



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 16, 2017 – 08:02 PM EDT

PDB ID : 3DLX  
Title : Crystal structure of human 3-oxoacid CoA transferase 1  
Authors : Kavanagh, K.L.; Shafqat, N.; Yue, W.W.; Picaud, S.; Murray, J.W.; Maclean, E.M.; von Delft, F.; Roos, A.K.; Arrowsmith, C.H.; Wikstrom, M.; Edwards, A.M.; Bountra, C.; Oppermann, U.; Structural Genomics Consortium (SGC)  
Deposited on : unknown  
Resolution : 2.20 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

<http://wwpdb.org/validation/2016/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  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

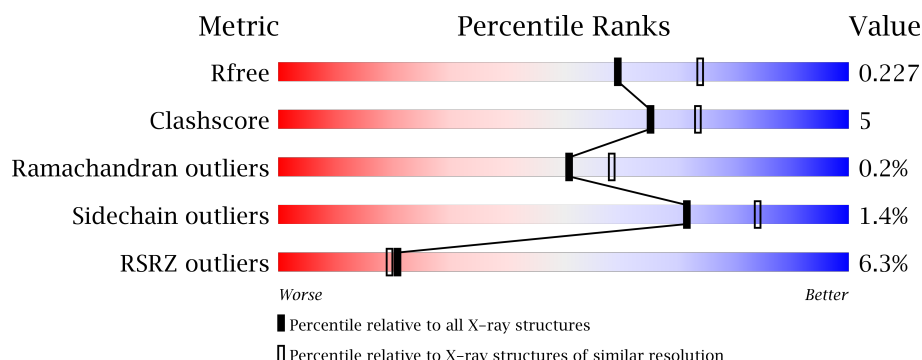
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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))
$R_{free}$	100719	4002 (2.20-2.20)
Clashscore	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)
RSRZ outliers	101464	4033 (2.20-2.20)

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. 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	489	<div> <div>6%</div> <div>84%</div> <div>12%</div> <div>•</div> </div>
1	B	489	<div> <div>7%</div> <div>82%</div> <div>12%</div> <div>• 5%</div> </div>
1	C	489	<div> <div>2%</div> <div>88%</div> <div>7%</div> <div>•</div> </div>
1	D	489	<div> <div>10%</div> <div>83%</div> <div>11%</div> <div>6%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14234 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 Succinyl-CoA:3-ketoacid-coenzyme A transferase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	470	Total	C	N	O	S	0	1	0
			3524	2238	601	666	19			
1	B	465	Total	C	N	O	S	0	0	0
			3449	2190	585	657	17			
1	C	467	Total	C	N	O	S	0	0	0
			3508	2225	599	665	19			
1	D	459	Total	C	N	O	S	0	0	0
			3360	2136	573	633	18			

There are 32 discrepancies between the modelled and reference sequences:

