



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:25 AM UTC

PDB ID : 1OPE / pdb_00001ope
Title : Deletion mutant of SUCCINYL-COA:3-KETOACID COA TRANSFERASE
FROM PIG HEART
Authors : Coros, A.M.; Swenson, L.; Wolodko, W.T.; Fraser, M.E.
Deposited on : 2003-03-05
Resolution : 2.50 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
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

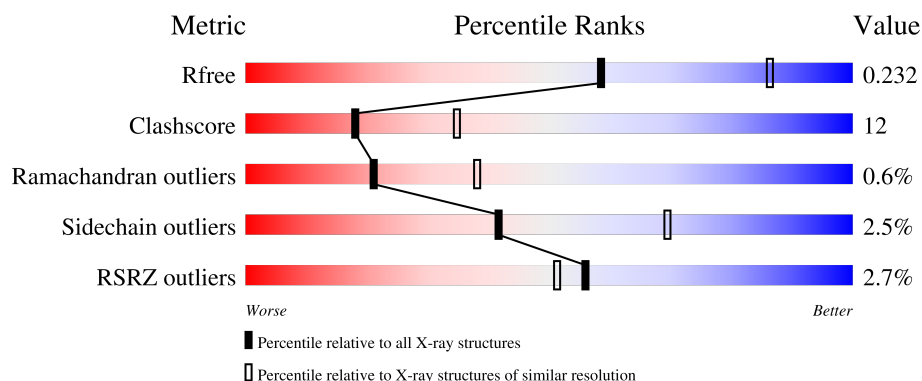
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

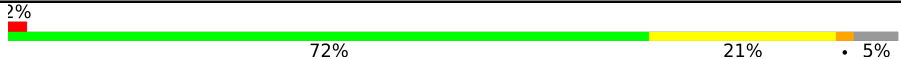
The reported resolution of this entry is 2.50 Å.

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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	475	 2% 72% 21% • 5%
1	B	475	 3% 72% 22% • •

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7202 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	453	Total	C	N	O	S	0	0	0
			3463	2201	590	654	18			
1	B	463	Total	C	N	O	S	0	0	0
			3531	2242	603	668	18			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLU	deletion	UNP Q29551
A	?	-	ASP	deletion	UNP Q29551
A	?	-	VAL	deletion	UNP Q29551
A	?	-	LYS	deletion	UNP Q29551
A	?	-	THR	deletion	UNP Q29551
A	?	-	ARG	deletion	UNP Q29551
B	?	-	GLU	deletion	UNP Q29551
B	?	-	ASP	deletion	UNP Q29551
B	?	-	VAL	deletion	UNP Q29551
B	?	-	LYS	deletion	UNP Q29551
B	?	-	THR	deletion	UNP Q29551
B	?	-	ARG	deletion	UNP Q29551

- Molecule 2 is MERCURY (II) ION (CCD ID: HG) (formula: Hg).

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

- Molecule 3 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	K 1	0	0
3	B	1	Total 1	K 1	0	0

