



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:01 AM UTC

PDB ID : 3GJB / pdb_00003gjb
Title : CytC3 with Fe(II) and alpha-ketoglutarate
Authors : Wong, C.; Drennan, C.L.
Deposited on : 2009-03-08
Resolution : 2.20 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<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

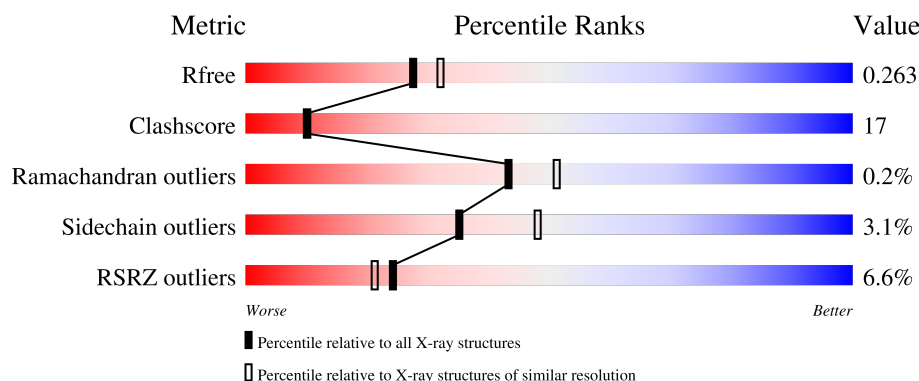
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	319	5% 56% 22% • 18%
1	B	319	6% 57% 25% • 15%

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	AKG	A	322	-	-	X	-
3	AKG	B	321	-	-	X	-
4	ACT	B	325	-	-	X	-
5	SO4	A	326	-	-	X	-
5	SO4	B	327	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 4530 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.

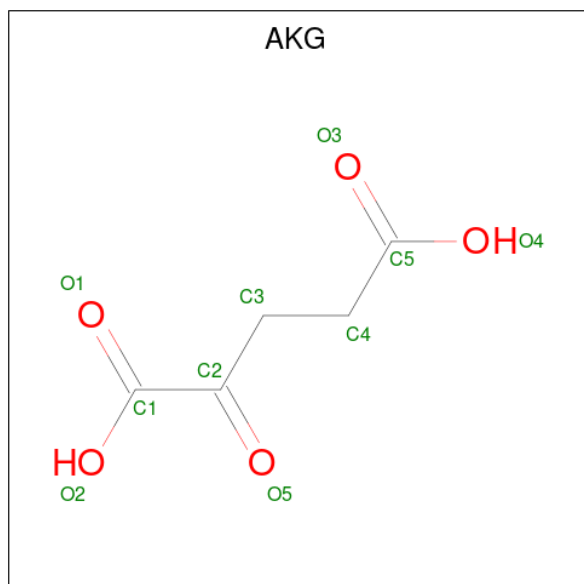
- Molecule 1 is a protein called CytC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	260	Total	C	N	O	S	0	0	0
			2068	1314	361	385	8			
1	B	271	Total	C	N	O	S	0	0	0
			2171	1373	379	410	9			

- Molecule 2 is FE (II) ION (CCD ID: FE2) (formula: Fe).

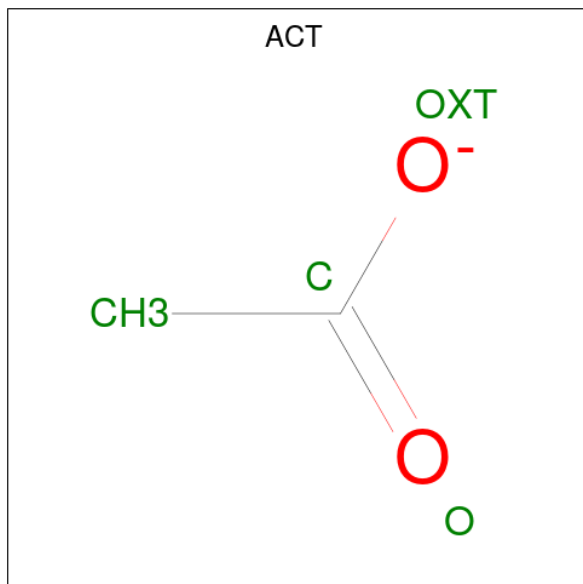
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Fe	0	0
			1	1		
2	B	1	Total	Fe	0	0
			1	1		

