



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 31, 2026 – 11:02 AM UTC

PDB ID : 3K6M / pdb_00003k6m
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

<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

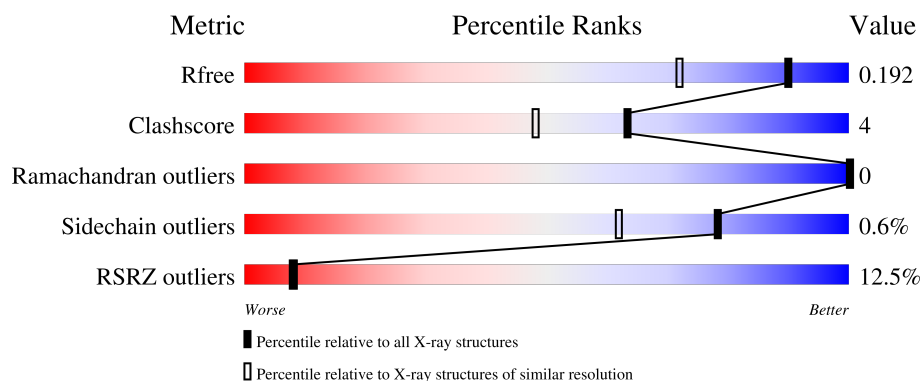
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	4037 (1.50-1.50)
Clashscore	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)
RSRZ outliers	180081	4039 (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 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	481	
1	B	481	
1	C	481	
1	D	481	

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 (CCD ID: 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 (CCD ID: GOL) (formula: C₃H₈O₃).



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

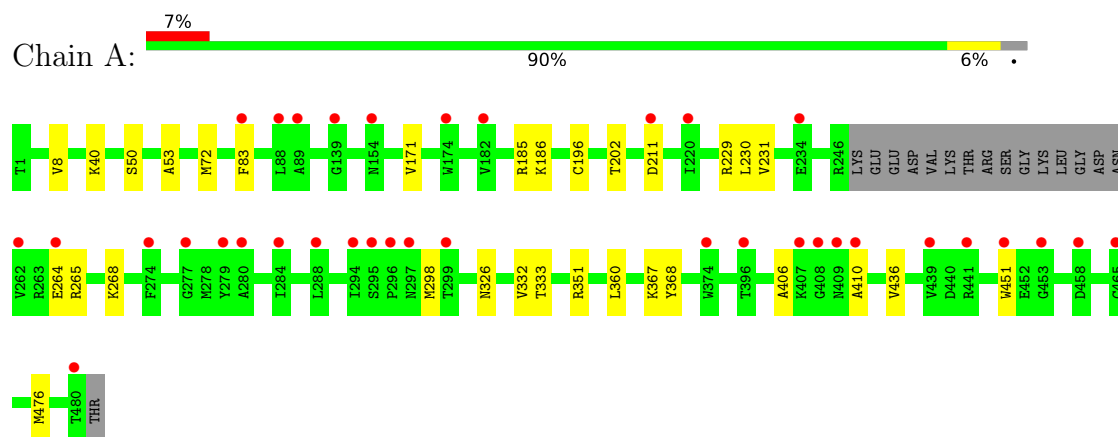
- Molecule 4 is water.

