



# Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 09:02 am BST

PDB ID : 1OOY  
Title : SUCCINYL-COA:3-KETOACID COA TRANSFERASE FROM PIG HEART  
Authors : Coros, A.M.; Swenson, L.; Wolodko, W.T.; Fraser, M.E.  
Deposited on : 2003-03-04  
Resolution : 1.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

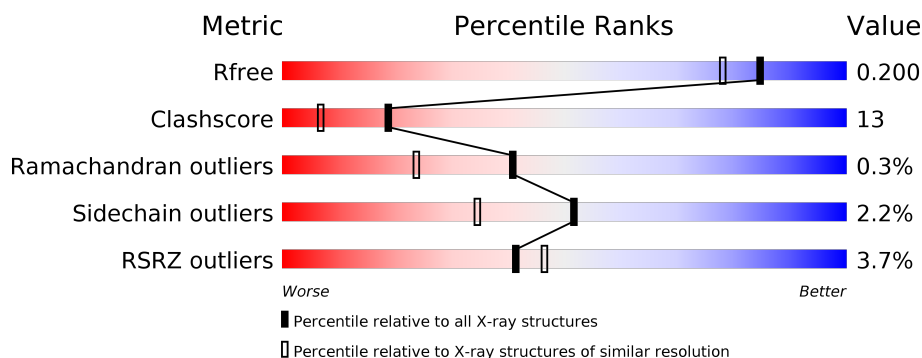
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 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))
$R_{free}$	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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	<div> <div>2%</div> <div> <div></div> <div>76%</div> <div>19%</div> <div>• •</div> </div> </div>
1	B	481	<div> <div>5%</div> <div> <div></div> <div>78%</div> <div>19%</div> <div>• •</div> </div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8252 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.

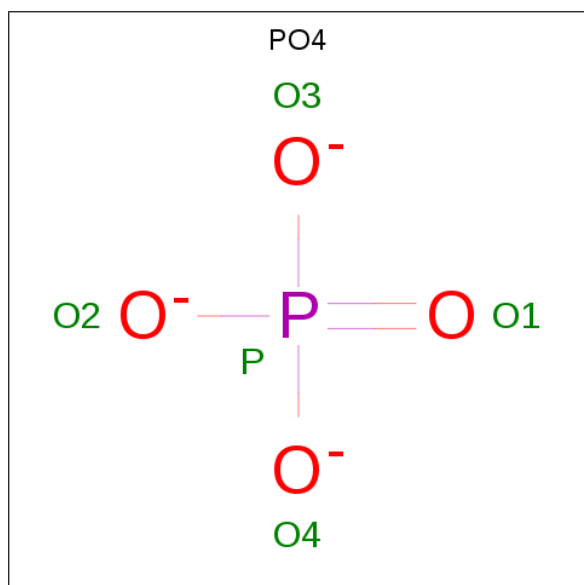
- Molecule 1 is a protein called Succinyl-CoA:3-ketoacid-coenzyme A transferase, mitochondrial precursor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	463	Total	C	N	O	S	0	28	0
			3624	2286	617	698	23			
1	B	468	Total	C	N	O	S	0	22	0
			3644	2301	623	699	21			

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	K	0	0
			2	2		
2	A	2	Total	K	0	0
			2	2		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	P	0	0
			5	4	1		