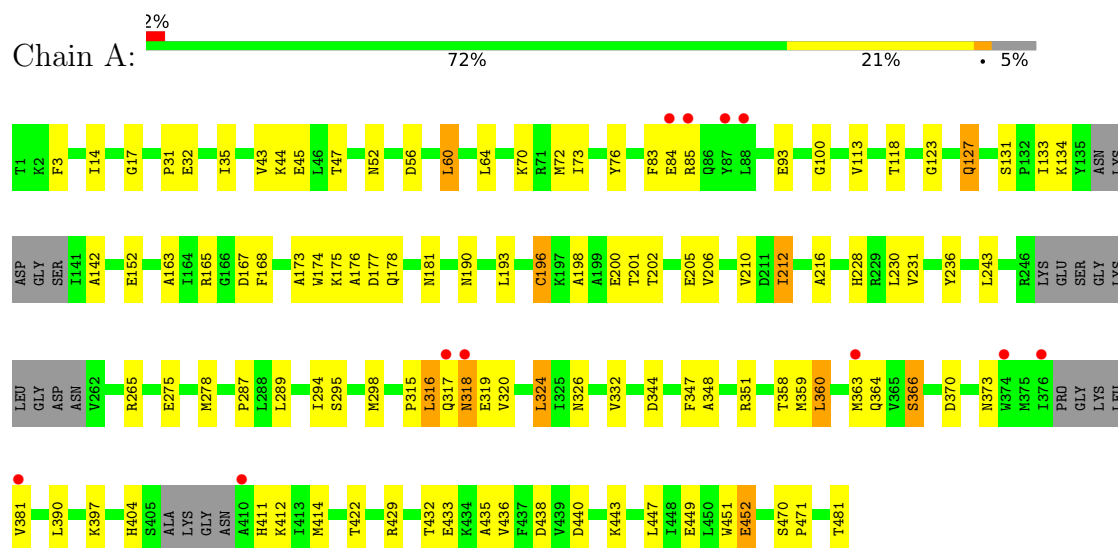
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	91	Total 91	O 91	0	0
4	B	111	Total 111	O 111	0	0

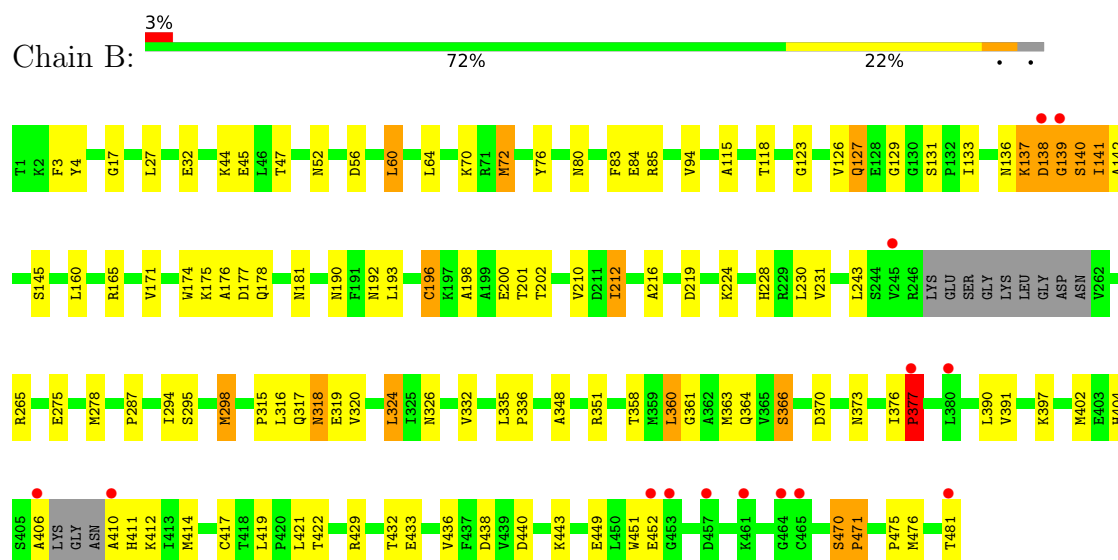
3 Residue-property plots [i](#)

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

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



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



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	147.64Å 68.70Å 103.50Å 90.00° 99.58° 90.00°	Depositor
Resolution (Å)	38.13 – 2.50 38.13 – 2.50	Depositor EDS
% Data completeness (in resolution range)	85.6 (38.13-2.50) 85.6 (38.13-2.50)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.93 (at 2.48Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.180 , 0.235 0.178 , 0.232	Depositor DCC
R_{free} test set	3093 reflections (10.01%)	wwPDB-VP
Wilson B-factor (Å ²)	21.2	Xtriage
Anisotropy	0.399	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 37.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7202	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.55% 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