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

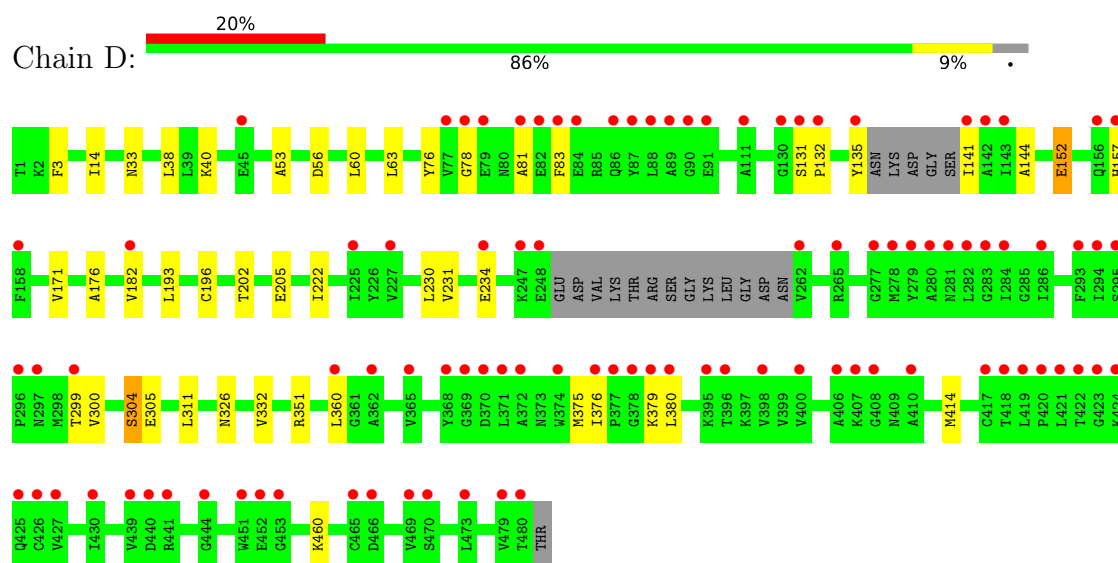
3 Residue-property plots [i](#)

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.

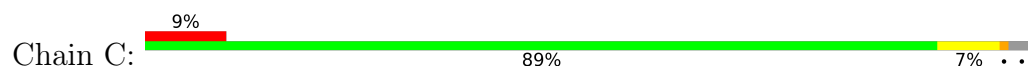
- Molecule 1: Succinyl-CoA:3-ketoacid-coenzyme A transferase 1, mitochondrial

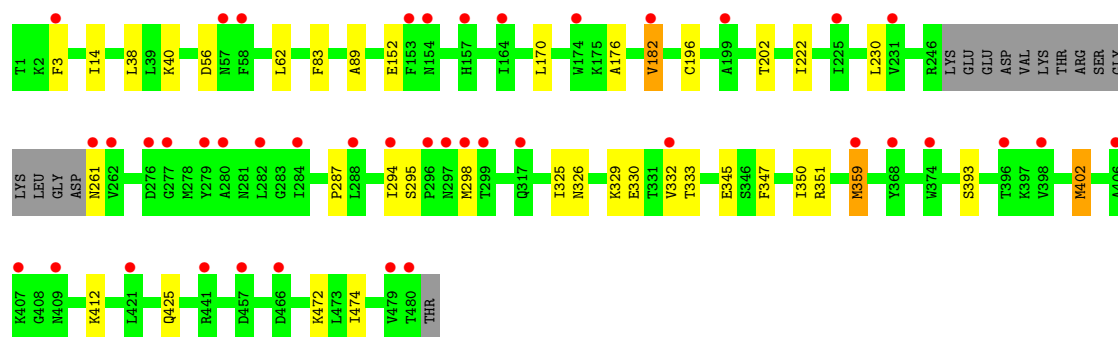


- Molecule 1: Succinyl-CoA:3-ketoacid-coenzyme A transferase 1, mitochondrial

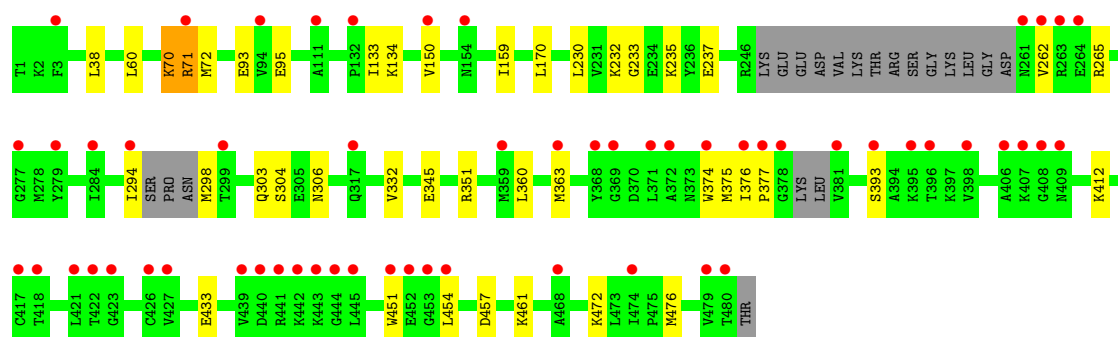
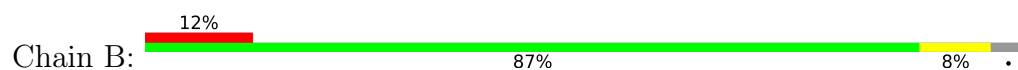


