Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 09:55 AM GMT

PDB ID	:	3K6M
Title	:	Dynamic domains of Succinyl-CoA:3-ketoacid-coenzyme A transferase from pig heart.
Authors	:	Coker, S.; Lloyd, A.; Mitchell, E.; Lewis, G.R.; Shoolingin-Jordan, P.; Coker, A.R.
Deposited on	:	2009-10-09
Resolution	:	1.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
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:

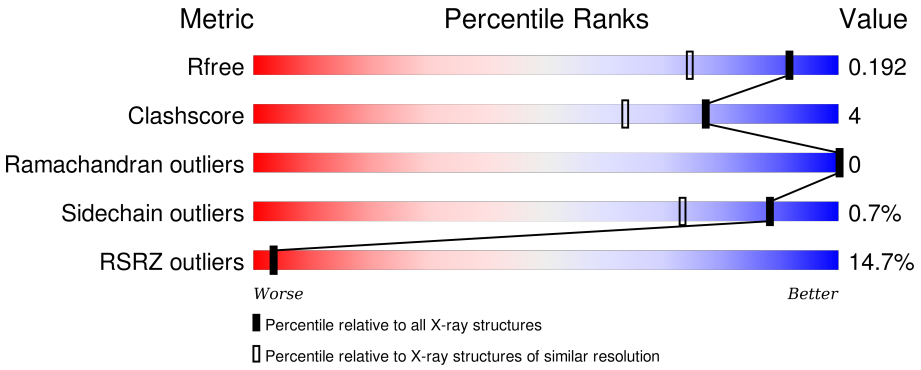
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2072 (1.50-1.50)
Clashscore	102246	2274 (1.50-1.50)
Ramachandran outliers	100387	2218 (1.50-1.50)
Sidechain outliers	100360	2216 (1.50-1.50)
RSRZ outliers	91569	2075 (1.50-1.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	481	15% 92% 5% ·
1	B	481	11% 89% 7% ·
1	C	481	11% 90% 7% ·
1	D	481	20% 86% 9% ·

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CL	A	6000	-	-	-	X
2	CL	D	6001	-	-	-	X
3	GOL	C	5000	-	-	-	X
3	GOL	C	5001	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16054 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.

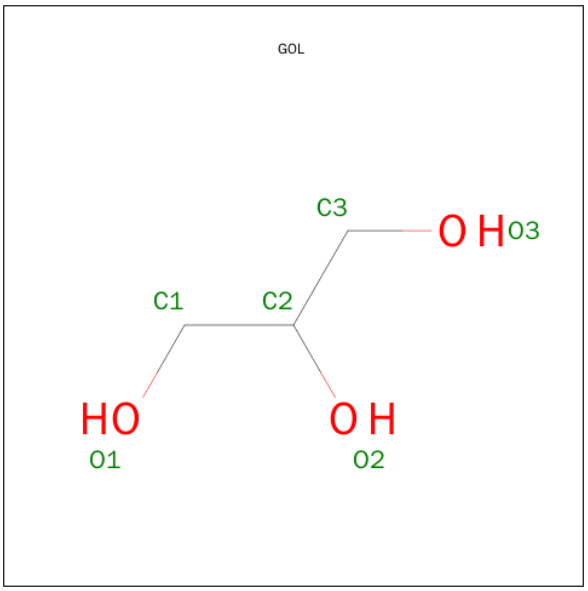
- Molecule 1 is a protein called Succinyl-CoA:3-ketoacid-coenzyme A transferase 1, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	465	Total	C	N	O	S	3	11	0
			3601	2292	610	678	21			
1	D	462	Total	C	N	O	S	2	19	0
			3623	2313	610	680	20			
1	C	466	Total	C	N	O	S	0	16	0
			3627	2311	613	680	23			
1	B	461	Total	C	N	O	S	16	17	0
			3608	2296	609	681	22			

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 4 is water.

