



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:18 PM UTC

PDB ID : 3DLX / pdb_00003dlx
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 : 2008-06-30
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

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

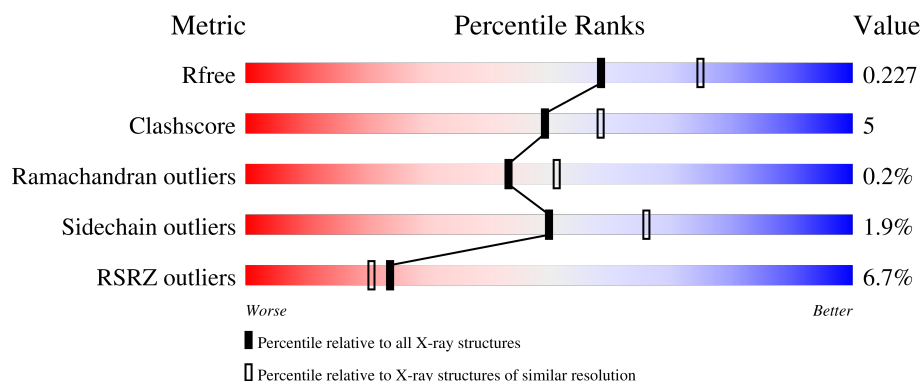
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (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 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	489	 6% 82% 13% . .
1	B	489	 6% 80% 14% . 5%
1	C	489	 2% 86% 9% .
1	D	489	 11% 81% 13% 6%

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:

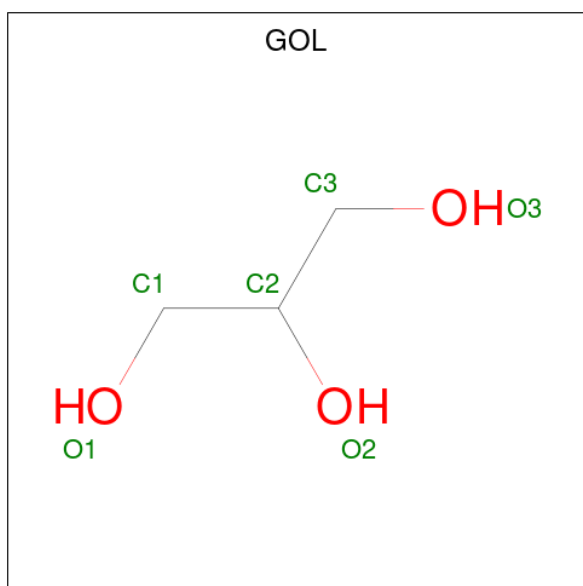
Chain	Residue	Modelled	Actual	Comment	Reference
A	39	MET	-	expression tag	UNP P55809
A	521	ALA	-	expression tag	UNP P55809
A	522	GLU	-	expression tag	UNP P55809
A	523	ASN	-	expression tag	UNP P55809
A	524	LEU	-	expression tag	UNP P55809
A	525	TYR	-	expression tag	UNP P55809
A	526	PHE	-	expression tag	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 (CCD ID: 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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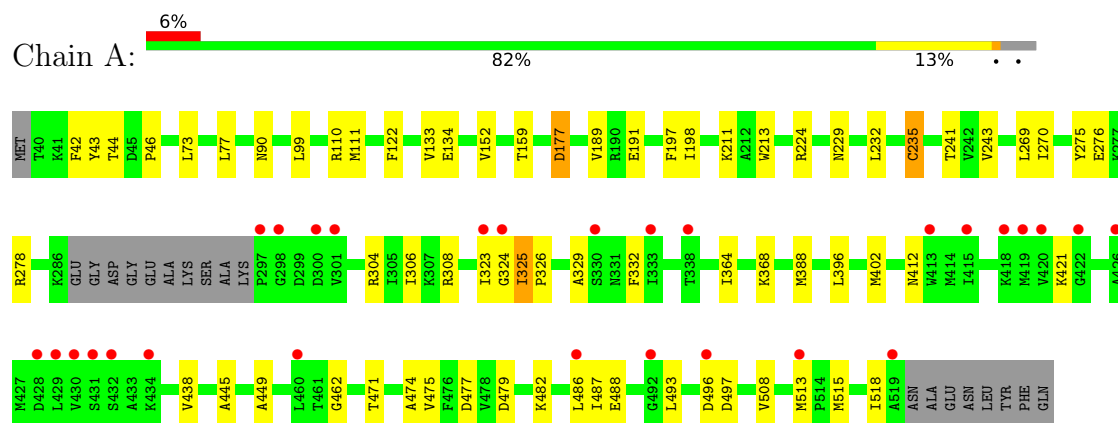
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	122	Total 125	O 125	0	3
3	D	78	Total 78	O 78	0	0