5.1 Standard geometry

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

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	1.03	2/3517 (0.1%)	1.28	30/4744 (0.6%)
1	B	1.07	2/3588 (0.1%)	1.27	37/4842 (0.8%)
All	All	1.05	4/7105 (0.1%)	1.27	67/9586 (0.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	298	MET	SD-CE	5.96	1.94	1.79
1	B	72	MET	SD-CE	5.68	1.93	1.79
1	A	359	MET	SD-CE	-5.51	1.65	1.79
1	A	73	ILE	CA-CB	5.37	1.60	1.53

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	404	HIS	N-CA-C	10.12	121.90	111.07
1	B	44	LYS	N-CA-C	9.46	120.74	108.34
1	B	404	HIS	N-CA-C	9.13	120.84	111.07
1	A	216	ALA	N-CA-C	-8.38	99.18	109.83
1	A	44	LYS	N-CA-C	8.31	120.58	108.86
1	B	216	ALA	N-CA-C	-8.29	97.31	109.50
1	A	165	ARG	CA-C-N	-7.78	115.55	122.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	165	ARG	C-N-CA	-7.78	115.55	122.47
1	B	316	LEU	N-CA-C	-7.58	99.81	110.50
1	A	348	ALA	N-CA-C	-7.38	103.31	111.36
1	B	452	GLU	CA-C-N	-7.00	115.11	123.44
1	B	452	GLU	C-N-CA	-7.00	115.11	123.44
1	A	452	GLU	CA-C-N	-6.94	115.18	123.44
1	A	452	GLU	C-N-CA	-6.94	115.18	123.44
1	B	47	THR	N-CA-C	-6.67	96.79	108.20
1	A	56	ASP	CA-C-N	-6.67	111.34	123.34
1	A	56	ASP	C-N-CA	-6.67	111.34	123.34
1	B	56	ASP	CA-C-N	-6.63	111.40	123.34
1	B	56	ASP	C-N-CA	-6.63	111.40	123.34
1	A	422	THR	N-CA-C	-6.59	105.37	113.41
1	B	471	PRO	N-CA-C	-6.54	105.99	114.03
1	B	165	ARG	CA-C-N	-6.53	115.63	122.69
1	B	165	ARG	C-N-CA	-6.53	115.63	122.69
1	A	471	PRO	N-CA-C	-6.53	106.00	114.03
1	A	212	ILE	N-CA-C	-6.48	101.22	109.58
1	B	64	LEU	N-CA-C	-6.46	103.47	112.45
1	B	193	LEU	CA-C-N	-6.42	112.39	119.19
1	B	193	LEU	C-N-CA	-6.42	112.39	119.19
1	B	422	THR	N-CA-C	-6.27	105.28	113.12
1	A	316	LEU	N-CA-C	-6.25	101.69	110.50
1	B	411	HIS	N-CA-C	6.20	119.26	109.96
1	B	212	ILE	N-CA-C	-6.20	101.55	109.30
1	A	47	THR	N-CA-C	-6.13	97.72	108.20
1	A	131	SER	CA-C-N	-6.11	113.39	119.99
1	A	131	SER	C-N-CA	-6.11	113.39	119.99
1	B	139	GLY	N-CA-C	-6.06	98.82	113.18
1	A	411	HIS	N-CA-C	6.04	118.46	109.59
1	A	438	ASP	N-CA-C	-6.02	99.85	109.96
1	A	64	LEU	N-CA-C	-6.00	104.31	111.69
1	B	94	VAL	N-CA-C	6.00	116.73	107.78
1	A	142	ALA	N-CA-C	-5.94	106.68	114.04
1	B	470	SER	CA-C-N	5.69	125.79	119.87
1	B	470	SER	C-N-CA	5.69	125.79	119.87
1	B	438	ASP	N-CA-C	-5.65	100.47	109.96
1	B	141	ILE	N-CA-C	5.64	116.70	108.58
1	A	193	LEU	CA-C-N	-5.63	113.22	119.19
1	A	193	LEU	C-N-CA	-5.63	113.22	119.19
1	B	140	SER	CB-CA-C	-5.61	108.49	116.34
1	B	348	ALA	N-CA-C	-5.59	105.27	111.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	129	GLY	N-CA-C	-5.55	103.74	112.61
1	A	167	ASP	N-CA-C	-5.51	104.91	111.69
1	A	70	LYS	N-CA-C	-5.49	106.26	113.12
1	A	470	SER	CA-C-N	5.49	125.58	119.87
1	A	470	SER	C-N-CA	5.49	125.58	119.87
1	B	219	ASP	N-CA-C	5.33	119.30	112.26
1	B	27	LEU	N-CA-C	-5.22	106.14	112.88
1	B	361	GLY	N-CA-C	-5.22	104.44	112.85
1	A	198	ALA	N-CA-C	5.21	118.94	112.59
1	B	475	PRO	N-CA-C	-5.16	103.17	111.38
1	A	32	GLU	N-CA-C	5.14	117.62	111.71
1	B	131	SER	N-CA-C	-5.10	103.36	109.83
1	B	198	ALA	N-CA-C	5.09	118.81	112.59
1	B	70	LYS	N-CA-C	-5.08	106.76	113.12
1	B	126	VAL	N-CA-C	-5.08	105.75	110.53
1	B	391	VAL	CB-CA-C	-5.07	105.71	112.46
1	B	32	GLU	N-CA-C	5.03	117.50	111.71
1	A	432	THR	N-CA-C	-5.03	102.45	109.69