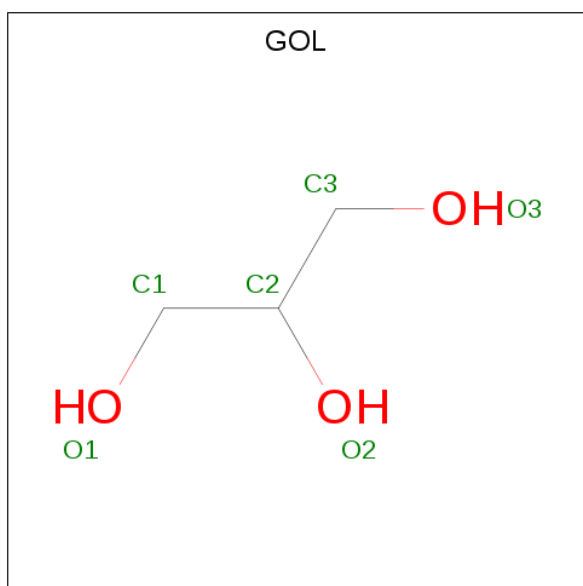
Chain	Residue	Modelled	Actual	Comment	Reference
A	39	MET	-	EXPRESSION TAG	UNP P55809
A	521	ALA	-	EXPRESSION TAG	UNP P55809
A	522	GLU	-	EXPRESSION TAG	UNP P55809
A	523	ASN	-	EXPRESSION TAG	UNP P55809
A	524	LEU	-	EXPRESSION TAG	UNP P55809
A	525	TYR	-	EXPRESSION TAG	UNP P55809
A	526	PHE	-	EXPRESSION TAG	UNP P55809
A	527	GLN	-	EXPRESSION TAG	UNP P55809
B	39	MET	-	EXPRESSION TAG	UNP P55809
B	521	ALA	-	EXPRESSION TAG	UNP P55809
B	522	GLU	-	EXPRESSION TAG	UNP P55809
B	523	ASN	-	EXPRESSION TAG	UNP P55809
B	524	LEU	-	EXPRESSION TAG	UNP P55809
B	525	TYR	-	EXPRESSION TAG	UNP P55809
B	526	PHE	-	EXPRESSION TAG	UNP P55809
B	527	GLN	-	EXPRESSION TAG	UNP P55809
C	39	MET	-	EXPRESSION TAG	UNP P55809
C	521	ALA	-	EXPRESSION TAG	UNP P55809
C	522	GLU	-	EXPRESSION TAG	UNP P55809
C	523	ASN	-	EXPRESSION TAG	UNP P55809
C	524	LEU	-	EXPRESSION TAG	UNP P55809

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Chain	Residue	Modelled	Actual	Comment	Reference
C	525	TYR	-	EXPRESSION TAG	UNP P55809
C	526	PHE	-	EXPRESSION TAG	UNP P55809
C	527	GLN	-	EXPRESSION TAG	UNP P55809
D	39	MET	-	EXPRESSION TAG	UNP P55809
D	521	ALA	-	EXPRESSION TAG	UNP P55809
D	522	GLU	-	EXPRESSION TAG	UNP P55809
D	523	ASN	-	EXPRESSION TAG	UNP P55809
D	524	LEU	-	EXPRESSION TAG	UNP P55809
D	525	TYR	-	EXPRESSION TAG	UNP P55809
D	526	PHE	-	EXPRESSION TAG	UNP P55809
D	527	GLN	-	EXPRESSION TAG	UNP P55809

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	110	Total	O	0	2
			112	112		
3	B	65	Total	O	0	1
			66	66		

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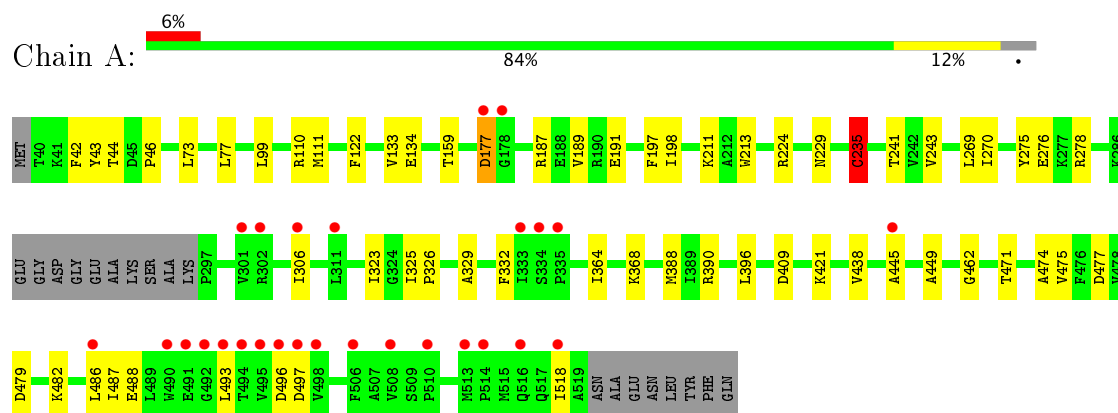
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	122	Total 125	O 125	0	3
3	D	78	Total 78	O 78	0	0