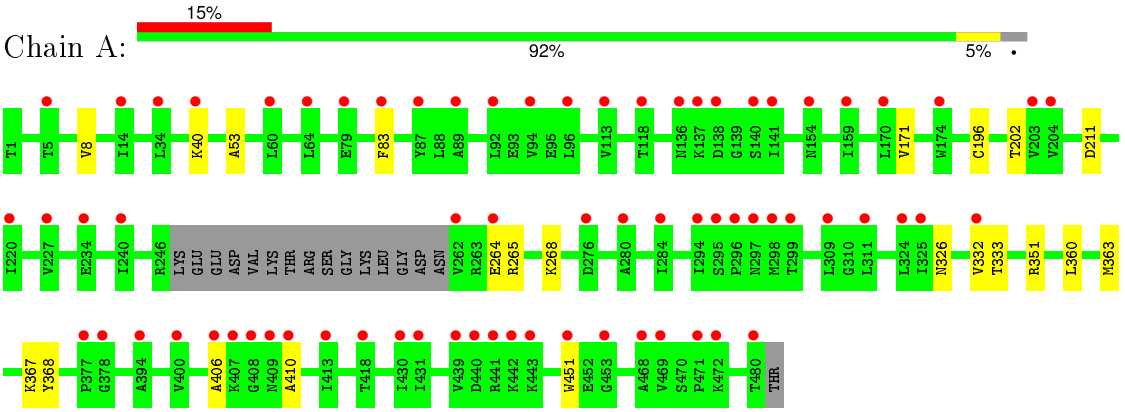
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	353	Total O 353 353	0	0
4	D	352	Total O 352 352	0	0
4	C	474	Total O 474 474	0	0
4	B	402	Total O 402 402	0	0

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.

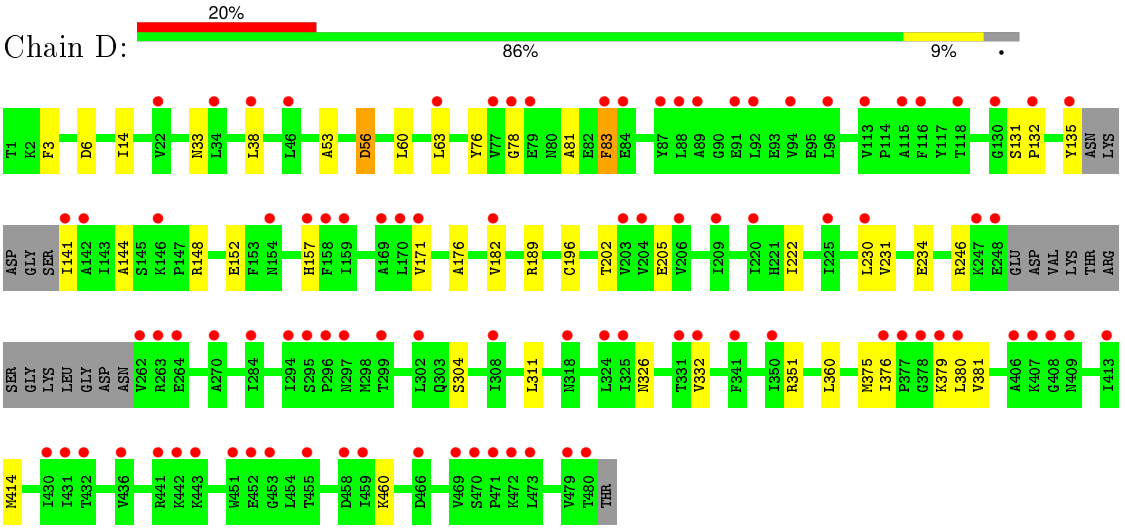
- Molecule 1: Succinyl-CoA:3-ketoacid-coenzyme A transferase 1, mitochondrial

Chain A:



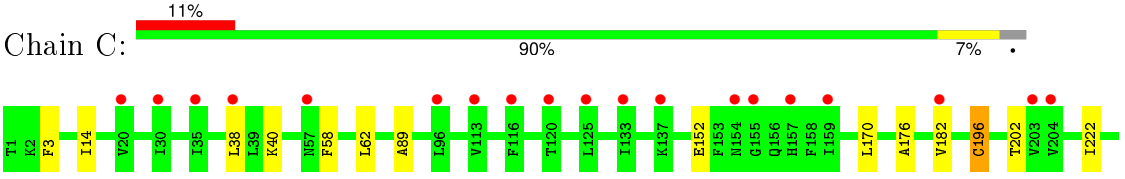
- Molecule 1: Succinyl-CoA:3-ketoacid-coenzyme A transferase 1, mitochondrial