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	236	TYR	Sidechain

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	3463	0	3529	79	1
1	B	3531	0	3601	93	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	91	0	0	3	0
4	B	111	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7202	0	7130	172	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 12.

All (172) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:LYS:HZ1	1:A:429:ARG:NH2	1.58	1.01
1:B:397:LYS:NZ	1:B:429:ARG:HH12	1.62	0.97
1:B:397:LYS:HZ1	1:B:429:ARG:NH2	1.62	0.94
1:B:397:LYS:NZ	1:B:429:ARG:HH22	1.65	0.94
1:A:397:LYS:NZ	1:A:429:ARG:HH22	1.67	0.92
1:A:397:LYS:NZ	1:A:429:ARG:HH12	1.68	0.92
1:B:397:LYS:HZ3	1:B:429:ARG:NH1	1.67	0.91
1:A:397:LYS:HZ3	1:A:429:ARG:HH12	0.91	0.88
1:B:123:GLY:H	1:B:127:GLN:HE21	1.22	0.87
1:B:376:ILE:HG23	1:B:377:PRO:HD2	1.53	0.87
1:A:397:LYS:HZ3	1:A:429:ARG:NH1	1.72	0.86
1:A:60:LEU:HD23	1:A:72:MET:CE	2.06	0.84
1:B:397:LYS:HZ1	1:B:429:ARG:HH22	0.85	0.84
1:A:363:MET:HE2	1:A:373:ASN:HA	1.58	0.84
1:B:397:LYS:HZ3	1:B:429:ARG:HH12	0.85	0.84
1:B:202:THR:H	1:B:228:HIS:CD2	1.97	0.83
1:A:123:GLY:H	1:A:127:GLN:HE21	1.27	0.82
1:A:294:ILE:HG23	1:A:298:MET:HE3	1.60	0.82
1:B:363:MET:HE2	1:B:373:ASN:HA	1.59	0.82
1:B:294:ILE:HG23	1:B:298:MET:HE3	1.63	0.81
1:B:140:SER:OG	1:B:141:ILE:N	2.11	0.81
1:B:60:LEU:HD23	1:B:72:MET:CE	2.11	0.81
1:A:201:THR:HA	1:A:228:HIS:HD2	1.47	0.80
1:A:202:THR:H	1:A:228:HIS:CD2	2.01	0.79
1:A:397:LYS:HZ1	1:A:429:ARG:HH22	0.82	0.79
1:B:140:SER:HG	1:B:141:ILE:H	1.33	0.77
1:A:265:ARG:HD2	1:A:451:TRP:CH2	2.19	0.76
1:B:265:ARG:HD2	1:B:451:TRP:CH2	2.21	0.76
1:B:397:LYS:NZ	1:B:429:ARG:NH1	2.30	0.74
1:B:376:ILE:CG2	1:B:377:PRO:HD2	2.18	0.73
1:B:202:THR:H	1:B:228:HIS:HD2	1.35	0.73
1:A:397:LYS:NZ	1:A:429:ARG:NH2	2.33	0.72
1:A:397:LYS:NZ	1:A:429:ARG:NH1	2.33	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:GLU:HG2	1:A:134:LYS:HB2	1.72	0.71
1:A:366:SER:HB3	1:A:370:ASP:HB2	1.74	0.69