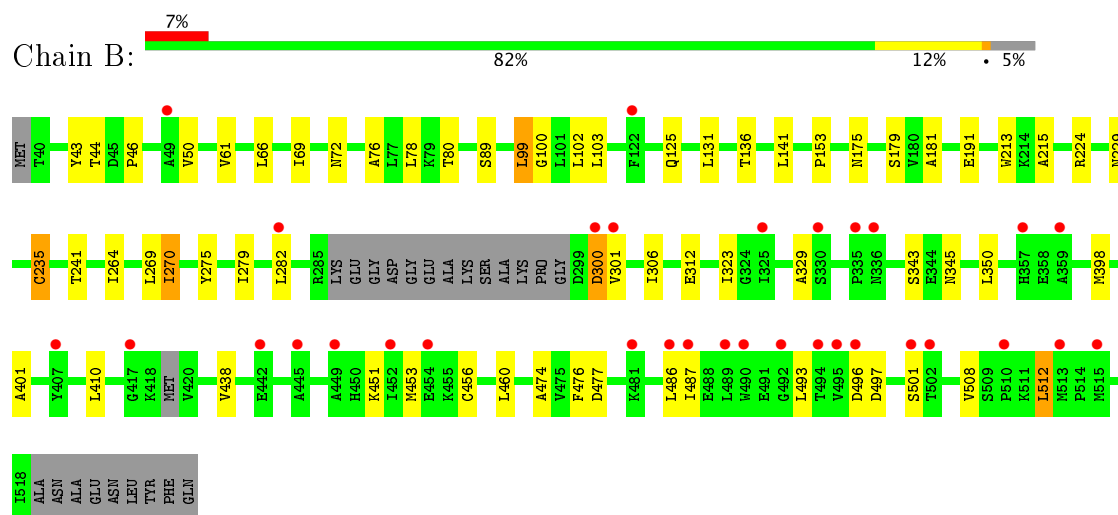
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

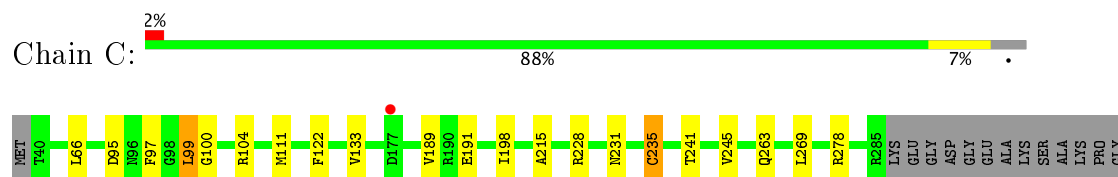
- Molecule 1: Succinyl-CoA:3-ketoacid-coenzyme A transferase 1

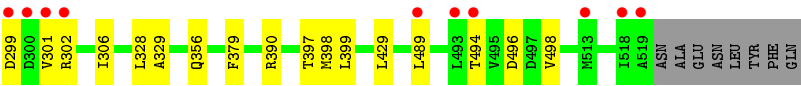


- Molecule 1: Succinyl-CoA:3-ketoacid-coenzyme A transferase 1

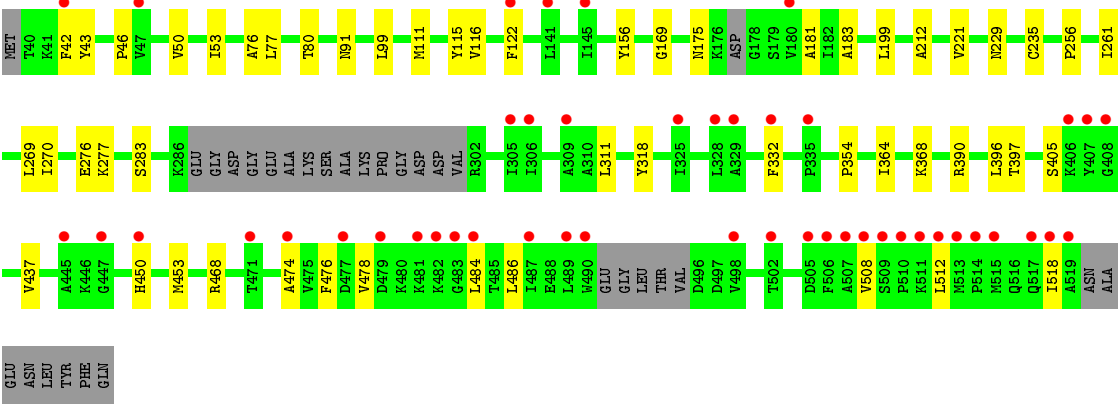
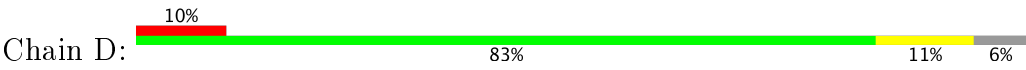