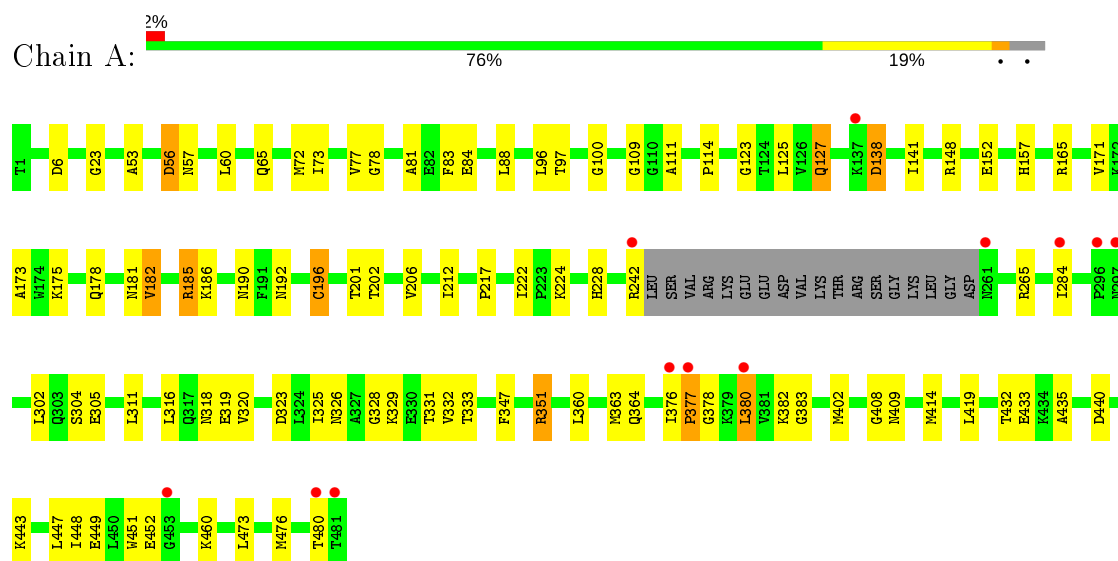
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	527	Total	O	0	0
			527	527		
4	B	448	Total	O	0	0
			448	448		

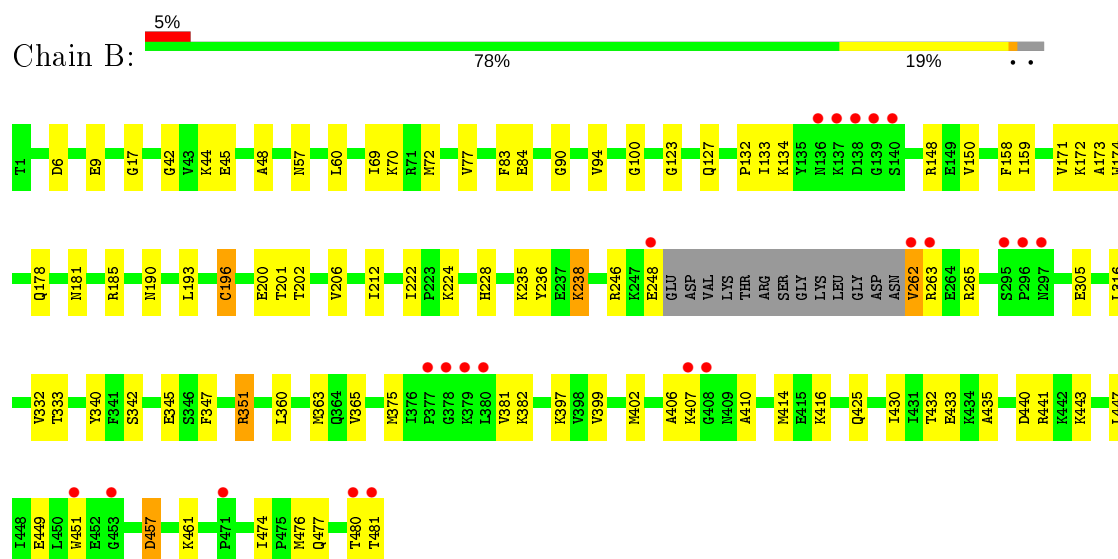
### 3 Residue-property plots [i](#)

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

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



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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.45Å 140.32Å 68.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.81 – 1.70 19.81 – 1.67	Depositor EDS
% Data completeness (in resolution range)	91.7 (19.81-1.70) 90.5 (19.81-1.67)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.67 (at 1.67Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.156 , 0.194 0.166 , 0.200	Depositor DCC
$R_{free}$ test set	9717 reflections (9.64%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	15.2	Xtriage
Anisotropy	0.170	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 51.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	8252	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.19% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: K, PO4