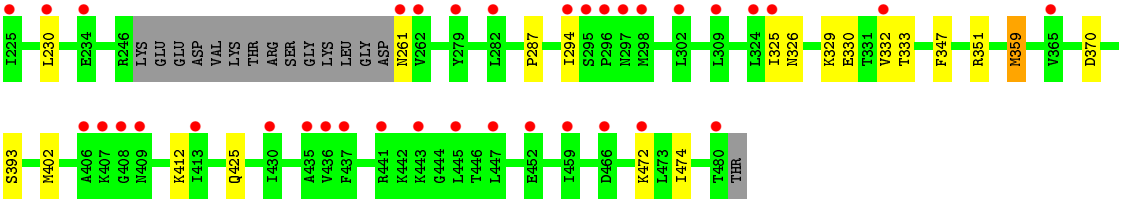
Chain D:



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

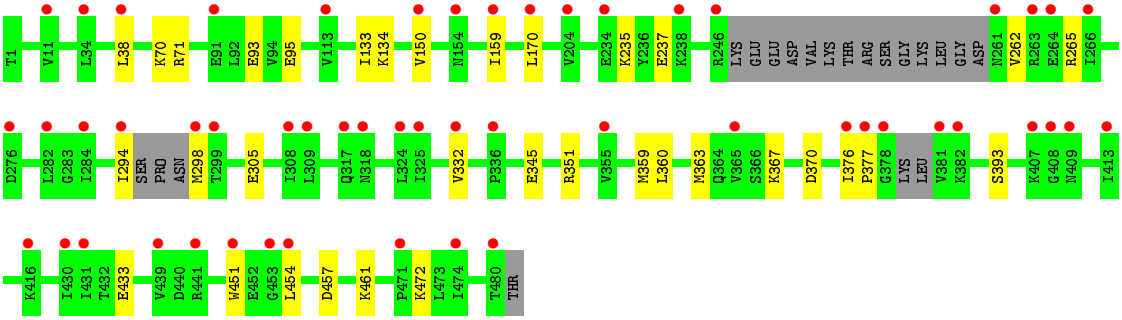
Chain C:





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

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	73.72Å 133.57Å 102.23Å 90.00° 104.98° 90.00°	Depositor
Resolution (Å)	20.00 – 1.50 19.79 – 1.50	Depositor EDS
% Data completeness (in resolution range)	97.6 (20.00-1.50) 97.6 (19.79-1.50)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$< I/\sigma(I) >$ [1]	2.05 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.165 , 0.185 0.173 , 0.192	Depositor DCC
R_{free} test set	14899 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	16.2	Xtriage
Anisotropy	0.076	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 50.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Outliers	1 of 296782 reflections (0.000%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	16054	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% 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, CL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.70	2/3689 (0.1%)	0.74	0/4976
1	B	0.71	4/3705 (0.1%)	0.76	3/4995 (0.1%)
1	C	0.84	5/3733 (0.1%)	0.83	1/5036 (0.0%)
1	D	0.74	0/3728	0.82	6/5030 (0.1%)
All	All	0.75	11/14855 (0.1%)	0.79	10/20037 (0.0%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	196[A]	CYS	CB-SG	-5.76	1.72	1.81
1	C	196[B]	CYS	CB-SG	-5.76	1.72	1.81
1	C	393[A]	SER	N-CA	5.59	1.57	1.46
1	C	393[B]	SER	N-CA	5.59	1.57	1.46
1	B	305[A]	GLU	CD-OE1	5.57	1.31	1.25
1	B	305[B]	GLU	CD-OE1	5.57	1.31	1.25
1	B	305[A]	GLU	CB-CG	-5.29	1.42	1.52
1	B	305[B]	GLU	CB-CG	-5.29	1.42	1.52
1	A	363[A]	MET	CG-SD	-5.14	1.67	1.81
1	A	363[B]	MET	CG-SD	-5.14	1.67	1.81
1	C	425	GLN	CD-NE2	-5.05	1.20	1.32

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	189	ARG	NE-CZ-NH1	5.93	123.27	120.30
1	B	359[A]	MET	CG-SD-CE	-5.47	91.45	100.20
1	B	359[B]	MET	CG-SD-CE	-5.47	91.45	100.20
1	B	370	ASP	CB-CG-OD1	5.45	123.21	118.30
1	D	189	ARG	NE-CZ-NH2	-5.45	117.57	120.30
1	D	6	ASP	CB-CG-OD2	5.38	123.14	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	148	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	D	246	ARG	NE-CZ-NH1	5.23	122.91	120.30
1	D	135	TYR	CB-CA-C	-5.15	100.09	110.40
1	C	370	ASP	CB-CG-OD1	5.09	122.88	118.30

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	3601	0	3704	19	0
1	B	3608	0	3705	27	0
1	C	3627	0	3748	31	0
1	D	3623	0	3734	32	0
2	A	1	0	0	0	0
2	D	1	0	0	0	0
3	C	12	0	16	0	0
4	A	353	0	0	1	0
4	B	402	0	0	6	0
4	C	474	0	0	5	0
4	D	352	0	0	2	0
All	All	16054	0	14907	108	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 4.