- Molecule 1: Succinyl-CoA:3-ketoacid-coenzyme A transferase 1





● Molecule 1: Succinyl-CoA:3-ketoacid-coenzyme A transferase 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.96Å 168.49Å 95.32Å 90.00° 105.86° 90.00°	Depositor
Resolution (Å)	48.11 – 2.20 48.13 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.4 (48.11-2.20) 98.4 (48.13-2.20)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.89 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.178 , 0.225 0.181 , 0.227	Depositor DCC
$R_{free}$ test set	1302 reflections (1.43%)	DCC
Wilson B-factor (Å <sup>2</sup> )	32.7	Xtriage
Anisotropy	0.293	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 68.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.029 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	14234	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.70% 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: 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	0.76	1/3589 (0.0%)	0.78	4/4858 (0.1%)
1	B	0.70	2/3509 (0.1%)	0.75	0/4759
1	C	0.77	1/3569 (0.0%)	0.81	1/4833 (0.0%)
1	D	0.71	1/3418 (0.0%)	0.74	2/4637 (0.0%)
All	All	0.73	5/14085 (0.0%)	0.77	7/19087 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	235	CYS	CB-SG	-8.30	1.68	1.82
1	B	179	SER	CB-OG	8.28	1.53	1.42
1	B	235	CYS	CB-SG	-7.88	1.68	1.82
1	A	235	CYS	CB-SG	-6.96	1.70	1.82
1	C	235	CYS	CB-SG	-5.78	1.72	1.81

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	390	ARG	NE-CZ-NH1	9.37	124.98	120.30
1	A	390	ARG	NE-CZ-NH2	-8.05	116.27	120.30
1	D	390	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	D	390	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	A	187	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	A	409	ASP	CB-CG-OD1	5.66	123.39	118.30
1	C	390	ARG	NE-CZ-NH2	-5.19	117.70	120.30

There are no chirality outliers.

There are no planarity outliers.

## 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	3524	0	3505	38	0
1	B	3449	0	3378	37	0
1	C	3508	0	3490	23	0
1	D	3360	0	3269	34	0
2	A	6	0	8	2	0
2	C	6	0	8	0	0
3	A	112	0	0	0	0
3	B	66	0	0	0	0
3	C	125	0	0	0	0
3	D	78	0	0	0	0
All	All	14234	0	13658	128	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 5.