1:B:201:THR:HA	1:B:228:HIS:HD2	1.57	0.69
1:B:366:SER:HB3	1:B:370:ASP:HB2	1.75	0.68
1:B:406:ALA:HB3	1:B:410:ALA:HB3	1.76	0.68
1:B:376:ILE:O	1:B:377:PRO:C	2.36	0.67
1:A:295:SER:HB3	1:A:298:MET:HE2	1.76	0.67
1:B:123:GLY:H	1:B:127:GLN:NE2	1.90	0.67
1:A:60:LEU:HD23	1:A:72:MET:HE1	1.78	0.65
1:A:440:ASP:OD2	1:A:443:LYS:N	2.26	0.64
1:B:136:ASN:O	1:B:138:ASP:N	2.31	0.64
1:B:295:SER:HB3	1:B:298:MET:HE2	1.81	0.63
1:A:196:CYS:O	1:A:202:THR:HG21	1.99	0.62
1:B:85:ARG:HG2	1:B:85:ARG:HH11	1.62	0.62
1:B:376:ILE:O	1:B:377:PRO:O	2.16	0.62
1:A:123:GLY:H	1:A:127:GLN:NE2	1.96	0.62
1:A:452:GLU:HG3	4:A:557:HOH:O	1.99	0.62
1:B:397:LYS:NZ	1:B:429:ARG:NH2	2.32	0.61
1:A:230:LEU:C	1:A:230:LEU:HD13	2.25	0.61
1:B:440:ASP:OD2	1:B:443:LYS:N	2.29	0.61
1:B:275:GLU:O	1:B:278:MET:HB3	2.00	0.61
1:A:318:ASN:HD22	1:A:318:ASN:C	2.09	0.61
1:A:201:THR:HA	1:A:228:HIS:CD2	2.31	0.60
1:A:363:MET:HE2	1:A:373:ASN:CA	2.30	0.60
1:B:3:PHE:CD2	1:B:230:LEU:HD12	2.36	0.60
1:B:136:ASN:C	1:B:138:ASP:N	2.59	0.59
1:B:176:ALA:HA	1:B:181:ASN:O	2.02	0.59
1:A:202:THR:H	1:A:228:HIS:HD2	1.48	0.59
1:B:287:PRO:HG2	1:B:360:LEU:HA	1.84	0.58
1:B:318:ASN:C	1:B:318:ASN:HD22	2.12	0.58
1:A:287:PRO:HG2	1:A:360:LEU:HA	1.87	0.57
1:B:326:ASN:HB3	1:B:332:VAL:HG11	1.86	0.57
1:B:201:THR:HA	1:B:228:HIS:CD2	2.37	0.57
1:B:85:ARG:HG2	1:B:85:ARG:NH1	2.19	0.56
1:B:363:MET:HE2	1:B:373:ASN:CA	2.31	0.56
1:A:176:ALA:HA	1:A:181:ASN:O	2.06	0.56
1:A:440:ASP:OD2	1:A:443:LYS:HG2	2.05	0.56
1:A:397:LYS:NZ	1:A:429:ARG:CZ	2.69	0.56
1:A:381:VAL:HA	4:A:541:HOH:O	2.05	0.56
1:B:397:LYS:NZ	1:B:429:ARG:CZ	2.68	0.55
1:A:265:ARG:HD2	1:A:451:TRP:CZ2	2.41	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:GLY:N	1:A:127:GLN:HE21	2.03	0.55
1:A:85:ARG:HG2	1:A:85:ARG:HH11	1.71	0.54
1:B:196:CYS:O	1:B:202:THR:HG21	2.07	0.54
1:A:318:ASN:HD22	1:A:319:GLU:N	2.05	0.54
1:B:178:GLN:HB2	1:B:212:ILE:HG13	1.89	0.53
1:B:265:ARG:HD2	1:B:451:TRP:CZ2	2.43	0.53
1:B:137:LYS:O	1:B:138:ASP:HB2	2.07	0.53
1:B:133:ILE:HD11	1:B:145:SER:HA	1.90	0.53