- Molecule 3 is 2-OXOGLUTARIC ACID (CCD ID: AKG) (formula: C₅H₆O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	5	5		
3	A	1	Total	C	O	0	0
			10	5	5		
3	B	1	Total	C	O	0	0
			10	5	5		

- Molecule 4 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	110	Total	O	0	0
			110	110		
6	B	107	Total	O	0	0
			107	107		

- Molecule 1: CytC3



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	88.99Å 88.99Å 248.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.49 – 2.20 44.49 – 2.20	Depositor EDS
% Data completeness (in resolution range)	95.1 (44.49-2.20) 95.1 (44.49-2.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.77 (at 2.20Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.227 , 0.259 0.231 , 0.263	Depositor DCC
R_{free} test set	5112 reflections (10.12%)	wwPDB-VP
Wilson B-factor (Å ²)	39.4	Xtriage
Anisotropy	0.606	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 44.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4530	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.15% 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: FE2, SO4, ACT, AKG

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	0.43	0/2124	1.02	15/2886 (0.5%)
1	B	0.41	0/2231	0.93	5/3031 (0.2%)
All	All	0.42	0/4355	0.97	20/5917 (0.3%)

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	154	THR	N-CA-C	-7.91	98.30	109.69
1	A	31	ILE	N-CA-C	-6.39	106.07	111.56
1	A	87	VAL	N-CA-C	6.28	116.95	110.36
1	A	301	ARG	N-CA-C	-6.26	100.58	109.96
1	A	69	ASP	N-CA-C	6.04	119.76	111.54
1	A	83	ARG	N-CA-C	6.04	116.99	109.57
1	B	301	ARG	N-CA-C	-5.74	101.79	110.28
1	B	154	THR	N-CA-C	-5.71	100.73	109.41
1	A	288	ALA	N-CA-C	-5.58	103.02	110.55
1	B	31	ILE	N-CA-C	-5.46	107.48	111.90
1	A	95	GLY	N-CA-C	5.42	117.10	111.95
1	A	20	PHE	N-CA-C	-5.42	105.45	111.36
1	A	98	LEU	N-CA-C	5.39	118.26	109.59
1	B	83	ARG	N-CA-C	5.23	117.14	109.71
1	B	87	VAL	N-CA-C	5.19	115.81	110.36
1	A	263	THR	N-CA-C	5.18	117.67	111.71
1	A	56	TYR	CA-C-N	5.12	125.13	120.21
1	A	56	TYR	C-N-CA	5.12	125.13	120.21
1	A	83	ARG	CA-C-N	5.05	124.66	119.05
1	A	83	ARG	C-N-CA	5.05	124.66	119.05

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	2068	0	1965	75	0
1	B	2171	0	2058	74	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	20	0	8	7	0
3	B	10	0	4	4	0
4	A	12	0	9	2	0
4	B	20	0	15	3	0
5	A	5	0	0	2	0
5	B	5	0	0	2	0
6	A	110	0	0	3	0
6	B	107	0	0	4	0
All	All	4530	0	4059	145	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 17.