All (128) 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:43:TYR:O	1:B:270:ILE:HG22	1.81	0.79
1:B:477:ASP:OD2	1:B:487:ILE:HG21	1.84	0.78
1:D:508:VAL:CG1	1:D:512:LEU:HD22	2.14	0.77
1:C:235:CYS:O	1:C:241:THR:HG21	1.84	0.77
1:D:508:VAL:HG11	1:D:512:LEU:HD22	1.68	0.75
1:D:43:TYR:HB2	1:D:270:ILE:HG22	1.69	0.74
1:B:474:ALA:HB1	1:B:486:LEU:HD11	1.68	0.73
1:C:494:THR:HG22	1:C:496:ASP:H	1.53	0.73
1:A:235:CYS:O	1:A:241:THR:HG21	1.91	0.71
1:A:42:PHE:CE2	1:A:269:LEU:HD23	2.28	0.68
1:D:42:PHE:CE2	1:D:269:LEU:HD23	2.29	0.67
1:B:474:ALA:HB1	1:B:486:LEU:CD1	2.25	0.66
1:D:175:ASN:ND2	1:D:181:ALA:HB2	2.11	0.66
1:B:78:LEU:HD23	1:B:102:LEU:HD23	1.80	0.63
1:C:99:LEU:CD2	1:C:111:MET:SD	2.87	0.63
1:B:508:VAL:CG1	1:B:512:LEU:HD22	2.28	0.63
1:A:474:ALA:HB1	1:A:486:LEU:CD1	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:302:ARG:HD3	1:C:328:LEU:HD13	1.83	0.60
1:B:215:ALA:HB1	1:B:269:LEU:HD21	1.84	0.60
1:B:215:ALA:CB	1:B:269:LEU:HD21	2.32	0.58
1:B:235:CYS:O	1:B:241:THR:HG21	2.03	0.58
1:A:477:ASP:OD2	1:A:487:ILE:HG21	2.04	0.58
1:D:474:ALA:HB1	1:D:486:LEU:CD1	2.33	0.58
1:A:396:LEU:HD11	1:A:438:VAL:HG23	1.87	0.57
1:A:211:LYS:HE2	1:A:275:TYR:CE1	2.39	0.57
1:D:478:VAL:HG22	1:D:484:LEU:CD2	2.34	0.57
1:A:43:TYR:HB2	1:A:270:ILE:HG22	1.87	0.56
1:A:306:ILE:HG23	1:A:329:ALA:HA	1.87	0.55
1:B:279:ILE:HD13	1:B:282:LEU:HD13	1.88	0.55
1:A:493:LEU:HD22	1:A:497:ASP:HB3	1.88	0.55
1:D:450:HIS:O	1:D:453:MET:HE1	2.06	0.55
1:D:311:LEU:HD21	1:D:518:ILE:HA	1.90	0.54
1:B:474:ALA:CB	1:B:486:LEU:HD11	2.36	0.54
1:D:478:VAL:HG22	1:D:484:LEU:HD23	1.89	0.54
1:D:474:ALA:HB1	1:D:486:LEU:HD11	1.89	0.53
1:D:76:ALA:O	1:D:80:THR:HG23	2.08	0.53
1:A:110:ARG:NH1	1:A:134:GLU:OE1	2.40	0.53
1:C:122:PHE:C	1:C:122:PHE:CD1	2.82	0.53
1:C:299:ASP:OD2	1:C:301:VAL:HG22	2.08	0.53
1:B:76:ALA:O	1:B:80:THR:HG23	2.09	0.52
1:C:99:LEU:HD21	1:C:111:MET:SD	2.50	0.52
1:B:343:SER:OG	1:B:345:ASN:OD1	2.27	0.51
1:B:89:SER:CB	1:B:99:LEU:CD2	2.88	0.51
1:C:302:ARG:HD3	1:C:328:LEU:CD1	2.40	0.51
1:A:211:LYS:CE	1:A:275:TYR:CE1	2.93	0.51
1:A:475:VAL:HB	1:A:488:GLU:HB2	1.93	0.51
1:B:72:ASN:ND2	1:B:275:TYR:CE1	2.79	0.50
1:D:212:ALA:HB1	1:D:221:VAL:HG13	1.94	0.50
1:D:332:PHE:O	1:D:518:ILE:HD13	2.12	0.50
1:A:479:ASP:HB3	1:A:482:LYS:HB2	1.94	0.50
1:D:169:GLY:HA2	1:D:183:ALA:HB1	1.94	0.50
1:A:189:VAL:HG22	1:A:198:ILE:HG22	1.95	0.49
1:B:343:SER:HB2	1:B:350:LEU:HD11	1.94	0.49
1:A:323:ILE:H	1:A:323:ILE:HD12	1.78	0.49
1:B:136:THR:HG21	1:B:141:LEU:HD13	1.95	0.48
1:C:215:ALA:HB1	1:C:269:LEU:HD21	1.95	0.48
1:C:263:GLN:HG3	1:D:318:TYR:OH	2.14	0.48
1:D:50:VAL:HG21	1:D:77:LEU:HD12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:PHE:CE2	1:A:269:LEU:CD2	2.96	0.47
1:C:99:LEU:HD23	1:C:111:MET:SD	2.54	0.47
1:A:177:ASP:N	1:A:177:ASP:OD2	2.39	0.47
1:D:99:LEU:HD23	1:D:111:MET:SD	2.55	0.47
1:D:276:GLU:O	1:D:277:LYS:C	2.53	0.47
1:A:445:ALA:HB3	1:A:449:ALA:HB3	1.97	0.47
1:C:100:GLY:O	1:C:104:ARG:HG2	2.15	0.47
1:C:189:VAL:HG22	1:C:198:ILE:HG22	1.97	0.47