All (108) 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:C:196[B]:CYS:SG	1:C:202[B]:THR:HG21	2.03	0.97
1:D:76[B]:TYR:CE2	1:D:78:GLY:HA2	2.01	0.95
1:C:3:PHE:CE2	1:C:230[B]:LEU:HD23	2.01	0.95
1:D:3:PHE:CE2	1:D:230[A]:LEU:HD23	2.01	0.94
1:D:196[B]:CYS:SG	1:D:202[B]:THR:HG21	2.13	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196[B]:CYS:SG	1:A:202[B]:THR:HG21	2.19	0.82
1:B:93[B]:GLU:HG3	1:B:133:ILE:HG22	1.68	0.76
1:C:326:ASN:HB3	1:C:332[B]:VAL:HG21	1.69	0.75
1:A:196[A]:CYS:O	1:A:202[A]:THR:HG21	1.90	0.71
1:D:76[B]:TYR:CE2	1:D:78:GLY:CA	2.76	0.68
1:C:332[A]:VAL:HG22	1:C:333:THR:H	1.59	0.68
1:C:332[A]:VAL:HG22	1:C:333:THR:N	2.09	0.66
1:A:326:ASN:HB3	1:A:332[B]:VAL:HG21	1.77	0.66
1:B:345[B]:GLU:HA	1:B:345[B]:GLU:OE1	1.95	0.66
1:A:332[B]:VAL:HG12	1:A:333:THR:N	2.11	0.65
1:B:472:LYS:HG2	1:B:472:LYS:O	1.96	0.65
1:D:53:ALA:HB3	1:D:83:PHE:CD1	2.31	0.65
1:B:95:GLU:HG3	4:B:820:HOH:O	1.97	0.64
1:D:414:MET:HE2	4:D:794:HOH:O	1.97	0.64
1:D:375[A]:MET:SD	1:D:380:LEU:O	2.56	0.63
1:B:93[B]:GLU:HG2	1:B:133:ILE:CG2	2.29	0.63
1:C:402[A]:MET:CE	1:C:412:LYS:HE2	2.30	0.61
1:A:332[B]:VAL:HG12	1:A:333:THR:O	2.00	0.61
1:B:93[B]:GLU:CG	1:B:133:ILE:HG22	2.31	0.60
1:C:402[A]:MET:HE2	1:C:412:LYS:HE2	1.84	0.60
1:B:93[B]:GLU:CG	1:B:133:ILE:CG2	2.79	0.60
1:D:132[A]:PRO:HD3	1:D:141:ILE:HD12	1.82	0.59
1:D:152:GLU:HB2	1:D:157[B]:HIS:CD2	2.37	0.59
1:B:351:ARG:HD3	4:B:545:HOH:O	2.04	0.58
1:C:196[B]:CYS:HG	1:C:202[B]:THR:HG21	1.70	0.57
1:D:131[A]:SER:O	1:D:144:ALA:HA	2.05	0.57
1:D:132[A]:PRO:CD	1:D:141:ILE:HD12	2.35	0.56
1:B:70:LYS:NZ	4:B:891:HOH:O	2.39	0.55
1:C:182:VAL:HG22	1:C:222:ILE:HB	1.87	0.55
1:B:265:ARG:HD3	1:B:451:TRP:CZ2	2.42	0.54
1:D:14:ILE:HD12	1:D:38[A]:LEU:HD21	1.89	0.54
1:C:3:PHE:CZ	1:C:230[B]:LEU:HD23	2.42	0.53
1:D:152:GLU:HB2	1:D:157[B]:HIS:NE2	2.24	0.53
1:C:38[A]:LEU:HD11	1:C:170:LEU:HD11	1.91	0.53
1:A:211:ASP:HB2	1:D:157[B]:HIS:CD2	2.44	0.52
1:A:332[B]:VAL:CG1	1:A:333:THR:N	2.74	0.52
1:C:196[B]:CYS:SG	1:C:202[B]:THR:CG2	2.89	0.51
1:B:451:TRP:HB3	1:B:454:LEU:HD12	1.93	0.51
1:B:150[A]:VAL:HG22	1:B:159:ILE:HG22	1.94	0.50
1:A:351:ARG:HD3	4:A:7042:HOH:O	2.11	0.50
1:B:294:ILE:HG23	1:B:298:MET:HE3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:294:ILE:HG23	1:B:298:MET:CE	2.43	0.49
1:D:56:ASP:OD1	1:D:81:ALA:HB3	2.12	0.49
1:D:326:ASN:HB3	1:D:332[A]:VAL:HG11	1.93	0.49
1:D:176:ALA:CB	1:D:230[B]:LEU:HD11	2.42	0.49
1:C:152:GLU:HG2	4:C:5565:HOH:O	2.12	0.49
1:C:472:LYS:O	1:C:474:ILE:HG23	2.13	0.49
1:B:265:ARG:HD3	1:B:451:TRP:CE2	2.48	0.48
1:C:14:ILE:HD12	1:C:38[A]:LEU:HD21	1.94	0.48
1:D:176:ALA:HB1	1:D:230[B]:LEU:HD11	1.95	0.48
1:C:330:GLU:O	1:C:332[B]:VAL:HG23	2.13	0.48
