1	C	198	ASN
1	C	201	ASN
1	D	50	GLN
1	D	110	ASN
1	D	198	ASN
1	D	213	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 ligands are modelled in this entry.

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	$\# Z > 2$
2	GOL	C	401	-	5,5,5	0.95	0	5,5,5	1.08	0
2	GOL	A	401	-	5,5,5	0.94	0	5,5,5	1.10	0
2	GOL	D	401	-	5,5,5	0.92	0	5,5,5	1.07	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
2	GOL	C	401	-	-	0/4/4/4	-
2	GOL	A	401	-	-	0/4/4/4	-
2	GOL	D	401	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	326/345 (94%)	0.82	30 (9%) 14 12	30, 49, 65, 77	0
1	B	326/345 (94%)	0.84	35 (10%) 11 8	36, 52, 69, 80	0
1	C	326/345 (94%)	0.65	17 (5%) 33 29	36, 48, 68, 84	0
1	D	325/345 (94%)	0.65	19 (5%) 29 25	30, 48, 66, 75	0
All	All	1303/1380 (94%)	0.74	101 (7%) 19 15	30, 49, 68, 84	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	88	PHE	7.4
1	A	89	PRO	5.8
1	C	325	MET	4.8
1	D	265	PRO	4.4
1	D	266	PHE	4.3
1	A	308	PHE	4.2
1	D	107	LEU	4.2
1	A	153	THR	3.9
1	B	158	PHE	3.8
1	C	190	ILE	3.8
1	A	87	ALA	3.7
1	C	323	TRP	3.7
1	B	26	ILE	3.7
1	A	248	VAL	3.6
1	B	287	VAL	3.6
1	C	82	THR	3.6
1	D	133	GLN	3.6
1	B	70	THR	3.6
1	A	14	PRO	3.5
1	A	325	MET	3.5
1	D	37	ARG	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	190	ILE	3.4
1	C	299	LEU	3.3
1	A	207	GLY	3.3
1	A	90	SER	3.2
1	B	136	LEU	3.2
1	B	265	PRO	3.2
1	A	112	THR	3.2
1	D	219	TYR	3.1
1	C	91	THR	3.0
1	C	265	PRO	3.0
1	B	99	PHE	2.9
1	D	33	TRP	2.9
1	B	268	ILE	2.8
1	C	221	TRP	2.8
1	A	312	GLY	2.8
1	A	265	PRO	2.8
1	B	221	TRP	2.8
1	A	111	ALA	2.8
1	B	69	GLY	2.7
1	B	218	VAL	2.7
1	B	266	PHE	2.7
1	A	222	ALA	2.7
1	A	254	LEU	2.7
1	C	175	GLY	2.7
1	B	186	ASN	2.7
1	A	137	VAL	2.7
1	B	325	MET	2.7
1	A	206	VAL	2.6
1	A	215	GLY	2.6
1	A	36	GLN	2.6
1	A	282	SER	2.6
1	B	267	PRO	2.6
1	D	73	ASP	2.6
1	B	122	LEU	2.5
1	D	261	CYS	2.5
1	D	230	PHE	2.5
1	C	260	ILE	2.5
1	B	11	THR	2.4
1	A	56	CYS	2.4
1	C	81	THR	2.4
1	A	136	LEU	2.4
1	D	278	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	188	GLY	2.4
1	B	244	LEU	2.4
1	B	27	VAL	2.4
1	D	137	VAL	2.3
1	D	153	THR	2.3
1	A	77	ILE	2.3
1	B	135	ILE	2.3
1	C	155	CYS	2.3
1	B	156	VAL	2.3
1	B	314	LEU	2.3
1	C	71	LEU	2.3
1	A	142	THR	2.3
1	C	264	THR	2.3
1	A	283	SER	2.3
1	A	272	LEU	2.3
1	B	95	VAL	2.2
1	A	57	ILE	2.2
1	B	154	THR	2.2
1	D	190	ILE	2.2
1	B	223	ALA	2.2
1	D	163	GLY	2.2
1	D	324	GLY	2.2
1	B	291	ASP	2.2
1	B	289	ALA	2.1
1	B	63	LEU	2.1
1	A	86	TYR	2.1
1	D	305	VAL	2.1
1	B	150	THR	2.1
1	B	37	ARG	2.1
1	B	219	TYR	2.1
1	D	241	SER	2.1
1	B	112	THR	2.1
1	C	173	THR	2.1
1	C	212	VAL	2.1
1	D	213	GLN	2.0
1	A	305	VAL	2.0
1	C	188	GLY	2.0
1	B	149	TYR	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($\text{\AA}^2$)	Q<0.9
2	GOL	A	401	6/6	-	-	44,45,46,47	6
2	GOL	C	401	6/6	-	-	54,56,60,62	6
2	GOL	D	401	6/6	-	-	44,46,46,47	6

6.5 Other polymers [i](#)

There are no such residues in this entry.