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	0.87	2/3823 (0.1%)	1.02	10/5154 (0.2%)
1	B	0.83	0/3813	0.98	4/5140 (0.1%)
All	All	0.85	2/7636 (0.0%)	1.00	14/10294 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	182[A]	VAL	CB-CG2	-5.77	1.40	1.52
1	A	182[B]	VAL	CB-CG2	-5.77	1.40	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	351	ARG	NE-CZ-NH2	-9.52	115.54	120.30
1	A	351	ARG	NE-CZ-NH1	8.23	124.42	120.30
1	B	148	ARG	NE-CZ-NH2	-7.92	116.34	120.30
1	A	185[A]	ARG	NE-CZ-NH1	6.13	123.36	120.30
1	A	185[B]	ARG	NE-CZ-NH1	6.13	123.36	120.30
1	A	378	GLY	N-CA-C	-6.06	97.94	113.10
1	A	148	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	A	185[A]	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	A	185[B]	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	B	351[A]	ARG	NE-CZ-NH2	-5.41	117.60	120.30
1	B	351[B]	ARG	NE-CZ-NH2	-5.41	117.60	120.30
1	B	246	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	A	73	ILE	N-CA-C	-5.27	96.77	111.00
1	A	351	ARG	CG-CD-NE	-5.10	101.09	111.80

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	3624	0	3660	93	0
1	B	3644	0	3690	103	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	B	5	0	0	0	0
4	A	527	0	0	22	1
4	B	448	0	0	19	0
All	All	8252	0	7350	193	1

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 13.