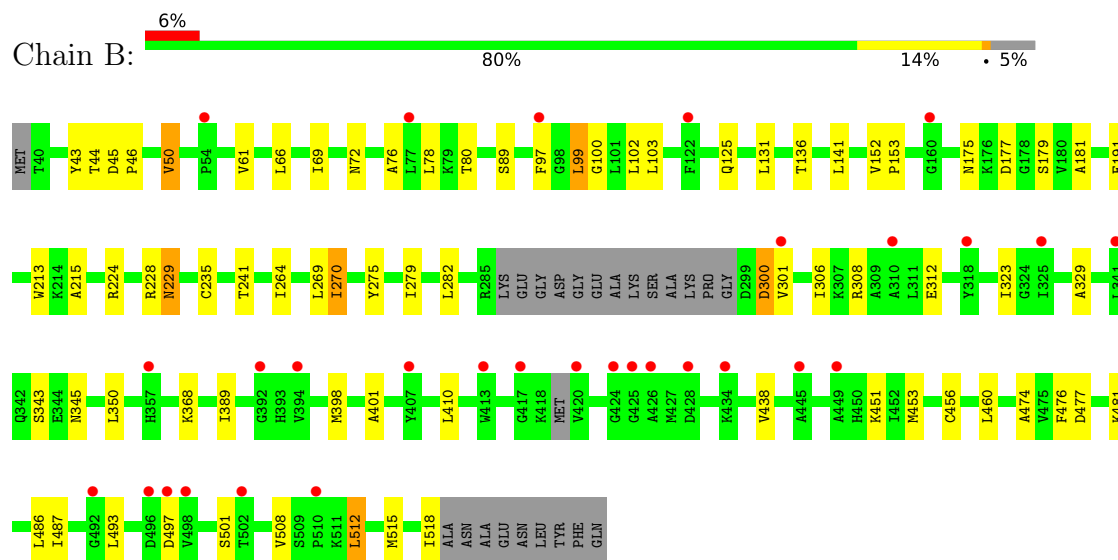
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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.

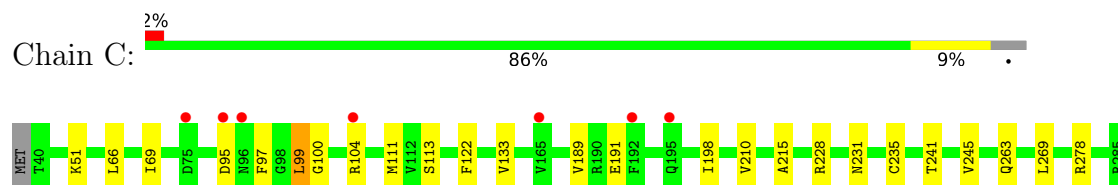
- Molecule 1: Succinyl-CoA:3-ketoacid-coenzyme A transferase 1