1:B:436:VAL:HB	1:B:449:GLU:HB2	1.91	0.53
1:A:83:PHE:C	1:A:83:PHE:CD1	2.87	0.52
1:B:243:LEU:HD21	1:B:317:GLN:OE1	2.11	0.51
1:A:230:LEU:HD13	1:A:231:VAL:N	2.25	0.51
1:B:60:LEU:HD23	1:B:72:MET:HE1	1.91	0.51
1:A:275:GLU:O	1:A:278:MET:HB3	2.11	0.51
1:B:83:PHE:C	1:B:83:PHE:CD1	2.88	0.51
1:B:265:ARG:HD2	1:B:451:TRP:CZ3	2.46	0.51
1:A:17:GLY:HA2	1:A:45:GLU:O	2.12	0.49
1:A:440:ASP:CG	1:A:443:LYS:HG2	2.37	0.49
1:B:230:LEU:C	1:B:230:LEU:HD13	2.37	0.49
1:B:295:SER:H	1:B:298:MET:CE	2.26	0.49
1:B:136:ASN:ND2	1:B:142:ALA:HB2	2.28	0.49
1:B:202:THR:N	1:B:228:HIS:HD2	2.07	0.49
1:A:174:TRP:CZ2	1:A:175:LYS:HE3	2.48	0.48
1:B:317:GLN:O	1:B:317:GLN:HG3	2.12	0.48
1:A:436:VAL:HB	1:A:449:GLU:HB2	1.96	0.48
1:B:440:ASP:OD2	1:B:443:LYS:HG2	2.14	0.48
1:A:178:GLN:HB2	1:A:212:ILE:HG13	1.95	0.47
1:A:326:ASN:HB3	1:A:332:VAL:HG11	1.95	0.47
1:A:265:ARG:HD2	1:A:451:TRP:CZ3	2.49	0.47
1:B:318:ASN:HD22	1:B:319:GLU:N	2.12	0.47
1:A:93:GLU:HA	1:A:133:ILE:O	2.14	0.47
1:B:230:LEU:HD13	1:B:231:VAL:N	2.29	0.47
1:A:85:ARG:HG2	1:A:85:ARG:NH1	2.29	0.47
1:B:402:MET:O	1:B:432:THR:HA	2.15	0.47
1:A:289:LEU:HA	1:A:289:LEU:HD23	1.75	0.46
1:B:174:TRP:CZ2	1:B:175:LYS:HE3	2.51	0.46
1:A:435:ALA:HB1	1:A:447:LEU:CD1	2.46	0.46
1:A:83:PHE:CD1	1:A:84:GLU:N	2.84	0.46
1:B:115:ALA:HB1	1:B:160:LEU:HD11	1.97	0.46
1:B:174:TRP:CE2	1:B:175:LYS:HE3	2.50	0.46
1:A:113:VAL:O	1:A:163:ALA:HB2	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:GLN:O	1:A:317:GLN:HG3	2.17	0.45
1:B:243:LEU:HD11	1:B:320:VAL:HG21	1.99	0.45
1:B:406:ALA:CB	1:B:410:ALA:HB3	2.45	0.45
1:A:177:ASP:HA	1:A:210:VAL:O	2.15	0.45
1:B:377:PRO:HD3	1:B:419:LEU:CD2	2.47	0.45
1:B:118:THR:OG1	1:B:351:ARG:HD2	2.17	0.45
1:B:433:GLU:OE1	1:B:433:GLU:N	2.46	0.45
1:A:243:LEU:HD21	1:A:317:GLN:OE1	2.16	0.44
1:B:138:ASP:OD1	1:B:138:ASP:C	2.60	0.44
1:B:123:GLY:N	1:B:127:GLN:HE21	2.01	0.44
1:B:171:VAL:HG13	1:B:192:ASN:HB3	2.00	0.44
1:A:3:PHE:CD2	1:A:230:LEU:HD12	2.53	0.44
1:B:406:ALA:N	1:B:410:ALA:O	2.50	0.44