All (145) 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:94:ILE:HD12	1:A:262:PRO:HD3	1.27	1.06
1:B:140:ARG:HG2	1:B:141:PRO:HD2	1.38	1.02
1:A:132:ILE:HG13	1:A:132:ILE:O	1.73	0.89
1:B:253:ARG:HD3	6:B:432:HOH:O	1.80	0.80
1:B:261:VAL:HG13	1:B:265:VAL:HB	1.68	0.76
1:A:131:GLN:HE22	3:A:322:AKG:H32	1.49	0.75
1:A:259:ARG:HH12	4:A:325:ACT:H2	1.52	0.75
1:B:35:GLU:H	1:B:35:GLU:CD	1.94	0.75
1:A:317:ILE:HG22	1:A:317:ILE:O	1.87	0.72
1:B:40:ARG:NH2	1:B:79:GLU:OE1	2.22	0.72
1:B:33:GLU:HB3	1:B:35:GLU:OE2	1.90	0.72
1:B:271:THR:O	1:B:274:LEU:HB3	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:THR:H	1:A:160:ASN:ND2	1.91	0.69
1:B:74:ILE:HD12	1:B:77:LEU:HD12	1.77	0.67
1:A:94:ILE:HD12	1:A:262:PRO:CD	2.17	0.67
1:A:107:PRO:HB3	1:A:254:MET:HE1	1.77	0.66
1:A:157:THR:H	1:A:160:ASN:HD21	1.40	0.66
1:A:55:ILE:HD13	1:A:72:LEU:HD12	1.77	0.66
1:B:220:GLN:HE21	1:B:220:GLN:HA	1.61	0.65
1:B:55:ILE:HD13	1:B:72:LEU:HD12	1.78	0.64
1:B:102:ARG:HD3	6:B:349:HOH:O	1.98	0.63
1:A:132:ILE:HD11	1:A:144:ILE:C	2.24	0.62
1:B:40:ARG:HH22	1:B:79:GLU:CD	2.09	0.61
1:B:220:GLN:HA	1:B:220:GLN:NE2	2.16	0.61
1:A:237:ASN:HD21	1:B:173:MET:HE2	1.66	0.61
1:A:122:THR:HA	3:A:322:AKG:H41	1.82	0.60
1:B:30:LYS:HE2	1:B:33:GLU:OE2	2.01	0.60
1:A:301:ARG:HH11	1:A:301:ARG:HG3	1.68	0.58
1:B:133:ILE:HD12	1:B:269:PRO:HG3	1.86	0.57
1:B:253:ARG:HH22	4:B:322:ACT:H1	1.69	0.57
1:A:132:ILE:HG12	1:A:144:ILE:O	2.04	0.57
1:A:102:ARG:HD3	6:A:327:HOH:O	2.04	0.56
1:A:35:GLU:CD	1:A:35:GLU:H	2.13	0.56
1:A:87:VAL:HG22	1:A:291:THR:HG21	1.86	0.56
1:A:37:MET:HG2	1:A:229:GLY:N	2.21	0.56
1:A:13:SER:OG	1:A:16:GLU:HG3	2.06	0.55
1:B:103:SER:HA	1:B:257:ALA:O	2.07	0.55
1:B:304:ARG:HD2	6:B:378:HOH:O	2.08	0.54
1:B:110:GLN:HA	1:B:245:HIS:ND1	2.22	0.53
1:A:174:ASN:HB2	1:B:144:ILE:HG12	1.89	0.53
1:B:69:ASP:OD1	1:B:102:ARG:HA	2.09	0.53
1:A:160:ASN:HD22	1:A:160:ASN:C	2.17	0.53
1:A:102:ARG:HG3	1:A:103:SER:N	2.24	0.53
1:A:121:ALA:HB2	1:B:239:MET:HE1	1.91	0.53
1:B:12:PHE:CE2	1:B:89:ARG:HB3	2.43	0.52
3:A:322:AKG:H31	5:B:327:SO4:O2	2.09	0.52
1:B:272:GLU:O	1:B:273:ASN:HB2	2.10	0.52
1:A:69:ASP:OD1	1:A:102:ARG:HA	2.10	0.52
1:B:102:ARG:HG3	1:B:103:SER:N	2.24	0.52
1:A:102:ARG:NH2	3:A:322:AKG:H32	2.24	0.52
1:A:103:SER:HA	1:A:257:ALA:O	2.10	0.52
1:A:123:PHE:O	3:A:322:AKG:O5	2.28	0.52
1:A:91:GLY:HA2	1:A:95:GLY:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:264:GLN:H	1:B:264:GLN:CD	2.15	0.51
1:A:102:ARG:HH22	1:A:131:GLN:HE22	1.57	0.51
1:B:84:PRO:HG2	1:B:85:GLU:OE1	2.11	0.51
1:A:133:ILE:HD12	1:A:269:PRO:HG3	1.92	0.50
1:B:165:LEU:O	1:B:222:TYR:HB3	2.12	0.50
1:A:133:ILE:CD1	1:A:269:PRO:HG3	2.42	0.49
1:B:132:ILE:HG23	1:B:265:VAL:HG11	1.93	0.49
1:A:87:VAL:HG22	1:A:291:THR:CG2	2.43	0.49
1:A:317:ILE:O	1:A:317:ILE:CG2	2.59	0.49
1:B:102:ARG:HH22	1:B:131:GLN:NE2	2.11	0.49
1:B:116:ASP:OD2	5:B:327:SO4:S	2.71	0.49
1:B:133:ILE:CD1	1:B:269:PRO:HG3	2.42	0.49
1:B:286:TYR:CG	1:B:287:GLY:N	2.80	0.49
1:A:107:PRO:HB3	1:A:254:MET:CE	2.42	0.49
1:A:64:ASN:HB2	6:A:372:HOH:O	2.12	0.48
1:A:19:ARG:NE	1:A:26:ILE:CD1	2.76	0.48
1:A:23:ASP:HB3	1:A:25:TYR:CE1	2.49	0.48
1:A:37:MET:HE3	1:A:37:MET:HA	1.95	0.48
1:B:91:GLY:HA2	1:B:95:GLY:O	2.14	0.48
1:A:262:PRO:HB2	1:A:264:GLN:OE1	2.14	0.47
1:B:131:GLN:O	1:B:132:ILE:HD13	2.14	0.47