- Molecule 1: Succinyl-CoA:3-ketoacid-coenzyme A transferase 1, mitochondrial





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



4 Data and refinement statistics

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 20.00 – 1.50	Depositor EDS
% Data completeness (in resolution range)	97.6 (20.00-1.50) 97.6 (20.00-1.50)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ 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 (4.90%)	wwPDB-VP
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 , 45.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	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.*

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: CL, 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	0.88	5/3689 (0.1%)	0.84	0/4976
1	B	0.86	9/3705 (0.2%)	0.83	0/4995
1	C	1.05	14/3733 (0.4%)	0.92	0/5036
1	D	0.91	5/3728 (0.1%)	0.89	1/5030 (0.0%)
All	All	0.93	33/14855 (0.2%)	0.87	1/20037 (0.0%)

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	402[A]	MET	SD-CE	-9.81	1.55	1.79
1	C	402[B]	MET	SD-CE	-9.81	1.55	1.79
1	A	231	VAL	C-O	-7.64	1.16	1.24
1	A	230	LEU	C-O	-7.16	1.15	1.24
1	D	152	GLU	C-N	6.82	1.43	1.33
1	B	230	LEU	C-O	-6.67	1.16	1.24
1	B	233	GLY	C-O	-6.49	1.17	1.23
1	A	229	ARG	C-O	-6.40	1.16	1.24
1	C	425	GLN	CD-NE2	-6.21	1.20	1.33
1	B	304	SER	C-O	-6.17	1.17	1.24
1	C	393[A]	SER	N-CA	6.06	1.53	1.46
1	C	393[B]	SER	N-CA	6.06	1.53	1.46
1	A	186	LYS	C-O	-5.99	1.18	1.24
1	C	345[A]	GLU	C-O	-5.95	1.17	1.24
1	C	345[B]	GLU	C-O	-5.95	1.17	1.24
1	C	56	ASP	C-O	-5.95	1.17	1.24
1	D	300	VAL	C-O	-5.87	1.17	1.24
1	D	304	SER	C-O	-5.82	1.17	1.24
1	D	305	GLU	C-O	-5.66	1.16	1.24
1	A	185	ARG	C-O	-5.62	1.17	1.24
1	B	232	LYS	C-O	-5.59	1.17	1.24
1	B	71[A]	ARG	C-O	-5.51	1.17	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	71[B]	ARG	C-O	-5.51	1.17	1.23
1	C	350	ILE	C-O	-5.46	1.18	1.24
1	C	402[A]	MET	C-O	-5.30	1.17	1.23
1	C	402[B]	MET	C-O	-5.30	1.17	1.23
1	C	425	GLN	C-O	-5.28	1.17	1.23
1	C	393[A]	SER	C-O	-5.22	1.17	1.24
1	C	393[B]	SER	C-O	-5.22	1.17	1.24
1	B	70	LYS	C-O	-5.20	1.16	1.23
1	B	303	GLN	C-O	-5.09	1.18	1.23
1	D	299	THR	C-O	-5.06	1.18	1.24
1	B	306	ASN	C-O	-5.04	1.17	1.24

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	135	TYR	CB-CA-C	-5.27	100.09	110.10