1:A:14:ILE:HG22	1:A:43:VAL:HG21	2.00	0.44
1:B:181:ASN:ND2	1:B:224:LYS:H	2.16	0.44
1:A:31:PRO:O	1:A:35:ILE:HG13	2.18	0.44
1:A:174:TRP:CE2	1:A:175:LYS:HE3	2.53	0.43
1:A:433:GLU:OE1	1:A:433:GLU:N	2.44	0.43
1:B:139:GLY:O	1:B:140:SER:HB3	2.17	0.43
1:A:52:ASN:HA	1:A:76:TYR:O	2.18	0.43
1:B:83:PHE:CD1	1:B:84:GLU:N	2.87	0.43
1:B:417:CYS:HB2	1:B:421:LEU:HD21	2.01	0.43
1:A:316:LEU:O	1:A:317:GLN:C	2.62	0.43
1:B:136:ASN:C	1:B:138:ASP:H	2.26	0.43
1:B:60:LEU:HD12	1:B:60:LEU:HA	1.57	0.43
1:A:202:THR:N	1:A:228:HIS:HD2	2.16	0.43
1:B:52:ASN:HA	1:B:76:TYR:O	2.19	0.42
1:B:315:PRO:HD3	1:B:332:VAL:HA	2.00	0.42
1:A:358:THR:HG21	1:A:390:LEU:HB3	2.01	0.42
1:B:177:ASP:HA	1:B:210:VAL:O	2.20	0.42
1:B:470:SER:HA	1:B:471:PRO:HD3	1.80	0.42
1:A:118:THR:OG1	1:A:351:ARG:HD2	2.19	0.42
1:A:295:SER:H	1:A:298:MET:CE	2.33	0.42
1:B:80:ASN:O	1:B:83:PHE:HB3	2.19	0.42
1:B:358:THR:HG21	1:B:390:LEU:HB3	2.01	0.42
1:A:173:ALA:HB3	1:A:206:VAL:HG12	2.02	0.42
1:B:397:LYS:CE	1:B:429:ARG:NH2	2.83	0.42
1:A:205:GLU:O	1:A:205:GLU:HG3	2.20	0.41
1:A:324:LEU:HD23	1:A:324:LEU:HA	1.90	0.41
1:A:100:GLY:HA2	1:A:347:PHE:CG	2.56	0.41
1:B:364:GLN:HA	1:B:412:LYS:O	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:PHE:HA	1:A:201:THR:O	2.21	0.41
1:A:205:GLU:HA	1:A:231:VAL:O	2.20	0.41
4:A:513:HOH:O	1:B:228:HIS:HE1	2.03	0.41
1:A:152:GLU:OE1	1:A:152:GLU:N	2.54	0.41
1:A:364:GLN:HA	1:A:412:LYS:O	2.19	0.41
1:B:3:PHE:CE2	1:B:230:LEU:HD12	2.56	0.41
1:A:344:ASP:OD1	1:A:344:ASP:N	2.52	0.41
1:A:315:PRO:HB2	1:A:319:GLU:HB2	2.02	0.41
1:B:17:GLY:HA2	1:B:45:GLU:O	2.21	0.41
1:A:481:THR:HG22	1:A:481:THR:O	2.21	0.41
1:B:481:THR:O	1:B:481:THR:HG22	2.20	0.41
1:B:324:LEU:HD23	1:B:324:LEU:HA	1.90	0.40
1:B:476:MET:HE3	1:B:476:MET:HB2	1.89	0.40
1:B:4:TYR:O	1:B:231:VAL:HG23	2.21	0.40
1:A:243:LEU:HD11	1:A:320:VAL:HG21	2.03	0.40
1:B:335:LEU:O	1:B:336:PRO:C	2.63	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)
1:A:152:GLU:OE1	1:A:152:GLU:OE1[2_555]	1.40	0.80