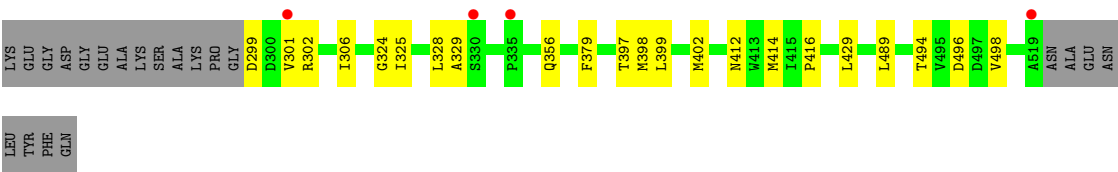


- Molecule 1: Succinyl-CoA:3-ketoacid-coenzyme A transferase 1

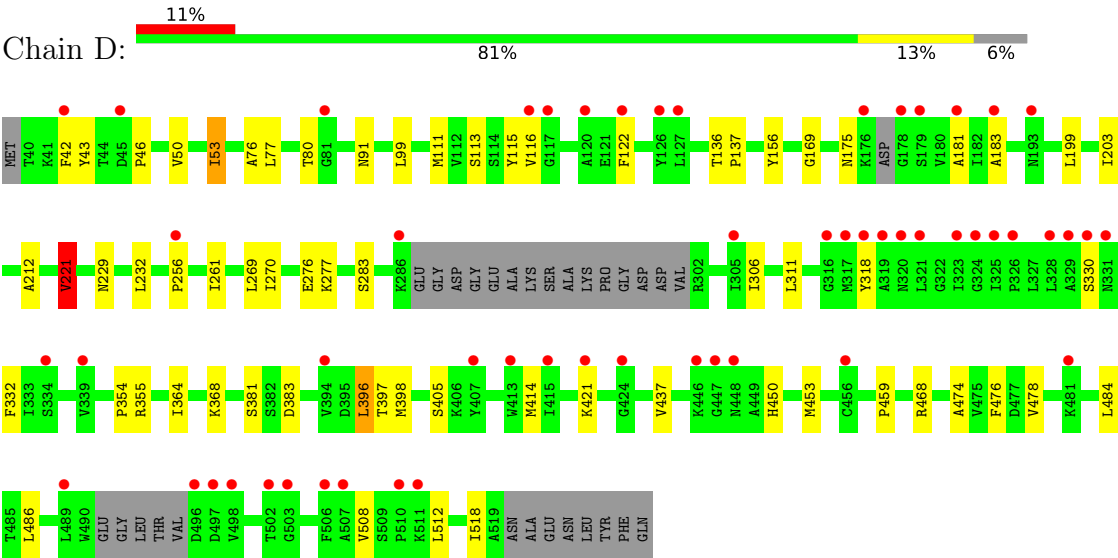


- Molecule 1: Succinyl-CoA:3-ketoacid-coenzyme A transferase 1





● 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, α , β , γ	60.96Å 168.49Å 95.32Å 90.00° 105.86° 90.00°	Depositor
Resolution (Å)	48.11 – 2.20 48.11 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.4 (48.11-2.20) 98.4 (48.11-2.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 (1.39%)	wwPDB-VP
Wilson B-factor (Å ²)	32.7	Xtriage
Anisotropy	0.293	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 62.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.029 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	14234	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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	0.98	1/3589 (0.0%)	0.97	4/4858 (0.1%)
1	B	0.89	2/3509 (0.1%)	0.95	7/4759 (0.1%)
1	C	1.00	3/3569 (0.1%)	1.02	2/4833 (0.0%)
1	D	0.92	2/3418 (0.1%)	0.95	4/4637 (0.1%)
All	All	0.95	8/14085 (0.1%)	0.97	17/19087 (0.1%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	325	ILE	CA-CB	9.69	1.60	1.53
1	D	203	ILE	CA-CB	5.86	1.61	1.54
1	A	152	VAL	CA-CB	5.77	1.59	1.53
1	C	210	VAL	C-O	-5.50	1.18	1.24
1	B	179	SER	CB-OG	5.43	1.53	1.42
1	D	221	VAL	CA-CB	5.29	1.62	1.54
1	C	69	ILE	CA-CB	5.26	1.59	1.53
1	B	389	ILE	CA-CB	5.19	1.60	1.54