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	22	0
1	B	3608	0	3705	30	0
1	C	3627	0	3748	34	0
1	D	3623	0	3734	33	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	3	0
All	All	16054	0	14907	118	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 (118) 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:B:294:ILE:HG23	1:B:298:MET:HE3	1.51	0.90
1:D:196[B]:CYS:SG	1:D:202[B]:THR:HG21	2.13	0.87
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:C:402[A]:MET:HE2	1:C:412:LYS:HE2	1.74	0.68
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:O	1:B:472:LYS:HG2	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: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:A:436:VAL:HG23	1:A:476:MET:HE2	1.80	0.61
1:B:93[B]:GLU:CG	1:B:133:ILE:HG22	2.31	0.60
1:B:93[B]:GLU:CG	1:B:133:ILE:CG2	2.79	0.60
1:B:60:LEU:HD23	1:B:72:MET:HE3	1.83	0.59
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:C:295:SER:H	1:C:298[A]:MET:HE2	1.68	0.59
1:B:60:LEU:CD2	1:B:72:MET:HE3	2.34	0.58
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:374:TRP:CZ3	1:B:375[A]:MET:HE2	2.42	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:50[B]:SER:OG	1:A:72:MET:HE1	2.09	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: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:B:70:LYS:NZ	4:B:891:HOH:O	2.39	0.49
1:C:472:LYS:O	1:C:474:ILE:HG23	2.13	0.49
1:C:14:ILE:HD12	1:C:38[A]:LEU:HD21	1.94	0.48
1:B:265:ARG:HD3	1:B:451:TRP:CE2	2.48	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:451:TRP:CE3	1:B:476:MET:HE2	2.50	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:412:LYS:NZ	4:B:860: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: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:3:PHE:CE2	1:C:230[B]:LEU:CD2	2.89	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:287:PRO:HB3	1:C:359[A]:MET:HB3	1.98	0.44
1:D:193:LEU:HD23	1:D:193:LEU:C	2.42	0.44
1:D:182:VAL:HG22	1:D:222:ILE:HB	1.99	0.44
1:A:406:ALA:HB3	1:A:410:ALA:HB3	2.00	0.44
1:D:176:ALA:CB	1:D:230[A]:LEU:HD21	2.47	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:D:33:ASN:OD1	1:D:234[A]:GLU:HG2	2.18	0.43
1:B:363[A]:MET:SD	1:B:376:ILE:HG23	2.58	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
1:C:40:LYS:HE3	4:C:5379:HOH:O	2.18	0.42
1:A:298:MET:HE2	1:A:298:MET:HB3	1.96	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:A:264[A]:GLU:OE2	1:A:268:LYS:HE3	2.19	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:C:83:PHE:CD2	1:C:83:PHE:C	2.96	0.41
1:D:40:LYS:NZ	4:D:850:HOH:O	2.31	0.41
1:D:304:SER:HB2	1:D:311:LEU:HD11	2.01	0.41
1:D:414:MET:HE2	4:D:794:HOH:O	2.21	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:C:89:ALA:HB2	4:C:5448:HOH:O	2.21	0.40
1:B:71[A]:ARG:HD3	4:B:820:HOH:O	2.21	0.40
1:C:359[B]:MET:HE3	1:C:359[B]:MET:HB2	1.90	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

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	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

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%)	86	75
1	B	392/393 (100%)	386 (98%)	6 (2%)	57	31
1	C	396/393 (101%)	393 (99%)	3 (1%)	73	54
1	D	394/393 (100%)	392 (100%)	2 (0%)	81	66
All	All	1572/1572 (100%)	1560 (99%)	12 (1%)	78	54

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	360	LEU
1	D	360	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	460	LYS
1	C	182	VAL
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	477	GLN
1	D	99	GLN
1	D	301	HIS
1	B	157	HIS
1	B	317	GLN
1	B	409	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	0.28	0
3	GOL	C	5001	-	5,5,5	0.69	0	5,5,5	0.68	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	-
3	GOL	C	5001	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	465/481 (96%)	0.97	36 (7%) 19 21	12, 25, 31, 37	12 (2%)
1	B	461/481 (95%)	1.11	58 (12%) 8 8	11, 24, 31, 43	19 (4%)
1	C	466/481 (96%)	1.05	42 (9%) 15 16	14, 24, 32, 39	16 (3%)
1	D	462/481 (96%)	1.40	96 (20%) 2 2	12, 24, 34, 42	20 (4%)
All	All	1854/1924 (96%)	1.13	232 (12%) 8 8	11, 24, 32, 43	67 (3%)