All (193) 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:69:ILE:HG21	1:B:72[A]:MET:CE	1.96	0.95
1:B:127[B]:GLN:OE1	1:B:150[B]:VAL:HG21	1.70	0.92
1:B:238:LYS:HG3	4:B:1283:HOH:O	1.73	0.89
1:A:84[B]:GLU:CG	1:A:380:LEU:HD21	2.03	0.89
1:A:84[B]:GLU:HG3	1:A:380:LEU:HD11	1.55	0.87
1:A:123:GLY:H	1:A:127:GLN:HE21	1.18	0.87
1:A:185[A]:ARG:CZ	1:A:186[A]:LYS:HZ3	1.90	0.85
1:A:185[A]:ARG:NH2	4:A:1320:HOH:O	2.09	0.84
1:B:69:ILE:HG21	1:B:72[A]:MET:HE2	1.60	0.83
1:B:236:TYR:HB3	1:B:238:LYS:HD3	1.61	0.82
1:B:440:ASP:HB3	1:B:443:LYS:HG3	1.64	0.79
1:A:284:ILE:HG23	4:A:1517:HOH:O	1.80	0.79
1:B:69:ILE:HG21	1:B:72[A]:MET:HE3	1.65	0.78
1:A:182[A]:VAL:CG2	1:A:222:ILE:HB	2.14	0.78
1:A:165:ARG:NH1	4:A:1092:HOH:O	2.15	0.77
1:B:48:ALA:HB3	1:B:72[A]:MET:HE2	1.68	0.75
1:B:238:LYS:HG3	4:B:1389:HOH:O	1.86	0.74
1:A:363[A]:MET:HE2	4:A:1178:HOH:O	1.91	0.71
1:B:60[A]:LEU:HD23	1:B:72[A]:MET:SD	2.31	0.71
1:A:440:ASP:HB3	1:A:443:LYS:HG3	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60[A]:LEU:CD2	1:B:72[A]:MET:SD	2.80	0.70
1:A:185[A]:ARG:CZ	1:A:186[A]:LYS:NZ	2.55	0.69
1:B:150[B]:VAL:HG22	1:B:159:ILE:HG22	1.73	0.68
1:A:53:ALA:HB2	1:A:72[B]:MET:HE1	1.74	0.68
1:B:236:TYR:HB3	1:B:238:LYS:CD	2.24	0.68
1:B:48:ALA:HB3	1:B:72[A]:MET:CE	2.24	0.68
1:B:345[B]:GLU:HG2	4:B:1326:HOH:O	1.92	0.67
1:B:69:ILE:HG13	1:B:72[A]:MET:HE3	1.76	0.67
1:A:111:ALA:O	1:B:351[B]:ARG:HD2	1.94	0.66
1:A:123:GLY:H	1:A:127:GLN:NE2	1.92	0.66
1:A:440:ASP:HB3	1:A:443:LYS:CG	2.25	0.66
1:B:201:THR:HA	1:B:228:HIS:HD2	1.60	0.66
1:A:185[A]:ARG:NH2	1:A:186[A]:LYS:NZ	2.43	0.66
1:A:178:GLN:HB2	1:A:212:ILE:HG13	1.78	0.65
1:A:84[B]:GLU:CD	1:A:380:LEU:HD21	2.16	0.65
1:B:57[B]:ASN:ND2	4:B:1218:HOH:O	2.09	0.65
1:B:238:LYS:CG	4:B:1389:HOH:O	2.46	0.64
1:B:172:LYS:HZ1	1:B:238:LYS:HE2	1.61	0.63
1:B:193:LEU:HD13	4:B:1394:HOH:O	1.99	0.62
1:B:69:ILE:CG2	1:B:72[A]:MET:HE2	2.30	0.62
1:A:363[A]:MET:CE	4:A:1178:HOH:O	2.47	0.62
1:A:56[A]:ASP:OD2	1:A:81:ALA:HB3	2.00	0.61
1:B:236:TYR:HB3	1:B:238:LYS:HE3	1.81	0.61
1:B:440:ASP:CB	1:B:443:LYS:HG3	2.30	0.61
1:B:440:ASP:OD2	1:B:443:LYS:HG2	2.00	0.61
1:A:201:THR:HA	1:A:228:HIS:HD2	1.65	0.61
1:A:182[A]:VAL:HG22	1:A:222:ILE:HB	1.82	0.60
1:A:265:ARG:HD3	1:A:451:TRP:CE3	2.37	0.60
1:A:57[B]:ASN:ND2	4:A:1211:HOH:O	2.34	0.60
1:A:84[B]:GLU:HG3	1:A:380:LEU:HD21	1.85	0.59
1:A:351:ARG:HD3	4:A:1022:HOH:O	2.02	0.59
1:B:414:MET:HG3	1:B:416:LYS:O	2.02	0.59
1:A:320:VAL:HG13	1:A:331:THR:HG21	1.85	0.59
1:A:138[A]:ASP:OD1	4:A:1516:HOH:O	2.16	0.59
1:B:123:GLY:H	1:B:127[B]:GLN:NE2	2.00	0.58
1:B:44:LYS:NZ	4:B:1299:HOH:O	2.30	0.58
1:B:236:TYR:CB	1:B:238:LYS:HE3	2.34	0.57
1:A:88:LEU:HD11	1:A:380:LEU:HD22	1.86	0.57
1:A:152[B]:GLU:OE1	1:A:157:HIS:HD2	1.87	0.57
1:B:238:LYS:HA	4:B:1283:HOH:O	2.03	0.57