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	324	GLY	CA-C-N	7.62	125.04	120.24
1	C	324	GLY	C-N-CA	7.62	125.04	120.24
1	A	325	ILE	CB-CA-C	-7.49	106.41	114.35
1	B	177	ASP	N-CA-C	6.70	118.58	111.28
1	D	113	SER	N-CA-C	6.12	118.37	109.07
1	B	45	ASP	CA-C-N	5.90	125.77	119.28
1	B	45	ASP	C-N-CA	5.90	125.77	119.28
1	B	152	VAL	N-CA-C	-5.74	101.46	107.60
1	B	177	ASP	CB-CA-C	-5.67	101.38	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	90	ASN	N-CA-C	5.53	117.31	111.28
1	D	330	SER	N-CA-C	5.48	117.25	111.28
1	B	97	PHE	N-CA-C	5.44	117.36	108.76
1	A	324	GLY	CA-C-N	5.26	123.55	120.24
1	A	324	GLY	C-N-CA	5.26	123.55	120.24
1	D	421	LYS	N-CA-C	5.21	119.49	113.18
1	D	355	ARG	N-CA-C	-5.21	103.52	110.55
1	B	50	VAL	N-CA-C	5.03	117.22	111.88

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	41	0
1	B	3449	0	3378	42	0
1	C	3508	0	3490	28	0
1	D	3360	0	3269	41	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	1	0
3	C	125	0	0	0	0
3	D	78	0	0	0	0
All	All	14234	0	13658	148	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 (148) 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:A:99:LEU:CD2	1:A:111:MET:HE3	2.11	0.80
1:B:43:TYR:O	1:B:270:ILE:HG22	1.81	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:312:GLU:HG3	1:B:398:MET:HE1	1.82	0.61
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:398:MET:HE2	1:B:438:VAL:HG11	1.84	0.59
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:C:122:PHE:C	1:C:122:PHE:CD1	2.82	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:B:308:ARG:HB2	1:B:515:MET:HE3	1.86	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: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:76:ALA:O	1:D:80:THR:HG23	2.08	0.53
1:D:474:ALA:HB1	1:D:486:LEU:HD11	1.89	0.53
1:A:110:ARG:NH1	1:A:134:GLU:OE1	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:99:LEU:HD21	1:C:111:MET:SD	2.50	0.52
1:D:276:GLU:O	1:D:277:LYS:C	2.53	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:C:402:MET:HE2	1:C:412:ASN:HA	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:488:GLU:OE2	1:A:513:MET:HE3	2.13	0.49
1:A:323:ILE:HD12	1:A:323:ILE:H	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:C:414:MET:HE2	1:C:416:PRO:HG3	1.95	0.48
1:D:50:VAL:HG21	1:D:77:LEU:HD12	1.95	0.48
1:A:42:PHE:CE2	1:A:269:LEU:CD2	2.96	0.47
1:A:99:LEU:HD22	1:A:111:MET:HE3	1.92	0.47
1:C:99:LEU:HD23	1:C:111:MET:SD	2.54	0.47
1:B:398:MET:HE2	1:B:438:VAL:CG1	2.45	0.47
1:B:308:ARG:CB	1:B:515:MET:HE3	2.45	0.47
1:A:177:ASP:OD2	1:A:177:ASP:N	2.39	0.47
1:D:99:LEU:HD23	1:D:111:MET:SD	2.55	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: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:D:396:LEU:HD21	1:D:398:MET:HE3	1.96	0.46
1:C:99:LEU:HD22	1:C:111:MET:HE1	1.97	0.46
1:C:215:ALA:HB2	1:C:245:VAL:HG11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:111:MET:HE3	1:C:113:SER:OG	2.17	0.45
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:D:450:HIS:O	1:D:453:MET:HE1	2.17	0.45
1:C:66:LEU:HD22	1:C:97:PHE:HD2	1.80	0.45
1:D:99:LEU:HD23	1:D:111:MET:HE1	1.99	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:D:381:SER:OG	1:D:383:ASP:OD1	2.33	0.45
1:C:379:PHE:CD2	1:D:256:PRO:HB2	2.52	0.45
1:C:398:MET:O	1:C:399:LEU:HD23	2.17	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:B:228:ARG:O	1:B:229:ASN:C	2.61	0.44
1:D:405:SER:HA	1:D:453:MET:O	2.18	0.44
1:A:122:PHE:CZ	1:A:133:VAL:HG21	2.53	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:368:LYS:NZ	3:B:586:HOH:O	2.50	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:D:232:LEU:C	1:D:232:LEU:HD23	2.43	0.42
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
1:D:175:ASN:CG	1:D:181:ALA:HB2	2.44	0.42
1:B:61:VAL:HG21	1:B:99:LEU:HD11	2.02	0.42
1:A:73:LEU:O	1:A:77:LEU:HD13	2.20	0.42
1:A:477:ASP:OD2	1:A:487:ILE:HD13	2.19	0.42
1:A:232:LEU:C	1:A:232:LEU:HD23	2.44	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:D:136:THR:O	1:D:137:PRO:C	2.63	0.42
1:A:159:THR:HA	2:A:1:GOL:H12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:414:MET:HE2	1:D:459:PRO:HG2	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:402:MET:HE2	1:A:412:ASN:HA	2.02	0.41
1:A:462:GLY:HA2	2:A:1:GOL:H31	2.02	0.41
1:D:450:HIS:O	1:D:453:MET:CE	2.69	0.41
1:B:398:MET:CE	1:B:438:VAL:HG11	2.48	0.41
1:B:401:ALA:HB2	1:B:410:LEU:HD11	2.02	0.41
1:A:308:ARG:HB2	1:A:515:MET:HE3	2.03	0.41
1:B:46:PRO:O	1:B:50:VAL:HG22	2.21	0.41
1:B:213:TRP:CE2	1:B:224:ARG:HD2	2.55	0.41
1:C:306:ILE:HG23	1:C:329:ALA:HA	2.02	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: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
1:C:99:LEU:CD2	1:C:111:MET:HE1	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	467/489 (96%)	455 (97%)	11 (2%)	1 (0%)	43 51
1	B	459/489 (94%)	450 (98%)	7 (2%)	2 (0%)	30 34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	463/489 (95%)	451 (97%)	12 (3%)	0	100	100
1	D	451/489 (92%)	431 (96%)	19 (4%)	1 (0%)	43	51
All	All	1840/1956 (94%)	1787 (97%)	49 (3%)	4 (0%)	43	51