All (232) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	130[A]	GLY	7.9
1	D	132[A]	PRO	5.6
1	B	453	GLY	5.5
1	B	381	VAL	5.4
1	D	141	ILE	5.4
1	D	87	TYR	5.2
1	D	279	TYR	5.2
1	D	83	PHE	5.2
1	D	374	TRP	5.2
1	D	88	LEU	5.1
1	D	131[A]	SER	4.8
1	D	380	LEU	4.8
1	B	377	PRO	4.8
1	D	248	GLU	4.5
1	B	441	ARG	4.5
1	D	262	VAL	4.5
1	C	480	THR	4.5
1	D	378	GLY	4.4
1	C	294	ILE	4.2
1	D	135	TYR	4.2
1	C	279	TYR	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	421	LEU	4.1
1	A	453	GLY	4.0
1	D	158	PHE	4.0
1	A	262	VAL	4.0
1	D	284	ILE	4.0
1	D	396	THR	3.9
1	D	280	ALA	3.9
1	D	395	LYS	3.8
1	D	77	VAL	3.7
1	D	377	PRO	3.7
1	B	451	TRP	3.7
1	D	422	THR	3.7
1	C	297	ASN	3.6
1	B	421	LEU	3.6
1	D	398	VAL	3.6
1	B	376	ILE	3.5
1	B	262	VAL	3.5
1	D	296	PRO	3.5
1	B	279	TYR	3.5
1	D	423	GLY	3.5
1	D	84	GLU	3.5
1	B	439	VAL	3.5
1	D	441	ARG	3.5
1	D	426	CYS	3.5
1	B	427	VAL	3.4
1	D	480	THR	3.4
1	D	407	LYS	3.3
1	B	398	VAL	3.3
1	D	427	VAL	3.3
1	A	279	TYR	3.3
1	B	261	ASN	3.3
1	D	294	ILE	3.3
1	B	396	THR	3.2
1	B	426	CYS	3.2
1	D	78	GLY	3.2
1	D	444	GLY	3.2
1	D	247	LYS	3.2
1	A	83	PHE	3.2
1	D	466	ASP	3.2
1	B	479	VAL	3.2
1	D	89	ALA	3.2
1	B	368	TYR	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	282	LEU	3.1
1	A	451	TRP	3.1
1	D	451	TRP	3.1
1	A	441	ARG	3.1
1	B	423	GLY	3.1
1	A	407	LYS	3.1
1	C	466	ASP	3.1
1	A	296	PRO	3.1
1	B	264	GLU	3.1
1	B	150[A]	VAL	3.0
1	D	473	LEU	3.0
1	A	409	ASN	3.0
1	A	410	ALA	3.0
1	D	142	ALA	3.0
1	C	280	ALA	3.0
1	D	91	GLU	3.0
1	A	480	THR	3.0
1	B	299	THR	3.0
1	A	280	ALA	3.0
1	D	419	LEU	3.0
1	B	444	GLY	2.9
1	D	425	GLN	2.9
1	D	452	GLU	2.9
1	C	288	LEU	2.9
1	D	299	THR	2.9
1	D	420	PRO	2.9
1	B	317	GLN	2.9
1	A	408	GLY	2.9
1	B	378	GLY	2.9
1	D	111	ALA	2.8
1	C	154	ASN	2.8
1	B	374	TRP	2.8
1	D	156	GLN	2.8
1	D	439	VAL	2.8
1	A	264[A]	GLU	2.8
1	D	372	ALA	2.8
1	B	284	ILE	2.8
1	D	406	ALA	2.7
1	B	440	ASP	2.7
1	D	297	ASN	2.7
1	D	376	ILE	2.7
1	D	368	TYR	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	369	GLY	2.7
1	C	396	THR	2.7
1	D	370	ASP	2.7
1	D	81	ALA	2.7
1	C	441	ARG	2.7
1	B	408	GLY	2.7
1	A	299	THR	2.7
1	C	261	ASN	2.7
1	B	422	THR	2.7
1	C	3	PHE	2.7
1	C	407	LYS	2.6
1	B	480	THR	2.6
1	D	379	LYS	2.6
1	C	57[A]	ASN	2.6
1	A	274	PHE	2.6
1	C	299	THR	2.6
1	C	409	ASN	2.6
1	D	86	GLN	2.6