1:A:84[B]:GLU:HG3	1:A:380:LEU:CD1	2.32	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60[A]:LEU:HD21	1:B:72[A]:MET:SD	2.46	0.56
1:B:236:TYR:HB3	1:B:238:LYS:CE	2.36	0.55
1:A:443:LYS:HE2	4:A:1294:HOH:O	2.06	0.55
1:A:284:ILE:HB	4:A:1518:HOH:O	2.06	0.55
1:A:78:GLY:HA3	1:A:382:LYS:HE3	1.88	0.55
1:B:375:MET:HE2	4:B:1437:HOH:O	2.06	0.55
1:A:332[B]:VAL:HG22	1:A:333:THR:H	1.73	0.54
1:B:474:ILE:HD12	1:B:477[A]:GLN:HE21	1.73	0.54
1:B:435:ALA:HB1	1:B:447:LEU:CD1	2.38	0.54
1:B:127[B]:GLN:OE1	1:B:150[B]:VAL:CG2	2.53	0.54
4:A:1117:HOH:O	1:B:228:HIS:HE1	1.91	0.54
1:A:316:LEU:N	1:A:319[B]:GLU:HG3	2.23	0.53
1:B:425[B]:GLN:NE2	1:B:441:ARG:NH2	2.57	0.53
1:A:185[A]:ARG:NH2	1:A:186[A]:LYS:HZ1	2.05	0.53
1:B:172:LYS:NZ	1:B:238:LYS:HE2	2.23	0.53
1:B:381:VAL:HG23	1:B:381:VAL:O	2.09	0.53
1:A:242:ARG:NH1	1:A:328:GLY:O	2.36	0.52
1:B:171:VAL:HG11	1:B:196[B]:CYS:SG	2.50	0.52
1:A:228:HIS:HE1	4:B:1066:HOH:O	1.92	0.52
1:A:6:ASP:OD2	4:A:1312:HOH:O	2.19	0.52
1:A:377:PRO:HD3	1:A:419:LEU:HD22	1.92	0.51
1:A:182[A]:VAL:HG23	1:A:222:ILE:HB	1.91	0.51
1:A:460:LYS:HE2	4:A:1424:HOH:O	2.09	0.51
1:B:238:LYS:CG	4:B:1283:HOH:O	2.43	0.51
1:A:480:THR:HB	4:A:1169:HOH:O	2.09	0.51
1:B:69:ILE:CG2	1:B:72[A]:MET:CE	2.79	0.51
1:A:97:THR:HG23	4:A:1010:HOH:O	2.11	0.51
1:B:425[B]:GLN:HE21	1:B:441:ARG:CZ	2.24	0.51
1:B:69:ILE:HG13	1:B:72[A]:MET:CE	2.40	0.50
1:B:222:ILE:HG22	1:B:222:ILE:O	2.10	0.50
1:A:171:VAL:HG11	1:A:196[B]:CYS:SG	2.52	0.50
1:A:449:GLU:HB3	1:A:476:MET:HA	1.93	0.50
1:A:326:ASN:HB3	1:A:332[A]:VAL:HG11	1.94	0.50
1:B:181:ASN:ND2	1:B:224:LYS:H	2.10	0.50
1:A:175:LYS:HD2	4:A:1368:HOH:O	2.11	0.50
1:B:481:THR:O	1:B:481:THR:HG22	2.12	0.49
1:A:173:ALA:HB1	1:A:182[B]:VAL:HG13	1.93	0.49
1:B:178:GLN:HB2	1:B:212:ILE:HG13	1.93	0.49
1:B:363:MET:HE1	4:B:1148:HOH:O	2.11	0.49
1:A:265:ARG:HD2	1:A:433:GLU:O	2.12	0.49
1:B:425[A]:GLN:HE21	1:B:441:ARG:HB2	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:ALA:HB3	1:A:206:VAL:HG12	1.93	0.48
1:B:480:THR:O	1:B:481:THR:OXT	2.30	0.48
1:A:304:SER:HB2	1:A:311:LEU:HD11	1.95	0.48
1:A:186[B]:LYS:NZ	4:A:1259:HOH:O	2.37	0.48
1:A:319[B]:GLU:OE1	4:A:1515:HOH:O	2.20	0.48
1:B:474:ILE:HD12	1:B:477[A]:GLN:NE2	2.28	0.48
1:B:397[B]:LYS:HE2	1:B:399:VAL:CG2	2.43	0.48
1:B:70:LYS:HE2	4:B:1358:HOH:O	2.14	0.48
1:A:141:ILE:HD11	4:A:1437:HOH:O	2.14	0.48
1:A:57[A]:ASN:OD1	1:A:65[A]:GLN:HG3	2.14	0.48
1:B:201:THR:HA	1:B:228:HIS:CD2	2.46	0.48
1:B:248:GLU:C	1:B:316:LEU:HD22	2.34	0.47
1:A:109:GLY:O	1:A:165:ARG:HD2	2.15	0.47
1:B:42:GLY:O	1:B:44:LYS:HE2	2.14	0.47
1:A:284:ILE:O	1:A:284:ILE:HG13	2.14	0.47
1:A:402:MET:O	1:A:432:THR:HA	2.15	0.47
1:B:351[A]:ARG:HD3	4:B:1053:HOH:O	2.14	0.47
1:B:425[B]:GLN:HE21	1:B:441:ARG:NH2	2.13	0.47
1:B:173:ALA:HB3	1:B:206:VAL:HG12	1.95	0.46
1:A:440:ASP:HB3	1:A:443:LYS:HG2	1.96	0.46