1:B:299:HIS:H	1:B:299:HIS:CD2	2.33	0.47
1:A:22:ARG:HB2	1:A:22:ARG:NH1	2.29	0.47
5:A:326:SO4:O1	3:B:321:AKG:H42	2.14	0.47
1:B:261:VAL:CG1	1:B:265:VAL:HB	2.40	0.47
1:A:154:THR:HG21	1:A:252:TYR:CE1	2.49	0.47
1:A:301:ARG:HG3	1:A:301:ARG:NH1	2.30	0.47
1:A:19:ARG:HE	1:A:26:ILE:CD1	2.28	0.47
1:B:19:ARG:HH21	1:B:26:ILE:HD11	1.79	0.47
1:A:222:TYR:HA	1:A:223:PRO:HD3	1.71	0.46
1:A:102:ARG:NH2	1:A:131:GLN:HE22	2.12	0.46
1:B:9:ASN:HD22	1:B:318:PRO:HB2	1.80	0.46
1:B:48:LEU:HD23	1:B:74:ILE:HD11	1.96	0.46
1:B:137:ASP:HB2	1:B:140:ARG:HD2	1.98	0.46
1:A:176:ASP:C	1:A:176:ASP:OD2	2.58	0.46
1:A:299:HIS:ND1	4:A:323:ACT:C	2.79	0.46
1:B:17:VAL:O	1:B:21:GLU:HG3	2.16	0.46
1:B:259:ARG:HH12	4:B:325:ACT:CH3	2.29	0.45
1:A:131:GLN:NE2	3:A:322:AKG:H32	2.23	0.45
1:B:102:ARG:HH22	1:B:131:GLN:HE22	1.65	0.45
1:A:262:PRO:HG2	1:A:265:VAL:HG23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:GLN:NE2	1:A:316:GLN:HA	2.32	0.45
1:B:175:TYR:CE2	1:B:177:GLU:HG2	2.53	0.44
1:B:234:PHE:HD1	1:B:235:TRP:O	2.00	0.44
1:A:83:ARG:HD3	1:A:84:PRO:HD2	1.98	0.44
1:A:174:ASN:CB	1:B:144:ILE:HG12	2.47	0.44
1:B:131:GLN:OE1	3:B:321:AKG:H32	2.18	0.44
1:B:71:HIS:CD2	1:B:81:ILE:HD13	2.52	0.44
1:B:133:ILE:HD12	1:B:269:PRO:CG	2.48	0.44
1:B:10:PHE:HB2	1:B:88:ASP:HB2	2.00	0.43
1:B:35:GLU:CD	1:B:35:GLU:N	2.71	0.43
1:B:86:ILE:HG23	1:B:149:VAL:HG21	2.00	0.43
1:A:83:ARG:HA	1:A:84:PRO:HD3	1.86	0.43
1:A:102:ARG:HH21	3:A:322:AKG:H32	1.84	0.43
1:B:9:ASN:ND2	1:B:318:PRO:HG2	2.33	0.43
1:A:56:TYR:HA	1:A:57:PRO:HD3	1.78	0.43
1:B:103:SER:HB2	1:B:256:PHE:CZ	2.53	0.43
1:A:120:ALA:HB2	6:A:402:HOH:O	2.17	0.43
1:B:297:TYR:CD1	1:B:297:TYR:N	2.87	0.43
1:A:110:GLN:HA	1:A:245:HIS:ND1	2.34	0.43
1:B:123:PHE:O	3:B:321:AKG:O5	2.37	0.43
1:B:146:THR:HG23	1:B:236:SER:HB3	2.00	0.43
1:B:220:GLN:HG3	1:B:243:LEU:CD1	2.49	0.42
1:B:276:GLU:HA	1:B:276:GLU:OE2	2.19	0.42
1:A:70:ARG:HA	1:A:70:ARG:HD2	1.84	0.42
1:B:122:THR:HA	3:B:321:AKG:H41	2.01	0.42
1:B:23:ASP:HB3	1:B:25:TYR:CE1	2.55	0.42
1:A:87:VAL:HG21	1:A:291:THR:HG23	2.01	0.42
1:B:259:ARG:HH12	4:B:325:ACT:H1	1.84	0.41
1:A:276:GLU:HA	1:A:276:GLU:OE1	2.19	0.41
1:A:87:VAL:CG2	1:A:291:THR:CG2	2.98	0.41
1:A:132:ILE:CD1	1:A:145:GLY:O	2.69	0.41
1:A:26:ILE:O	1:A:26:ILE:HG23	2.21	0.41
1:B:294:VAL:HG23	6:B:406:HOH:O	2.20	0.41
1:A:87:VAL:CG2	1:A:291:THR:HG23	2.50	0.41
1:A:116:ASP:OD2	5:A:326:SO4:S	2.79	0.41
1:A:237:ASN:ND2	1:B:173:MET:HE2	2.33	0.41
1:A:316:GLN:O	1:A:317:ILE:C	2.64	0.41
1:B:30:LYS:HE2	1:B:33:GLU:CD	2.46	0.41
1:B:25:TYR:CB	1:B:234:PHE:HB3	2.51	0.41
1:A:13:SER:O	1:A:17:VAL:HG23	2.21	0.40
1:A:40:ARG:O	1:A:44:ILE:HG13	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:GLN:OE1	1:A:249:LYS:HE2	2.21	0.40
1:A:175:TYR:O	1:B:141:PRO:HA	2.21	0.40
1:A:41:TRP:O	1:A:45:ARG:HB2	2.22	0.40
1:B:152:ALA:HB1	1:B:154:THR:O	2.21	0.40
1:B:13:SER:O	1:B:17:VAL:HG23	2.22	0.40
1:B:56:TYR:HA	1:B:57:PRO:HD3	1.86	0.40
1:B:94:ILE:HG13	1:B:98:LEU:HD21	2.03	0.40
1:B:317:ILE:HA	1:B:318:PRO:HD2	1.88	0.40
1:A:73:ASP:O	1:A:308:ARG:NH1	2.50	0.40
1:A:266:GLN:CG	1:A:269:PRO:HB3	2.52	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	252/319 (79%)	247 (98%)	5 (2%)	0	100	100
1	B	265/319 (83%)	257 (97%)	7 (3%)	1 (0%)	30	34
All	All	517/638 (81%)	504 (98%)	12 (2%)	1 (0%)	43	51