1:B:457:ASP:O	1:B:461:LYS:HG3	2.13	0.48
1:C:332[A]:VAL:CG2	1:C:333:THR:N	2.77	0.48
1:D:196[B]:CYS:SG	1:D:202[B]:THR:CG2	2.96	0.47
1:B:93[B]:GLU:HG3	1:B:133:ILE:CG2	2.41	0.46
1:C:332[A]:VAL:CG2	1:C:333:THR:H	2.28	0.46
1:B:367:LYS:NZ	4:B:847:HOH:O	2.48	0.46
1:A:332[B]:VAL:HG12	1:A:333:THR:H	1.79	0.46
1:B:70:LYS:NZ	1:B:93[A]:GLU:OE1	2.47	0.46
1:C:3:PHE:CE2	1:C:230[B]:LEU:CD2	2.89	0.46
1:A:171:VAL:HG11	1:A:196[A]:CYS:SG	2.56	0.46
1:D:351:ARG:HD3	4:D:549:HOH:O	2.16	0.46
1:C:294:ILE:HD12	4:C:5472:HOH:O	2.17	0.45
1:C:176:ALA:CB	1:C:230[B]:LEU:HD21	2.47	0.45
1:C:325:ILE:HD12	1:C:329:LYS:HA	1.98	0.45
1:B:38[B]:LEU:HD11	1:B:170:LEU:HD11	1.99	0.45
1:A:196[B]:CYS:SG	1:A:202[B]:THR:CG2	3.00	0.45
1:A:265:ARG:HD3	1:A:451:TRP:CD2	2.52	0.45
1:C:287:PRO:HB3	1:C:359[A]:MET:HB3	1.98	0.44
1:D:182:VAL:HG22	1:D:222:ILE:HB	1.99	0.44
1:D:176:ALA:CB	1:D:230[A]:LEU:HD21	2.47	0.44
1:A:406:ALA:HB3	1:A:410:ALA:HB3	2.00	0.44
1:A:8:VAL:HG21	1:A:40[B]:LYS:HD3	1.99	0.43
1:A:53:ALA:HB3	1:A:83:PHE:CD1	2.54	0.43
1:D:205:GLU:HA	1:D:231:VAL:O	2.19	0.43
1:C:261:ASN:N	4:C:5515:HOH:O	2.51	0.43
1:B:363[A]:MET:SD	1:B:376:ILE:HG23	2.58	0.43
1:D:33:ASN:OD1	1:D:234[A]:GLU:HG2	2.18	0.43
1:D:60:LEU:CD2	1:D:63:LEU:HD12	2.48	0.43
1:C:332[A]:VAL:HG22	1:C:333:THR:O	2.19	0.43
1:A:332[B]:VAL:CG1	1:A:333:THR:H	2.32	0.42
1:D:3:PHE:CZ	1:D:230[A]:LEU:HD23	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:40:LYS:HE3	4:C:5379:HOH:O	2.18	0.42
1:D:171:VAL:HG11	1:D:196[A]:CYS:SG	2.60	0.42
1:B:235:LYS:HE2	1:B:237:GLU:HG2	2.02	0.42
1:B:71[A]:ARG:CD	4:B:820:HOH:O	2.66	0.42
1:A:367:LYS:HD2	1:A:368:TYR:CE1	2.55	0.42
1:C:347:PHE:O	1:C:351[B]:ARG:HB2	2.20	0.42
1:D:375[A]:MET:HE1	1:D:381:VAL:HA	2.01	0.41
1:D:141:ILE:O	1:D:141:ILE:HG23	2.20	0.41
1:D:376:ILE:HG21	1:D:379:LYS:HD2	2.01	0.41
1:A:264[A]:GLU:OE2	1:A:268:LYS:HE3	2.19	0.41
1:D:304:SER:HB2	1:D:311:LEU:HD11	2.01	0.41
1:B:472:LYS:O	1:B:472:LYS:CG	2.66	0.41
1:A:265:ARG:HD3	1:A:451:TRP:CE3	2.56	0.41
1:B:71[A]:ARG:HD3	4:B:820:HOH:O	2.21	0.40
1:C:89:ALA:HB2	4:C:5448:HOH:O	2.21	0.40
1:B:93[A]:GLU:HG2	1:B:134:LYS:HD2	2.03	0.40
1:B:262:VAL:HG13	1:B:433:GLU:HB3	2.03	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	472/481 (98%)	464 (98%)	8 (2%)	0	100	100
1	B	470/481 (98%)	463 (98%)	7 (2%)	0	100	100
1	C	478/481 (99%)	469 (98%)	9 (2%)	0	100	100
1	D	475/481 (99%)	464 (98%)	11 (2%)	0	100	100
All	All	1895/1924 (98%)	1860 (98%)	35 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	390/393 (99%)	389 (100%)	1 (0%)	94	86
1	B	392/393 (100%)	386 (98%)	6 (2%)	72	44
1	C	396/393 (101%)	393 (99%)	3 (1%)	86	70
1	D	394/393 (100%)	390 (99%)	4 (1%)	82	62
All	All	1572/1572 (100%)	1558 (99%)	14 (1%)	88	65