1:B:100:GLY:HA2	1:B:347:PHE:CG	2.50	0.46
1:A:302:LEU:HB2	1:A:311:LEU:HB2	1.97	0.46
1:B:236:TYR:CG	1:B:238:LYS:HE3	2.50	0.46
1:A:181:ASN:ND2	1:A:224:LYS:H	2.13	0.46
1:A:440:ASP:CB	1:A:443:LYS:HG2	2.45	0.46
1:B:193:LEU:HD23	1:B:193:LEU:C	2.36	0.46
1:A:448:ILE:C	1:A:473:LEU:HD12	2.37	0.45
1:B:235:LYS:CE	4:B:1433:HOH:O	2.64	0.45
1:A:408:GLY:O	1:A:409[B]:ASN:HB2	2.16	0.45
1:A:443:LYS:CE	4:A:1294:HOH:O	2.63	0.45
1:B:449:GLU:HB3	1:B:476:MET:HA	1.99	0.45
1:B:174:TRP:HZ3	4:B:1429:HOH:O	1.98	0.45
1:B:174:TRP:CE2	1:B:185:ARG:HD2	2.52	0.45
1:B:17:GLY:HA2	1:B:45:GLU:O	2.16	0.45
1:A:56[B]:ASP:O	1:A:57[B]:ASN:CG	2.55	0.45
1:B:132:PRO:HG2	4:B:1437:HOH:O	2.17	0.45
1:B:305:GLU:HB2	1:B:347:PHE:CZ	2.52	0.45
1:B:90:GLY:O	1:B:134[B]:LYS:HE3	2.17	0.45
1:B:365:VAL:HG11	1:B:430:ILE:HD11	1.99	0.45
1:B:457:ASP:O	1:B:461:LYS:HG3	2.16	0.45
1:A:77:VAL:HG21	1:A:83:PHE:CZ	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60[A]:LEU:HD21	1:B:72[A]:MET:HE1	1.98	0.44
1:B:406:ALA:HB3	1:B:410:ALA:HB3	1.98	0.44
1:B:193:LEU:HD13	1:B:342[B]:SER:OG	2.17	0.44
1:B:265:ARG:HD2	1:B:433:GLU:O	2.17	0.44
1:A:325:ILE:HD12	1:A:329:LYS:HA	2.00	0.44
1:B:94:VAL:O	1:B:133:ILE:HA	2.18	0.44
1:A:83:PHE:C	1:A:83:PHE:CD1	2.91	0.44
1:A:100:GLY:HA2	1:A:347:PHE:CG	2.53	0.43
1:A:377:PRO:CD	1:A:419:LEU:HD22	2.48	0.43
1:B:265:ARG:HD3	1:B:451:TRP:CE3	2.53	0.43
1:A:88:LEU:HD11	1:A:380:LEU:CD2	2.47	0.43
1:B:363:MET:CE	4:B:1148:HOH:O	2.66	0.43
1:B:69:ILE:CG2	1:B:72[A]:MET:HE3	2.44	0.43
1:B:83:PHE:C	1:B:83:PHE:CD1	2.92	0.43
1:A:171:VAL:HG13	1:A:192:ASN:HB3	2.02	0.42
1:A:96:LEU:HD13	1:A:383:GLY:HA2	2.01	0.42
1:B:262:VAL:HG13	1:B:263:ARG:H	1.82	0.42
1:B:42:GLY:O	1:B:44:LYS:CE	2.67	0.42
1:A:217:PRO:HB2	1:B:340:TYR:CE2	2.54	0.42
1:A:185[A]:ARG:HD3	1:A:323:ASP:OD2	2.19	0.42
1:A:114:PRO:HG3	1:B:158:PHE:CG	2.55	0.42
1:A:305:GLU:HB2	1:A:347:PHE:CZ	2.54	0.42
1:A:409[B]:ASN:ND2	4:A:1396:HOH:O	2.53	0.42
1:B:77:VAL:HG21	1:B:83:PHE:CZ	2.55	0.42
1:B:84:GLU:HG3	1:B:382:LYS:NZ	2.34	0.41
1:B:402:MET:O	1:B:432:THR:HA	2.19	0.41
1:A:125:LEU:HD23	1:A:125:LEU:HA	1.91	0.41
1:A:435:ALA:HB1	1:A:447:LEU:CD1	2.51	0.41
1:A:23:GLY:HA3	1:A:192:ASN:OD1	2.21	0.41
1:B:363:MET:HB2	1:B:363:MET:HE2	1.47	0.41
1:B:83:PHE:CZ	1:B:94:VAL:HG21	2.56	0.41
1:A:65[B]:GLN:HG3	4:A:1403:HOH:O	2.21	0.41
1:B:375:MET:HE3	4:B:1098:HOH:O	2.21	0.41
1:A:364:GLN:NE2	1:A:414:MET:HE1	2.36	0.40
1:B:332:VAL:HG22	1:B:333:THR:H	1.86	0.40
1:B:6:ASP:OD2	1:B:9:GLU:HG2	2.20	0.40
1:B:60[A]:LEU:CD2	1:B:72[A]:MET:HE1	2.51	0.40
1:A:222:ILE:HD12	1:A:222:ILE:HG23	1.83	0.40
1:B:316:LEU:HA	1:B:316:LEU:HD23	1.85	0.40
1:A:182[A]:VAL:HG22	1:A:222:ILE:CB	2.50	0.40
1:B:425[B]:GLN:NE2	1:B:441:ARG:HH21	2.17	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1502:HOH:O	4:A:1502:HOH:O[2_555]	1.04	1.16

