Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:10 AM GMT

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	:	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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

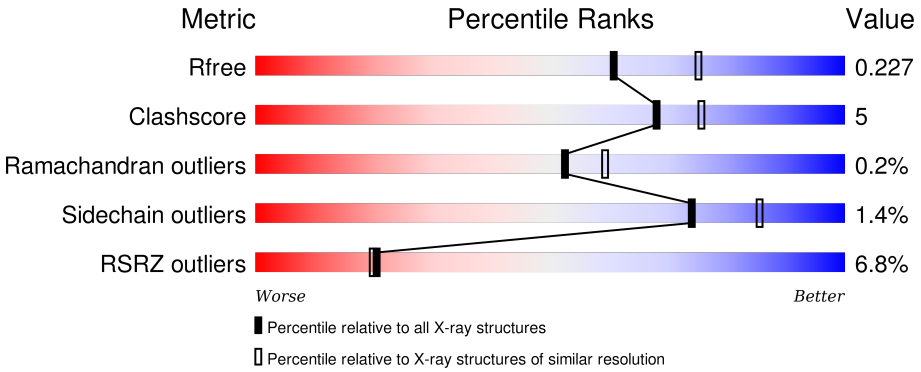
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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}	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (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 >=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 <=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% 84% 12% •
1	B	489	7% 82% 12% • 5%
1	C	489	2% 88% 7% •
1	D	489	11% 83% 11% 6%

2 Entry composition (i)

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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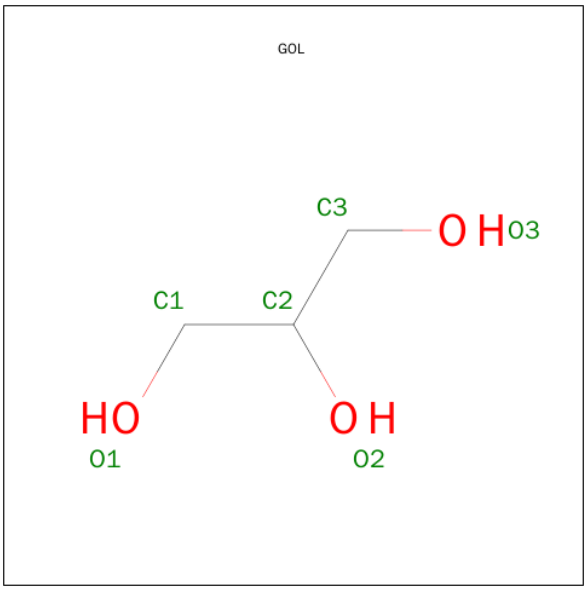
Chain	Residue	Modelled	Actual	Comment	Reference
C	525	TYR	-	EXPRESSION TAG	UNP P55809
C	526	PHE	-	EXPRESSION TAG	UNP P55809
C	527	GLN	-	EXPRESSION TAG	UNP P55809
D	39	MET	-	EXPRESSION TAG	UNP P55809
D	521	ALA	-	EXPRESSION TAG	UNP P55809
D	522	GLU	-	EXPRESSION TAG	UNP P55809
D	523	ASN	-	EXPRESSION TAG	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 6 3 3	0	0
2	C	1	Total C O 6 3 3	0	0

- Molecule 3 is water.

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

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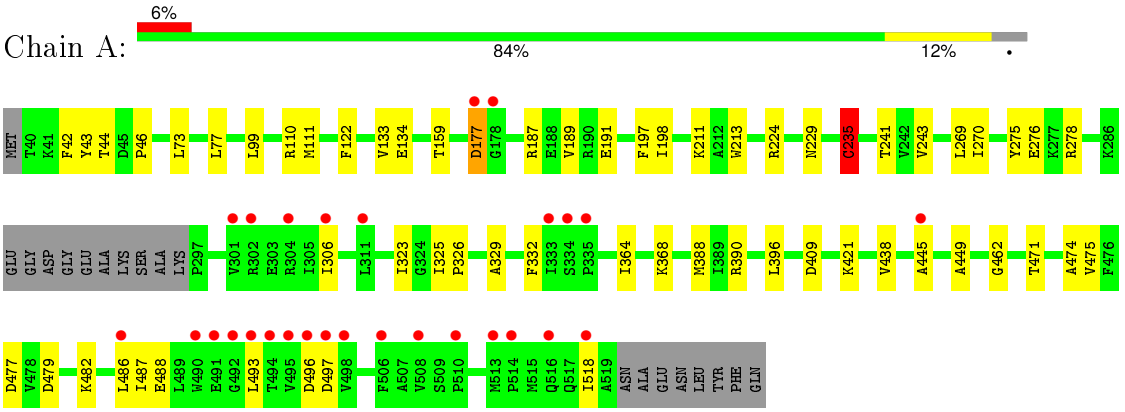
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	122	Total O 125 125	0	3
3	D	78	Total O 78 78	0	0

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 errors 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.