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	9	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	216/273 (79%)	207 (96%)	9 (4%)	26	36
1	B	230/273 (84%)	225 (98%)	5 (2%)	45	61
All	All	446/546 (82%)	432 (97%)	14 (3%)	35	48

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

Mol	Chain	Res	Type
1	A	36	GLU
1	A	48	LEU
1	A	70	ARG
1	A	119	GLN
1	A	132	ILE
1	A	160	ASN
1	A	163	LEU
1	A	239	MET
1	A	291	THR
1	B	30	LYS
1	B	35	GLU
1	B	261	VAL
1	B	264	GLN
1	B	299	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	GLN
1	A	60	ASN
1	A	64	ASN
1	A	119	GLN
1	A	131	GLN
1	A	160	ASN
1	A	174	ASN
1	A	316	GLN
1	B	9	ASN
1	B	42	ASN
1	B	47	GLN
1	B	170	HIS
1	B	220	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 15 ligands modelled in this entry, 2 are monoatomic - leaving 13 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	AKG	A	322	-	9,9,9	1.06	0	11,11,11	1.43	2 (18%)
4	ACT	B	323	-	3,3,3	0.59	0	3,3,3	0.86	0
3	AKG	B	321	-	9,9,9	1.17	1 (11%)	11,11,11	1.45	2 (18%)
4	ACT	A	323	-	3,3,3	0.47	0	3,3,3	0.85	0
5	SO4	A	326	-	4,4,4	0.32	0	6,6,6	0.14	0
4	ACT	B	322	-	3,3,3	0.46	0	3,3,3	0.84	0
4	ACT	B	325	-	3,3,3	0.55	0	3,3,3	0.86	0
4	ACT	B	324	-	3,3,3	0.51	0	3,3,3	0.83	0
3	AKG	A	321	2	9,9,9	0.91	1 (11%)	11,11,11	1.39	1 (9%)
4	ACT	A	325	-	3,3,3	0.52	0	3,3,3	0.77	0
4	ACT	B	326	-	3,3,3	0.56	0	3,3,3	0.84	0
4	ACT	A	324	-	3,3,3	0.47	0	3,3,3	0.82	0
5	SO4	B	327	-	4,4,4	0.39	0	6,6,6	0.11	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	AKG	A	322	-	-	0/9/9/9	-
3	AKG	A	321	2	-	0/9/9/9	-
3	AKG	B	321	-	-	0/9/9/9	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	321	AKG	C2-C1	-2.07	1.50	1.53
3	B	321	AKG	C3-C2	2.06	1.53	1.51