1	D	157[A]	HIS	2.6
1	A	234	GLU	2.6
1	B	409	ASN	2.6
1	C	359[A]	MET	2.6
1	D	281	ASN	2.5
1	A	211	ASP	2.5
1	C	298[A]	MET	2.5
1	D	360	LEU	2.5
1	D	408	GLY	2.5
1	C	262	VAL	2.5
1	D	182	VAL	2.5
1	C	398	VAL	2.5
1	D	417	CYS	2.4
1	B	468	ALA	2.4
1	D	371	LEU	2.4
1	D	79	GLU	2.4
1	C	406	ALA	2.4
1	D	424	LYS	2.4
1	C	296	PRO	2.4
1	A	284	ILE	2.4
1	B	371	LEU	2.4
1	A	396	THR	2.4
1	C	58	PHE	2.4
1	B	3	PHE	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	439	VAL	2.4
1	C	231	VAL	2.4
1	C	157	HIS	2.4
1	B	294	ILE	2.4
1	A	295	SER	2.4
1	A	154	ASN	2.4
1	D	234[A]	GLU	2.4
1	B	442	LYS	2.3
1	D	295	SER	2.3
1	D	453	GLY	2.3
1	A	465	CYS	2.3
1	D	465	CYS	2.3
1	B	417	CYS	2.3
1	B	443	LYS	2.3
1	A	374	TRP	2.3
1	C	374	TRP	2.3
1	D	143	ILE	2.3
1	B	406	ALA	2.3
1	D	418	THR	2.3
1	D	277	GLY	2.3
1	B	277	GLY	2.3
1	B	407	LYS	2.3
1	D	225	ILE	2.3
1	D	286	ILE	2.3
1	B	452	GLU	2.3
1	A	458	ASP	2.2
1	D	400	VAL	2.2
1	A	288	LEU	2.2
1	B	454	LEU	2.2
1	C	164	ILE	2.2
1	C	284	ILE	2.2
1	B	395	LYS	2.2
1	D	227	VAL	2.2
1	D	365	VAL	2.2
1	C	332[A]	VAL	2.2
1	A	220	ILE	2.2
1	A	294	ILE	2.2
1	D	278	MET	2.2
1	C	225	ILE	2.2
1	A	89	ALA	2.2
1	A	174	TRP	2.2
1	D	362	ALA	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	410	ALA	2.2
1	B	372	ALA	2.2
1	A	139	GLY	2.2
1	B	154	ASN	2.2
1	D	293	PHE	2.2
1	D	469	VAL	2.2
1	B	445	LEU	2.1
1	D	90	GLY	2.1
1	B	418	THR	2.1
1	D	470	SER	2.1
1	B	263	ARG	2.1
1	D	45	GLU	2.1
1	C	457	ASP	2.1
1	A	182	VAL	2.1
1	B	94	VAL	2.1
1	D	265	ARG	2.1
1	D	369	GLY	2.1
1	C	277	GLY	2.1
1	C	317	GLN	2.1
1	B	132	PRO	2.1
1	D	282	LEU	2.1
1	A	297	ASN	2.1
1	B	363[A]	MET	2.1
1	D	82	GLU	2.1
1	D	440	ASP	2.1
1	B	359[A]	MET	2.1
1	C	199	ALA	2.1
1	C	368	TYR	2.1
1	B	71[A]	ARG	2.1
1	A	277	GLY	2.1
1	C	276	ASP	2.1
1	C	153	PHE	2.0
1	D	479	VAL	2.0
1	C	182	VAL	2.0
1	A	88	LEU	2.0
1	D	430	ILE	2.0
1	B	474	ILE	2.0
1	D	283	GLY	2.0
1	C	174	TRP	2.0
1	B	111	ALA	2.0
1	C	479	VAL	2.0
1	C	421	LEU	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	393[A]	SER	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
3	GOL	C	5000	6/6	0.90	0.21	20,21,23,24	0
3	GOL	C	5001	6/6	0.93	0.12	25,28,29,30	0
2	CL	D	6001	1/1	0.98	0.21	15,15,15,15	1
2	CL	A	6000	1/1	0.99	0.16	19,19,19,19	1

6.5 Other polymers [i](#)

There are no such residues in this entry.