1:A:99:LEU:CD2	1:A:111:MET:CE	2.93	0.47
1:D:397:THR:CG2	1:D:437:VAL:HG22	2.45	0.47
1:C:397:THR:HG21	1:C:429:LEU:HB3	1.97	0.47
1:C:215:ALA:HB2	1:C:245:VAL:HG11	1.98	0.46
1:B:312:GLU:HG3	1:B:398:MET:HE1	1.98	0.46
1:A:46:PRO:HB3	1:A:270:ILE:HD13	1.96	0.46
1:A:388:MET:HG2	1:B:264:ILE:HD13	1.98	0.46
1:B:508:VAL:HG11	1:B:512:LEU:HD22	1.98	0.46
1:D:46:PRO:HB3	1:D:270:ILE:HD13	1.97	0.46
1:A:276:GLU:OE1	1:A:278:ARG:NE	2.49	0.45
1:B:125:GLN:HB3	1:B:131:LEU:HB2	1.98	0.45
1:C:122:PHE:CZ	1:C:133:VAL:HG21	2.52	0.45
1:A:99:LEU:CD2	1:A:111:MET:HE1	2.46	0.45
1:C:66:LEU:HD22	1:C:97:PHE:HD2	1.80	0.45
1:B:175:ASN:OD1	1:B:181:ALA:HB2	2.17	0.45
1:A:325:ILE:N	1:A:326:PRO:CD	2.80	0.45
1:C:398:MET:O	1:C:399:LEU:HD23	2.17	0.45
1:C:379:PHE:CD2	1:D:256:PRO:HB2	2.52	0.45
1:B:100:GLY:HA2	1:B:103:LEU:HD12	1.98	0.44
1:A:364:ILE:HD12	1:A:368:LYS:HA	1.99	0.44
1:A:306:ILE:HG23	1:A:329:ALA:CA	2.47	0.44
1:D:405:SER:HA	1:D:453:MET:O	2.18	0.44
1:B:398:MET:CE	1:B:438:VAL:HG11	2.48	0.44
1:A:122:PHE:CZ	1:A:133:VAL:HG21	2.53	0.43
1:A:99:LEU:HD23	1:A:111:MET:HE1	2.01	0.43
1:A:493:LEU:HD22	1:A:497:ASP:CB	2.49	0.43
1:B:300:ASP:OD2	1:B:301:VAL:HG13	2.19	0.43
1:B:451:LYS:HA	1:B:453:MET:CE	2.49	0.43
1:D:261:ILE:HD13	1:D:261:ILE:HA	1.95	0.43
1:D:468:ARG:HA	1:D:476:PHE:O	2.19	0.43
1:D:156:TYR:CE2	1:D:199:LEU:HD13	2.54	0.43
1:C:228:ARG:O	1:C:231:ASN:HB2	2.19	0.42
1:D:212:ALA:CB	1:D:221:VAL:HG13	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:VAL:HG21	1:B:99:LEU:HD11	2.02	0.42
1:A:477:ASP:OD2	1:A:487:ILE:HD13	2.19	0.42
1:A:73:LEU:O	1:A:77:LEU:HD13	2.20	0.42
1:A:332:PHE:O	1:A:518:ILE:HD13	2.19	0.42
1:C:489:LEU:HD13	1:C:498:VAL:HG21	2.00	0.42
1:D:91:ASN:HA	1:D:115:TYR:O	2.19	0.42
1:A:213:TRP:CE2	1:A:224:ARG:HD2	2.54	0.42
1:D:508:VAL:HG13	1:D:512:LEU:HD22	2.00	0.42
1:B:66:LEU:HA	1:B:69:ILE:HG13	2.01	0.42
1:A:159:THR:HA	2:A:1:GOL:H12	2.02	0.42
1:A:243:VAL:HB	1:A:269:LEU:HD12	2.01	0.41
1:B:493:LEU:HD22	1:B:497:ASP:HB3	2.02	0.41
1:D:50:VAL:O	1:D:53:ILE:HG13	2.20	0.41
1:D:283:SER:O	1:D:354:PRO:HD2	2.19	0.41
1:A:462:GLY:HA2	2:A:1:GOL:H31	2.02	0.41
1:B:401:ALA:HB2	1:B:410:LEU:HD11	2.02	0.41
1:B:213:TRP:CE2	1:B:224:ARG:HD2	2.55	0.41
1:B:46:PRO:O	1:B:50:VAL:HG22	2.21	0.41
1:C:306:ILE:HG23	1:C:329:ALA:HA	2.02	0.41
1:B:312:GLU:HG3	1:B:398:MET:CE	2.51	0.41
1:C:302:ARG:O	1:C:306:ILE:HD12	2.21	0.41
1:A:471:THR:HG1	1:A:474:ALA:H	1.67	0.40
1:B:306:ILE:HG23	1:B:329:ALA:HA	2.03	0.40
1:D:116:VAL:HB	1:D:122:PHE:CE1	2.55	0.40
1:D:450:HIS:O	1:D:453:MET:CE	2.69	0.40
1:B:476:PHE:CE1	1:B:486:LEU:HD13	2.57	0.40
1:A:197:PHE:CD1	1:B:153:PRO:HG3	2.56	0.40
1:B:456:CYS:HB2	1:B:460:LEU:HD21	2.04	0.40
1:D:364:ILE:HD12	1:D:368:LYS:HA	2.02	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	467/489 (96%)	455 (97%)	11 (2%)	1 (0%)	51	58
1	B	459/489 (94%)	450 (98%)	7 (2%)	2 (0%)	38	41
1	C	463/489 (95%)	451 (97%)	12 (3%)	0	100	100
1	D	451/489 (92%)	431 (96%)	19 (4%)	1 (0%)	51	58
All	All	1840/1956 (94%)	1787 (97%)	49 (3%)	4 (0%)	51	58