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%)	356 (98%)	8 (2%)	45	61
1	B	351/396 (89%)	342 (97%)	9 (3%)	40	55
1	C	365/396 (92%)	359 (98%)	6 (2%)	55	71
1	D	334/396 (84%)	330 (99%)	4 (1%)	63	78
All	All	1414/1584 (89%)	1387 (98%)	27 (2%)	50	66

All (27) 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	304	ARG
1	A	421	LYS
1	A	496	ASP
1	A	508	VAL

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Mol	Chain	Res	Type
1	B	44	THR
1	B	99	LEU
1	B	191	GLU
1	B	270	ILE
1	B	300	ASP
1	B	323	ILE
1	B	481	LYS
1	B	501	SER
1	B	518	ILE
1	C	51	LYS
1	C	95	ASP
1	C	99	LEU
1	C	191	GLU
1	C	278	ARG
1	C	356	GLN
1	D	53	ILE
1	D	221	VAL
1	D	306	ILE
1	D	396	LEU

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

Mol	Chain	Res	Type
1	A	107	GLN
1	A	138	GLN
1	A	263	GLN
1	B	464	GLN
1	B	516	GLN
1	C	96	ASN
1	C	357	HIS
1	D	175	ASN
1	D	357	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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](#)

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	0.47	0	5,5,5	0.71	0
2	GOL	C	1	-	5,5,5	0.45	0	5,5,5	0.73	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	-
2	GOL	C	1	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1	GOL	C1-C2-C3-O3
2	C	1	GOL	O2-C2-C3-O3
2	C	1	GOL	O1-C1-C2-C3
2	C	1	GOL	O1-C1-C2-O2

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, 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	470/489 (96%)	0.57	28 (5%)	27	24	16, 35, 44, 51	1 (0%)
1	B	465/489 (95%)	0.80	30 (6%)	25	22	31, 36, 43, 50	0
1	C	467/489 (95%)	0.55	11 (2%)	59	56	28, 36, 43, 52	0
1	D	459/489 (93%)	1.01	55 (11%)	9	6	28, 36, 45, 48	0
All	All	1861/1956 (95%)	0.73	124 (6%)	24	21	16, 36, 44, 52	1 (0%)