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	360	LEU
1	D	56	ASP
1	D	83	PHE
1	D	360	LEU
1	D	460	LYS
1	C	58	PHE
1	C	359[A]	MET
1	C	359[B]	MET
1	B	332[A]	VAL
1	B	332[B]	VAL
1	B	360	LEU
1	B	377	PRO
1	B	393[A]	SER
1	B	393[B]	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	301	HIS
1	B	99	GLN
1	B	154	ASN
1	B	411	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

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	$\#\|Z\| > 2$
3	GOL	C	5000	-	5,5,5	0.16	0	5,5,5	0.23	0
3	GOL	C	5001	-	5,5,5	0.66	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
3	GOL	C	5000	-	-	0/4/4/4	0/0/0/0
3	GOL	C	5001	-	-	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.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	465/481 (96%)	1.02	71 (15%)	3 3	18, 25, 31, 37	1 (0%)
1	B	461/481 (95%)	0.96	53 (11%)	6 6	18, 24, 32, 43	2 (0%)
1	C	466/481 (96%)	0.95	55 (11%)	6 5	20, 24, 32, 39	0
1	D	462/481 (96%)	1.23	94 (20%)	1 1	17, 25, 34, 42	1 (0%)
All	All	1854/1924 (96%)	1.04	273 (14%)	3 3	17, 25, 32, 43	4 (0%)

All (273) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	381	VAL	12.9
1	B	377	PRO	9.7
1	D	378	GLY	8.1
1	A	296	PRO	7.8
1	D	248	GLU	7.0
1	D	141	ILE	6.8
1	D	296	PRO	6.7
1	C	297	ASN	6.5
1	C	296	PRO	6.4
1	A	407	LYS	6.3
1	D	407	LYS	6.3
1	D	480	THR	6.3
1	B	408	GLY	6.1
1	B	376	ILE	6.0
1	A	262	VAL	6.0
1	C	407	LYS	5.7
1	B	480	THR	5.6
1	A	297	ASN	5.5
1	D	408	GLY	5.3
1	C	261	ASN	5.1
1	A	137	LYS	5.1