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	229	ASN
1	D	229	ASN
1	A	229	ASN
1	B	512	LEU

### 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	364/396 (92%)	358 (98%)	6 (2%)	68	81
1	B	351/396 (89%)	343 (98%)	8 (2%)	56	69
1	C	365/396 (92%)	360 (99%)	5 (1%)	71	84
1	D	334/396 (84%)	333 (100%)	1 (0%)	94	97
All	All	1414/1584 (89%)	1394 (99%)	20 (1%)	71	84

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

Mol	Chain	Res	Type
1	A	44	THR
1	A	177	ASP
1	A	191	GLU
1	A	235	CYS
1	A	421	LYS
1	A	496	ASP
1	B	44	THR

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Mol	Chain	Res	Type
1	B	99	LEU
1	B	191	GLU
1	B	270	ILE
1	B	300	ASP
1	B	323	ILE
1	B	496	ASP
1	B	501	SER
1	C	95	ASP
1	C	99	LEU
1	C	191	GLU
1	C	278	ARG
1	C	356	GLN
1	D	396	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	357	HIS
1	D	175	ASN
1	D	357	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

2 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	A	1	-	5,5,5	0.48	0	5,5,5	0.64	0
2	GOL	C	1	-	5,5,5	0.45	0	5,5,5	0.61	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	A	1	-	-	0/4/4/4	0/0/0/0
2	GOL	C	1	-	-	0/4/4/4	0/0/0/0

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.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	GOL	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 ⓘ

### 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	470/489 (96%)	0.40	27 (5%) 24 24	28, 35, 44, 51	0
1	B	465/489 (95%)	0.43	32 (6%) 18 16	31, 36, 43, 50	0
1	C	467/489 (95%)	0.18	11 (2%) 59 57	28, 36, 43, 52	0
1	D	459/489 (93%)	0.63	47 (10%) 7 7	28, 36, 45, 48	0
All	All	1861/1956 (95%)	0.41	117 (6%) 21 19	28, 36, 44, 52	0