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	321	AKG	C3-C2-C1	2.60	120.28	115.86
3	A	321	AKG	O2-C1-C2	2.53	120.61	113.59
3	A	322	AKG	O2-C1-C2	2.36	120.13	113.59
3	B	321	AKG	O2-C1-C2	2.26	119.87	113.59
3	A	322	AKG	C3-C2-C1	2.18	119.56	115.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	322	AKG	7	0
3	B	321	AKG	4	0
4	A	323	ACT	1	0
5	A	326	SO4	2	0
4	B	322	ACT	1	0
4	B	325	ACT	2	0
4	A	325	ACT	1	0
5	B	327	SO4	2	0

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	260/319 (81%)	0.38	15 (5%) 29 25	34, 43, 64, 96	0
1	B	271/319 (84%)	0.50	20 (7%) 20 18	32, 46, 71, 89	0
All	All	531/638 (83%)	0.44	35 (6%) 24 21	32, 44, 68, 96	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	175	TYR	5.6
1	A	317	ILE	4.5
1	B	8	ALA	4.3
1	A	132	ILE	4.0
1	A	221	ALA	3.9
1	A	174	ASN	3.6
1	A	140	ARG	3.6
1	A	169	THR	3.4
1	B	177	GLU	3.4
1	B	273	ASN	3.2
1	B	217	ASP	3.1
1	B	173	MET	3.0
1	A	222	TYR	2.9
1	A	94	ILE	2.9
1	B	137	ASP	2.9
1	B	218	GLU	2.9
1	B	274	LEU	2.8
1	B	220	GLN	2.7
1	B	219	SER	2.6
1	A	8	ALA	2.5
1	B	319	SER	2.4
1	B	58	ASP	2.4
1	A	176	ASP	2.4
1	A	18	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	302	ILE	2.4
1	B	304	ARG	2.4
1	B	15	GLU	2.3
1	A	274	LEU	2.2
1	B	140	ARG	2.2
1	B	221	ALA	2.2
1	A	137	ASP	2.2
1	A	58	ASP	2.2
1	B	172	SER	2.1
1	B	222	TYR	2.1
1	B	296	GLU	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(Å ²)	Q<0.9
4	ACT	B	326	4/4	0.66	0.31	69,70,71,72	0
4	ACT	B	325	4/4	0.71	0.31	69,71,72,72	0
3	AKG	B	321	10/10	0.75	0.24	65,70,77,80	0
3	AKG	A	322	10/10	0.76	0.24	53,61,73,76	0
4	ACT	A	323	4/4	0.77	0.23	58,58,59,60	0
3	AKG	A	321	10/10	0.78	0.20	58,67,68,71	0
4	ACT	A	325	4/4	0.81	0.24	62,62,64,65	0
5	SO4	B	327	5/5	0.81	0.17	67,67,70,70	0
4	ACT	B	324	4/4	0.83	0.21	71,71,71,71	0
5	SO4	A	326	5/5	0.84	0.17	71,73,74,74	0
4	ACT	B	322	4/4	0.87	0.24	64,64,64,65	0
4	ACT	B	323	4/4	0.91	0.17	52,53,54,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	ACT	A	324	4/4	0.95	0.14	44,46,48,50	0
2	FE2	A	320	1/1	0.99	0.05	51,51,51,51	0
2	FE2	B	320	1/1	1.00	0.01	48,48,48,48	0

6.5 Other polymers [i](#)

There are no such residues in this entry.