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Mol	Chain	Res	Type	RSRZ
1	B	453	GLY	4.9
1	A	471	PRO	4.8
1	A	409	ASN	4.8
1	A	441	ARG	4.8
1	D	413	ILE	4.8
1	D	380	LEU	4.7
1	C	408	GLY	4.7
1	D	297	ASN	4.7
1	A	408	GLY	4.7
1	A	406	ALA	4.7
1	A	480	THR	4.7
1	D	472	LYS	4.6
1	D	88	LEU	4.6
1	A	378	GLY	4.6
1	A	284	ILE	4.5
1	D	379	LYS	4.5
1	C	154	ASN	4.5
1	A	453	GLY	4.5
1	B	317	GLN	4.4
1	D	431	ILE	4.4
1	D	262	VAL	4.3
1	D	284	ILE	4.2
1	D	377	PRO	4.1
1	B	261	ASN	4.1
1	D	441	ARG	4.1
1	D	332[A]	VAL	4.0
1	B	378	GLY	4.0
1	B	284	ILE	4.0
1	D	453	GLY	3.9
1	B	430	ILE	3.9
1	D	466	ASP	3.9
1	C	294	ILE	3.8
1	C	332[A]	VAL	3.8
1	A	264[A]	GLU	3.8
1	A	394	ALA	3.8
1	D	376	ILE	3.7
1	A	332[A]	VAL	3.7
1	D	452	GLU	3.7
1	C	413	ILE	3.6
1	B	431	ILE	3.6
1	C	325	ILE	3.6
1	C	137	LYS	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	276	ASP	3.6
1	D	325	ILE	3.6
1	B	332[A]	VAL	3.6
1	D	132[A]	PRO	3.5
1	A	325	ILE	3.5
1	D	94	VAL	3.5
1	B	471	PRO	3.5
1	D	87	TYR	3.4
1	A	472	LYS	3.4
1	D	92	LEU	3.4
1	D	247	LYS	3.4
1	D	206	VAL	3.3
1	D	158	PHE	3.3
1	D	459	ILE	3.3
1	B	299	THR	3.3
1	A	431	ILE	3.3
1	A	410	ALA	3.3
1	D	473	LEU	3.3
1	C	447	LEU	3.3
1	C	459	ILE	3.2
1	B	409	ASN	3.2
1	A	96	LEU	3.2
1	C	230[A]	LEU	3.2
1	D	203	VAL	3.2
1	A	440	ASP	3.2
1	D	458	ASP	3.2
1	D	84	GLU	3.1
1	D	96	LEU	3.1
1	B	451	TRP	3.1
1	A	442	LYS	3.1
1	C	282	LEU	3.1
1	D	471	PRO	3.1
1	D	146	LYS	3.1
1	A	138	ASP	3.1
1	B	441	ARG	3.1
1	C	466	ASP	3.0
1	B	298	MET	3.0
1	A	294	ILE	3.0
1	B	413	ILE	3.0
1	C	204	VAL	3.0
1	C	409	ASN	3.0
1	A	299	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	140	SER	3.0
1	D	135	TYR	3.0
1	D	455	THR	3.0
1	C	480	THR	3.0
1	C	445	LEU	3.0
1	B	34	LEU	3.0
1	C	430	ILE	3.0
1	A	276	ASP	2.9
1	D	264	GLU	2.9
1	A	154	ASN	2.9
1	B	154	ASN	2.9
1	A	94	VAL	2.9
1	D	432	THR	2.9
1	A	413	ILE	2.9
1	D	157[A]	HIS	2.9
1	D	204	VAL	2.9
1	A	451	TRP	2.9
1	A	309	LEU	2.8
1	B	416	LYS	2.8
1	D	77	VAL	2.8
1	A	324	LEU	2.8
1	A	400	VAL	2.8
1	A	469	VAL	2.8
1	B	204	VAL	2.8
1	D	442	LYS	2.8
1	B	294	ILE	2.8
1	D	263	ARG	2.8
1	D	443	LYS	2.8
1	C	406	ALA	2.8
1	D	170	LEU	2.7
1	C	365	VAL	2.7
1	C	436	VAL	2.7
1	B	318	ASN	2.7
1	A	204	VAL	2.7
1	D	113	VAL	2.7
1	B	407	LYS	2.7
1	B	150[A]	VAL	2.7
1	D	406	ALA	2.7
1	B	234	GLU	2.7
1	C	435	ALA	2.7
1	D	38[A]	LEU	2.7
1	A	298	MET	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	451	TRP	2.6
1	D	318	ASN	2.6
1	D	79	GLU	2.6
1	D	230[A]	LEU	2.6