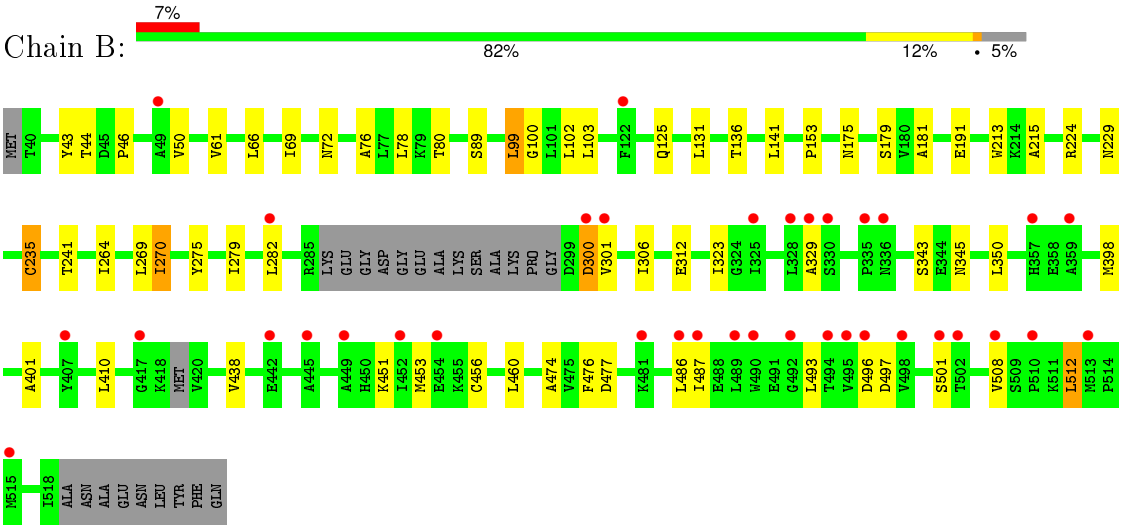
- Molecule 1: Succinyl-CoA:3-ketoacid-coenzyme A transferase 1

Chain A:



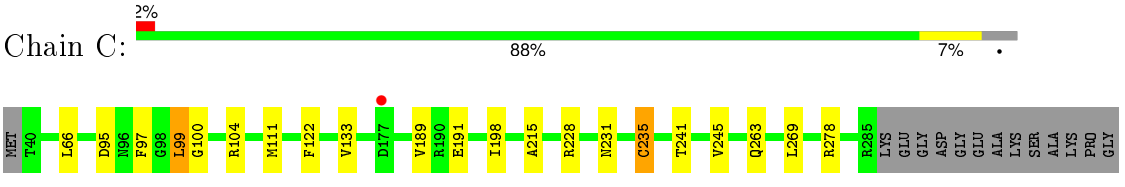
- Molecule 1: Succinyl-CoA:3-ketoacid-coenzyme A transferase 1

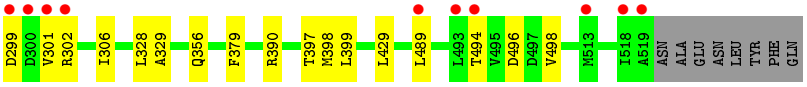
Chain B:



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

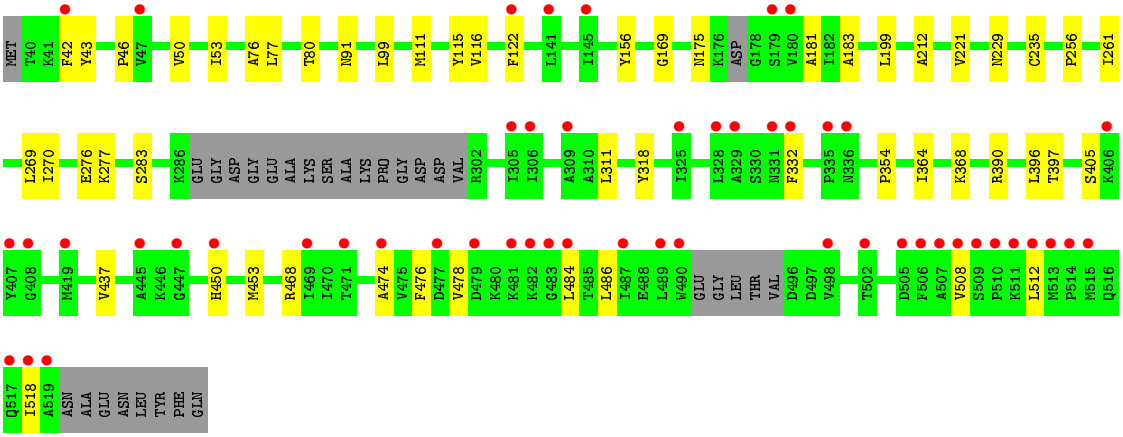
Chain C:





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

Chain D:



4 Data and refinement statistics (i)

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 48.13 – 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
$< I/\sigma(I) >$ [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 (1.43%)	DCC
Wilson B-factor (Å^2)	32.7	Xtriage
Anisotropy	0.293	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 68.3	EDS
Estimated twinning fraction	0.029 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 92058 reflections	Xtriage
F_o,F_c correlation	0.95	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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(^{o})	Ideal(^{o})
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 (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	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:D:474:ALA:HB1	1:D:486:LEU:CD1	2.33	0.58
1:A:477:ASP:OD2	1:A:487:ILE:HG21	2.04	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:D:450:HIS:O	1:D:453:MET:HE1	2.06	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: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:CD1	1:C:122:PHE:C	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:332:PHE:O	1:D:518:ILE:HD13	2.12	0.50
1:D:212:ALA:HB1	1:D:221:VAL:HG13	1.94	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:D:99:LEU:HD23	1:D:111:MET:SD	2.55	0.47
1:A:177:ASP:N	1:A:177:ASP:OD2	2.39	0.47
1:D:276:GLU:O	1:D:277:LYS:C	2.53	0.47
1:C:100:GLY:O	1:C:104:ARG:HG2	2.15	0.47
1:A:445:ALA:HB3	1:A:449:ALA:HB3	1.97	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:D:46:PRO:HB3	1:D:270:ILE:HD13	1.97	0.46
1:B:508:VAL:HG11	1:B:512:LEU:HD22	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:A:276:GLU:OE1	1:A:278:ARG:NE	2.49	0.45
1:C:122:PHE:CZ	1:C:133:VAL:HG21	2.52	0.45
1:B:125:GLN:HB3	1:B:131:LEU:HB2	1.98	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:99:LEU:HD23	1:A:111:MET:HE1	2.01	0.43
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: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:212:ALA:CB	1:D:221:VAL:HG13	2.49	0.42
1:C:228:ARG:O	1:C:231:ASN:HB2	2.19	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:C:489:LEU:HD13	1:C:498:VAL:HG21	2.00	0.42
1:A:332:PHE:O	1:A:518:ILE:HD13	2.19	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:D:50:VAL:O	1:D:53:ILE:HG13	2.20	0.41
1:B:493:LEU:HD22	1:B:497:ASP:HB3	2.02	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:C:306:ILE:HG23	1:C:329:ALA:HA	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:302:ARG:O	1:C:306:ILE:HD12	2.21	0.41
1:B:312:GLU:HG3	1:B:398:MET:CE	2.51	0.41
1:A:471:THR:HG1	1:A:474:ALA:H	1.67	0.40
1:D:450:HIS:O	1:D:453:MET:CE	2.69	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

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%)	52 59
1	B	459/489 (94%)	450 (98%)	7 (2%)	2 (0%)	39 42
1	C	463/489 (95%)	451 (97%)	12 (3%)	0	100 100
1	D	451/489 (92%)	431 (96%)	19 (4%)	1 (0%)	52 59
All	All	1840/1956 (94%)	1787 (97%)	49 (3%)	4 (0%)	52 59

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 (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	364/396 (92%)	358 (98%)	6 (2%)	70 82
1	B	351/396 (89%)	343 (98%)	8 (2%)	58 71
1	C	365/396 (92%)	360 (99%)	5 (1%)	74 85
1	D	334/396 (84%)	333 (100%)	1 (0%)	94 98
All	All	1414/1584 (89%)	1394 (99%)	20 (1%)	74 85

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	0.44	0	5,5,5	0.63	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^{th} 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%)	0.46	28 (5%) 25 25	28, 35, 44, 51	0
1	B	465/489 (95%)	0.50	36 (7%) 16 16	31, 36, 43, 50	0
1	C	467/489 (95%)	0.24	11 (2%) 62 61	28, 36, 43, 52	0
1	D	459/489 (93%)	0.70	52 (11%) 7 6	28, 36, 45, 48	0
All	All	1861/1956 (95%)	0.47	127 (6%) 20 20	28, 36, 44, 52	0