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	443/475 (93%)	428 (97%)	14 (3%)	1 (0%)	43	63
1	B	457/475 (96%)	435 (95%)	18 (4%)	4 (1%)	14	27
All	All	900/950 (95%)	863 (96%)	32 (4%)	5 (1%)	21	38

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	137	LYS
1	B	138	ASP
1	B	377	PRO
1	A	190	ASN
1	B	190	ASN

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	371/387 (96%)	362 (98%)	9 (2%)	43	70
1	B	378/387 (98%)	368 (97%)	10 (3%)	40	68
All	All	749/774 (97%)	730 (98%)	19 (2%)	42	69

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	LEU
1	A	127	GLN
1	A	196	CYS
1	A	200	GLU
1	A	318	ASN
1	A	324	LEU
1	A	360	LEU
1	A	366	SER
1	A	414	MET
1	B	60	LEU
1	B	127	GLN
1	B	196	CYS
1	B	200	GLU
1	B	318	ASN
1	B	324	LEU
1	B	360	LEU
1	B	366	SER
1	B	377	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	414	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	127	GLN
1	A	181	ASN
1	A	228	HIS
1	A	297	ASN
1	A	301	HIS
1	A	318	ASN
1	A	373	ASN
1	A	425	GLN
1	A	477	GLN
1	B	65	GLN
1	B	127	GLN
1	B	136	ASN
1	B	181	ASN
1	B	228	HIS
1	B	297	ASN
1	B	301	HIS
1	B	318	ASN
1	B	373	ASN
1	B	425	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

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, 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	453/475 (95%)	-0.24	11 (2%) 59 55	7, 21, 50, 74	0
1	B	463/475 (97%)	-0.31	14 (3%) 52 48	6, 20, 50, 62	0
All	All	916/950 (96%)	-0.27	25 (2%) 56 51	6, 21, 50, 74	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	377	PRO	4.8
1	B	406	ALA	4.4
1	A	410	ALA	3.4
1	A	87	TYR	3.1
1	A	381	VAL	2.9
1	B	380	LEU	2.9
1	B	410	ALA	2.7
1	A	374	TRP	2.7
1	A	88	LEU	2.7
1	A	363	MET	2.6
1	A	318	ASN	2.6
1	B	138	ASP	2.5
1	B	245	VAL	2.4
1	B	461	LYS	2.4
1	B	464	GLY	2.3
1	B	453	GLY	2.3
1	B	465	CYS	2.3
1	A	376	ILE	2.3
1	B	457	ASP	2.2
1	A	84	GLU	2.2
1	A	85	ARG	2.1
1	A	317	GLN	2.1
1	B	481	THR	2.1
1	B	452	GLU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	139	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	HG	B	483	1/1	0.88	0.23	46,46,46,46	1
2	HG	B	482	1/1	0.93	0.20	59,59,59,59	1
2	HG	A	482	1/1	0.93	0.18	43,43,43,43	1
2	HG	A	483	1/1	0.95	0.15	49,49,49,49	1
3	K	A	484	1/1	0.96	0.06	45,45,45,45	0
3	K	B	484	1/1	0.97	0.06	42,42,42,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.