## 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	487/481 (101%)	472 (97%)	14 (3%)	1 (0%)	47 30
1	B	486/481 (101%)	471 (97%)	13 (3%)	2 (0%)	34 18
All	All	973/962 (101%)	943 (97%)	27 (3%)	3 (0%)	41 24

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	407	LYS
1	A	190	ASN
1	B	190	ASN

### 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	405/393 (103%)	390 (96%)	15 (4%)	34 15
1	B	404/393 (103%)	396 (98%)	8 (2%)	55 38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	809/786 (103%)	786 (97%)	23 (3%)	52 25

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56[A]	ASP
1	A	56[B]	ASP
1	A	60[A]	LEU
1	A	60[B]	LEU
1	A	127	GLN
1	A	138[A]	ASP
1	A	138[B]	ASP
1	A	196[A]	CYS
1	A	196[B]	CYS
1	A	318	ASN
1	A	360	LEU
1	A	376	ILE
1	A	377	PRO
1	A	380	LEU
1	A	452	GLU
1	B	196[A]	CYS
1	B	196[B]	CYS
1	B	200[A]	GLU
1	B	200[B]	GLU
1	B	238	LYS
1	B	262	VAL
1	B	360	LEU
1	B	457	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	86	GLN
1	A	127	GLN
1	A	157	HIS
1	A	181	ASN
1	A	228	HIS
1	A	297	ASN
1	A	318	ASN
1	B	86	GLN
1	B	154	ASN

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Mol	Chain	Res	Type
1	B	181	ASN
1	B	228	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 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 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	PO4	B	997	-	4,4,4	1.43	0	6,6,6	0.43	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 [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	463/481 (96%)	-0.30	12 (2%) 56 60	9, 15, 29, 49	0
1	B	468/481 (97%)	-0.12	22 (4%) 31 35	9, 17, 37, 58	0
All	All	931/962 (96%)	-0.21	34 (3%) 41 46	9, 16, 35, 58	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	481	THR	7.2
1	B	407	LYS	6.6
1	A	481	THR	6.5
1	A	376	ILE	5.9
1	B	137	LYS	5.5
1	B	139	GLY	5.0
1	B	138	ASP	4.6
1	B	379	LYS	4.6
1	A	377	PRO	4.6
1	A	297	ASN	4.3
1	A	261	ASN	4.1
1	B	380	LEU	3.9
1	A	296	PRO	3.6
1	B	480	THR	3.6
1	B	408	GLY	3.5
1	B	136	ASN	3.3
1	A	480	THR	3.3
1	B	377	PRO	3.3
1	B	248	GLU	3.3
1	B	296	PRO	3.1
1	B	378	GLY	3.1
1	B	297	ASN	3.1
1	B	262	VAL	2.8
1	B	453	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	242	ARG	2.7
1	A	284	ILE	2.7
1	B	451	TRP	2.6
1	B	140	SER	2.6
1	B	471	PRO	2.5
1	A	380	LEU	2.5
1	A	137	LYS	2.5
1	B	295	SER	2.4
1	B	263	ARG	2.2
1	A	453	GLY	2.1

## 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. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	PO4	B	997	5/5	0.94	0.17	56,56,56,57	0
2	K	B	995	1/1	0.95	0.07	27,27,27,27	0
2	K	A	994	1/1	0.97	0.06	23,23,23,23	0
2	K	B	996	1/1	0.99	0.07	30,30,30,30	0
2	K	A	993	1/1	1.00	0.03	16,16,16,16	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.