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	498	VAL	7.4
1	D	511	LYS	7.2
1	C	301	VAL	6.5
1	D	510	PRO	6.4
1	D	483	GLY	6.4
1	D	507	ALA	6.2
1	B	492	GLY	6.0
1	D	489	LEU	5.8
1	A	301	VAL	5.7
1	D	487	ILE	5.6
1	A	498	VAL	5.4
1	B	301	VAL	5.0
1	D	329	ALA	4.8
1	D	506	PHE	4.8
1	D	481	LYS	4.7
1	D	509	SER	4.7
1	B	357	HIS	4.5
1	D	502	THR	4.4
1	B	496	ASP	4.3
1	D	513	MET	4.3
1	B	417	GLY	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	508	VAL	3.9
1	D	407	TYR	3.9
1	D	484	LEU	3.9
1	D	450	HIS	3.8
1	C	299	ASP	3.8
1	D	328	LEU	3.7
1	A	497	ASP	3.7
1	A	494	THR	3.7
1	A	333	ILE	3.6
1	D	474	ALA	3.5
1	D	490	TRP	3.5
1	D	406	LYS	3.4
1	A	334	SER	3.4
1	A	492	GLY	3.4
1	D	517	GLN	3.4
1	D	471	THR	3.4
1	D	445	ALA	3.4
1	B	502	THR	3.3
1	D	447	GLY	3.3
1	D	515	MET	3.3
1	B	300	ASP	3.2
1	A	518	ILE	3.2
1	B	486	LEU	3.0
1	A	490	TRP	3.0
1	B	336	ASN	3.0
1	D	122	PHE	3.0
1	D	514	PRO	2.9
1	B	513	MET	2.9
1	D	42	PHE	2.9
1	D	180	VAL	2.8
1	A	495	VAL	2.8
1	C	513	MET	2.8
1	B	449	ALA	2.7
1	C	177	ASP	2.7
1	D	479	ASP	2.7
1	D	518	ILE	2.7
1	A	496	ASP	2.7
1	D	519	ALA	2.6
1	A	311	LEU	2.6
1	B	490	TRP	2.6
1	C	494	THR	2.6
1	B	445	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	325	ILE	2.6
1	A	513	MET	2.6
1	B	494	THR	2.5
1	B	510	PRO	2.5
1	D	482	LYS	2.5
1	D	335	PRO	2.5
1	A	177	ASP	2.5
1	A	493	LEU	2.5
1	A	306	ILE	2.5
1	D	305	ILE	2.5
1	D	505	ASP	2.5
1	A	486	LEU	2.5
1	B	501	SER	2.5
1	D	306	ILE	2.5
1	D	325	ILE	2.5
1	A	302	ARG	2.4
1	B	515	MET	2.4
1	A	516	GLN	2.4
1	A	510	PRO	2.4
1	B	454	GLU	2.4
1	B	282	LEU	2.4
1	A	445	ALA	2.4
1	B	442	GLU	2.4
1	A	335	PRO	2.4
1	D	47	VAL	2.4
1	D	332	PHE	2.4
1	B	481	LYS	2.4
1	C	300	ASP	2.3
1	C	518	ILE	2.3
1	B	335	PRO	2.3
1	C	302	ARG	2.3
1	D	145	ILE	2.3
1	A	506	PHE	2.3
1	D	309	ALA	2.3
1	B	495	VAL	2.3
1	C	493	LEU	2.2
1	A	491	GLU	2.2
1	D	512	LEU	2.2
1	D	408	GLY	2.2
1	B	122	PHE	2.2
1	D	141	LEU	2.2
1	B	407	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	49	ALA	2.1
1	A	514	PRO	2.1
1	B	330	SER	2.1
1	B	452	ILE	2.1
1	B	487	ILE	2.1
1	B	489	LEU	2.1
1	B	359	ALA	2.1
1	C	489	LEU	2.0
1	C	519	ALA	2.0
1	D	508	VAL	2.0
1	A	178	GLY	2.0
1	D	477	ASP	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	GOL	C	1	6/6	0.94	0.13	-1.26	27,33,36,37	0
2	GOL	A	1	6/6	0.96	0.11	-2.58	41,43,45,46	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.