All (124) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	492	GLY	5.1
1	B	420	VAL	4.1
1	D	507	ALA	3.9
1	A	492	GLY	3.7
1	D	502	THR	3.7
1	D	496	ASP	3.7
1	D	510	PRO	3.4
1	B	496	ASP	3.3
1	D	506	PHE	3.3
1	C	519	ALA	3.2
1	A	323	ILE	3.2
1	A	297	PRO	3.1
1	D	511	LYS	3.1
1	A	519	ALA	3.1
1	D	339	VAL	2.9
1	D	498	VAL	2.9
1	D	330	SER	2.9
1	D	334	SER	2.9
1	D	193	ASN	2.9
1	D	448	ASN	2.8
1	A	431	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	325	ILE	2.8
1	A	513	MET	2.7
1	D	122	PHE	2.7
1	C	75	ASP	2.7
1	A	432	SER	2.7
1	D	331	ASN	2.7
1	A	333	ILE	2.7
1	B	497	ASP	2.7
1	B	498	VAL	2.7
1	B	510	PRO	2.6
1	B	425	GLY	2.6
1	A	428	ASP	2.6
1	A	301	VAL	2.6
1	B	77	LEU	2.6
1	D	127	LEU	2.6
1	A	413	TRP	2.6
1	A	496	ASP	2.6
1	B	502	THR	2.6
1	D	316	GLY	2.6
1	A	430	VAL	2.6
1	A	419	MET	2.5
1	D	320	ASN	2.5
1	D	328	LEU	2.5
1	B	424	GLY	2.5
1	B	122	PHE	2.5
1	D	394	VAL	2.5
1	D	481	LYS	2.5
1	D	329	ALA	2.5
1	B	417	GLY	2.5
1	A	420	VAL	2.4
1	B	394	VAL	2.4
1	A	460	LEU	2.4
1	B	449	ALA	2.4
1	D	117	GLY	2.4
1	B	325	ILE	2.4
1	A	434	LYS	2.4
1	B	413	TRP	2.4
1	B	428	ASP	2.4
1	D	256	PRO	2.4
1	D	318	TYR	2.4
1	A	300	ASP	2.4
1	A	338	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	176	LYS	2.4
1	D	413	TRP	2.4
1	A	426	ALA	2.3
1	B	97	PHE	2.3
1	D	489	LEU	2.3
1	C	95	ASP	2.3
1	D	421	LYS	2.3
1	D	183	ALA	2.3
1	A	330	SER	2.3
1	D	323	ILE	2.3
1	A	324	GLY	2.3
1	B	318	TYR	2.3
1	D	407	TYR	2.3
1	D	179	SER	2.2
1	A	415	ILE	2.2
1	B	301	VAL	2.2
1	D	116	VAL	2.2
1	C	335	PRO	2.2
1	C	330	SER	2.2
1	B	341	LEU	2.2
1	D	447	GLY	2.2
1	D	456	CYS	2.2
1	D	120	ALA	2.2
1	D	45	ASP	2.2
1	D	497	ASP	2.2
1	B	434	LYS	2.2
1	D	324	GLY	2.2
1	D	181	ALA	2.2
1	C	301	VAL	2.1
1	A	298	GLY	2.1
1	A	422	GLY	2.1
1	D	81	GLY	2.1
1	B	426	ALA	2.1
1	B	445	ALA	2.1
1	D	286	LYS	2.1
1	D	415	ILE	2.1
1	C	192	PHE	2.1
1	D	42	PHE	2.1
1	B	160	GLY	2.1
1	A	418	LYS	2.1
1	A	486	LEU	2.1
1	B	407	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	165	VAL	2.1
1	D	178	GLY	2.1
1	B	310	ALA	2.1
1	A	429	LEU	2.1
1	B	357	HIS	2.1
1	D	321	LEU	2.1
1	C	96	ASN	2.1
1	D	326	PRO	2.1
1	D	424	GLY	2.1
1	D	446	LYS	2.0
1	D	317	MET	2.0
1	C	195	GLN	2.0
1	D	305	ILE	2.0
1	D	126	TYR	2.0
1	C	104	ARG	2.0
1	B	392	GLY	2.0
1	D	503	GLY	2.0
1	D	319	ALA	2.0
1	B	54	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	C	1	6/6	0.89	0.15	27,33,36,37	0
2	GOL	A	1	6/6	0.90	0.15	41,43,45,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.