1	D	469	VAL	2.6
1	C	125	LEU	2.6
1	B	336	PRO	2.6
1	D	430	ILE	2.6
1	C	437	PHE	2.6
1	A	79	GLU	2.6
1	B	170	LEU	2.6
1	B	309	LEU	2.6
1	D	142	ALA	2.6
1	C	35	ILE	2.6
1	B	246	ARG	2.6
1	A	443	LYS	2.6
1	D	479	VAL	2.6
1	C	203	VAL	2.6
1	A	40[A]	LYS	2.6
1	D	154	ASN	2.5
1	C	225	ILE	2.5
1	A	295	SER	2.5
1	C	182	VAL	2.5
1	D	324	LEU	2.5
1	D	118	THR	2.5
1	A	141	ILE	2.5
1	D	409	ASN	2.5
1	D	78	GLY	2.5
1	A	227	VAL	2.5
1	A	64	LEU	2.5
1	D	34	LEU	2.5
1	C	96	LEU	2.5
1	A	118	THR	2.5
1	D	331	THR	2.5
1	C	30	ILE	2.5
1	A	34	LEU	2.5
1	A	280	ALA	2.5
1	B	264	GLU	2.5
1	A	159	ILE	2.5
1	D	220	ILE	2.5
1	B	474	ILE	2.5
1	A	418	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	113	VAL	2.4
1	D	171	VAL	2.4
1	C	157	HIS	2.4
1	C	302	LEU	2.4
1	B	454	LEU	2.4
1	A	83	PHE	2.4
1	D	436	VAL	2.4
1	B	308	ILE	2.4
1	B	439	VAL	2.4
1	D	63	LEU	2.4
1	A	174	TRP	2.4
1	A	234	GLU	2.4
1	D	91	GLU	2.4
1	A	439	VAL	2.4
1	C	57[A]	ASN	2.4
1	C	113	VAL	2.4
1	C	262	VAL	2.4
1	A	430	ILE	2.4
1	D	294	ILE	2.4
1	B	325	ILE	2.4
1	D	302	LEU	2.4
1	C	38[A]	LEU	2.4
1	C	120	THR	2.4
1	B	324	LEU	2.4
1	C	443	LYS	2.3
1	C	234	GLU	2.3
1	A	87	TYR	2.3
1	C	452	GLU	2.3
1	D	308	ILE	2.3
1	B	159	ILE	2.3
1	C	298[A]	MET	2.2
1	A	89	ALA	2.2
1	A	203	VAL	2.2
1	B	263	ARG	2.2
1	A	92	LEU	2.2
1	C	295	SER	2.2
1	D	209	ILE	2.2
1	B	266	ILE	2.2
1	B	382	LYS	2.2
1	A	136	ASN	2.2
1	C	279	TYR	2.2
1	D	295	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	11	VAL	2.2
1	C	159	ILE	2.2
1	D	182	VAL	2.1
1	A	311	LEU	2.1
1	D	89	ALA	2.1
1	A	14	ILE	2.1
1	B	91[A]	GLU	2.1
1	D	116	PHE	2.1
1	D	115	ALA	2.1
1	C	20	VAL	2.1
1	B	113	VAL	2.1
1	B	365	VAL	2.1
1	A	170	LEU	2.1
1	B	282	LEU	2.1
1	A	240	ILE	2.1
1	C	441	ARG	2.1
1	D	22	VAL	2.1
1	B	355	VAL	2.1
1	D	46	LEU	2.1
1	C	309	LEU	2.1
1	C	324	LEU	2.1
1	A	220	ILE	2.1
1	D	350	ILE	2.1
1	C	133	ILE	2.1
1	D	270	ALA	2.1
1	A	377	PRO	2.1
1	C	116	PHE	2.1
1	C	155	GLY	2.1
1	C	472	LYS	2.1
1	B	38[A]	LEU	2.1
1	D	299	THR	2.0
1	A	468	ALA	2.0
1	D	470	SER	2.0
1	D	159	ILE	2.0
1	D	225	ILE	2.0
1	D	83	PHE	2.0
1	D	341	PHE	2.0
1	A	5	THR	2.0
1	A	60	LEU	2.0
1	B	238	LYS	2.0
1	D	130[A]	GLY	2.0
1	D	169	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
3	GOL	C	5000	6/6	0.92	0.20	8.19	20,21,23,24	0
2	CL	A	6000	1/1	0.99	0.17	5.25	19,19,19,19	1
2	CL	D	6001	1/1	0.99	0.19	4.94	15,15,15,15	1
3	GOL	C	5001	6/6	0.92	0.26	4.67	25,28,29,30	0

6.5 Other polymers (i)

There are no such residues in this entry.