All (127) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	498	VAL	7.7
1	D	511	LYS	7.3
1	C	301	VAL	6.7
1	D	510	PRO	6.6
1	D	483	GLY	6.6
1	D	507	ALA	6.4
1	B	492	GLY	6.3
1	D	489	LEU	6.0
1	A	301	VAL	6.0
1	D	487	ILE	5.8
1	A	498	VAL	5.6
1	B	301	VAL	5.2
1	D	329	ALA	5.0
1	D	506	PHE	5.0
1	D	509	SER	4.8
1	D	481	LYS	4.8
1	B	357	HIS	4.7
1	D	502	THR	4.6
1	B	496	ASP	4.5
1	D	513	MET	4.5
1	B	417	GLY	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	508	VAL	4.1
1	D	407	TYR	4.0
1	D	484	LEU	4.0
1	D	450	HIS	3.9
1	C	299	ASP	3.9
1	D	328	LEU	3.9
1	A	497	ASP	3.8
1	A	494	THR	3.8
1	A	333	ILE	3.7
1	D	474	ALA	3.7
1	D	490	TRP	3.6
1	A	334	SER	3.5
1	D	471	THR	3.5
1	A	492	GLY	3.5
1	D	406	LYS	3.5
1	D	445	ALA	3.5
1	D	517	GLN	3.5
1	B	502	THR	3.5
1	D	447	GLY	3.4
1	D	515	MET	3.4
1	B	300	ASP	3.4
1	A	518	ILE	3.3
1	A	490	TRP	3.2
1	B	486	LEU	3.2
1	B	336	ASN	3.1
1	D	122	PHE	3.1
1	D	514	PRO	3.1
1	D	42	PHE	3.0
1	B	513	MET	3.0
1	D	180	VAL	3.0
1	A	495	VAL	2.9
1	C	513	MET	2.9
1	B	449	ALA	2.9
1	C	177	ASP	2.9
1	D	518	ILE	2.9
1	D	479	ASP	2.8
1	A	496	ASP	2.8
1	D	519	ALA	2.8
1	A	311	LEU	2.8
1	B	490	TRP	2.8
1	C	494	THR	2.7
1	B	325	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	445	ALA	2.7
1	A	513	MET	2.7
1	B	494	THR	2.7
1	B	510	PRO	2.7
1	D	335	PRO	2.7
1	A	493	LEU	2.6
1	A	306	ILE	2.6
1	D	305	ILE	2.6
1	A	177	ASP	2.6
1	D	505	ASP	2.6
1	A	486	LEU	2.6
1	D	482	LYS	2.6
1	B	501	SER	2.6
1	D	306	ILE	2.6
1	D	325	ILE	2.6
1	D	47	VAL	2.5
1	A	510	PRO	2.5
1	A	445	ALA	2.5
1	B	282	LEU	2.5
1	B	515	MET	2.5
1	A	335	PRO	2.5
1	A	302	ARG	2.5
1	A	516	GLN	2.5
1	B	454	GLU	2.5
1	D	332	PHE	2.5
1	B	442	GLU	2.5
1	C	518	ILE	2.5
1	B	335	PRO	2.5
1	C	300	ASP	2.5
1	D	145	ILE	2.4
1	B	481	LYS	2.4
1	B	495	VAL	2.4
1	A	506	PHE	2.4
1	D	309	ALA	2.4
1	C	302	ARG	2.4
1	C	493	LEU	2.4
1	D	512	LEU	2.3
1	D	408	GLY	2.3
1	A	491	GLU	2.3
1	B	122	PHE	2.3
1	D	141	LEU	2.3
1	B	407	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	49	ALA	2.2
1	B	452	ILE	2.2
1	B	487	ILE	2.2
1	B	489	LEU	2.2
1	A	514	PRO	2.2
1	B	330	SER	2.2
1	B	359	ALA	2.2
1	D	508	VAL	2.2
1	C	489	LEU	2.2
1	C	519	ALA	2.2
1	A	178	GLY	2.1
1	B	508	VAL	2.1
1	D	477	ASP	2.1
1	D	469	ILE	2.1
1	B	328	LEU	2.1
1	D	331	ASN	2.0
1	D	419	MET	2.0
1	D	179	SER	2.0
1	B	498	VAL	2.0
1	D	336	ASN	2.0
1	A	304	ARG	2.0
1	B	329	ALA	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^{th} 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^2)	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.