



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:55 AM UTC

PDB ID : 5GK6 / pdb_00005gk6
Title : Structure of E.Coli fructose 1,6-bisphosphate aldolase, Citrate bound form
Authors : Tran, T.H.; Huynh, K.H.; Ho, T.H.; Kang, L.W.
Deposited on : 2016-07-03
Resolution : 1.80 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

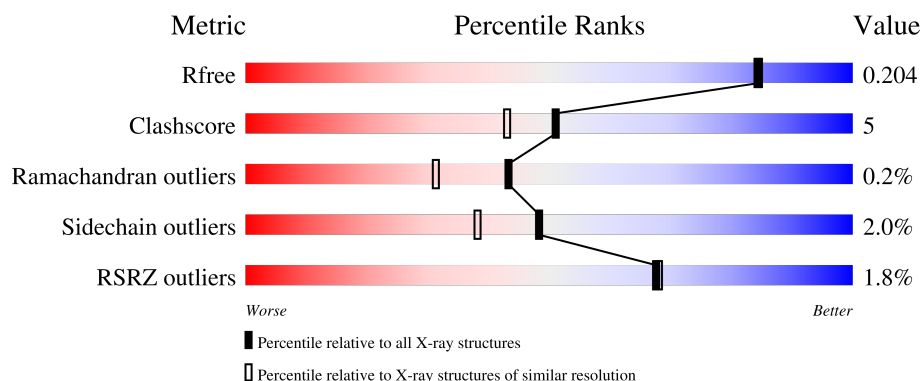
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	359	
1	B	359	

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	CIT	B	402	-	X	-	-
4	PEG	A	403	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5651 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.

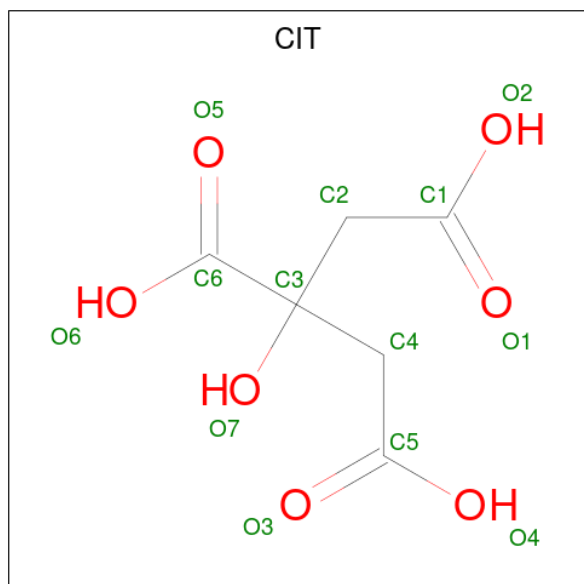
- Molecule 1 is a protein called Fructose-bisphosphate aldolase class 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	333	Total	C	N	O	S	0	2	0
			2583	1643	435	494	11			
1	B	331	Total	C	N	O	S	0	4	0
			2590	1648	436	495	11			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

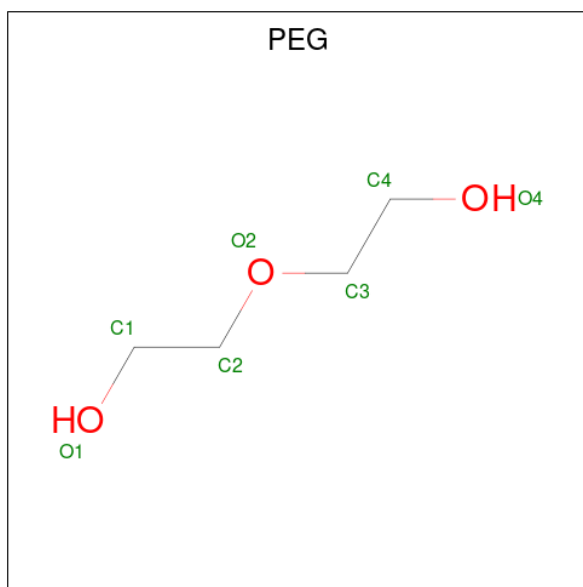
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		

- Molecule 3 is CITRIC ACID (CCD ID: CIT) (formula: C₆H₈O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	6	7		
3	B	1	Total	C	O	0	0
			13	6	7		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		

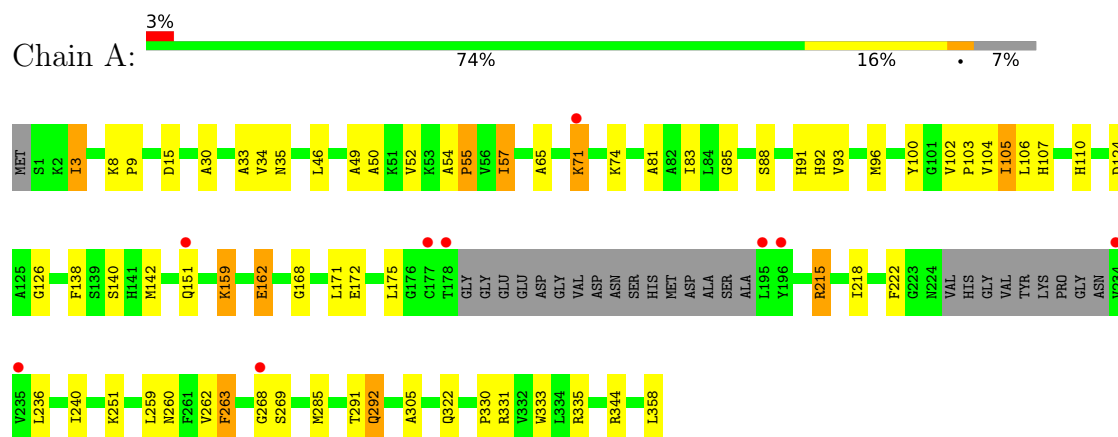
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	228	Total	O	0	0
			228	228		
5	B	215	Total	O	0	0
			215	215		

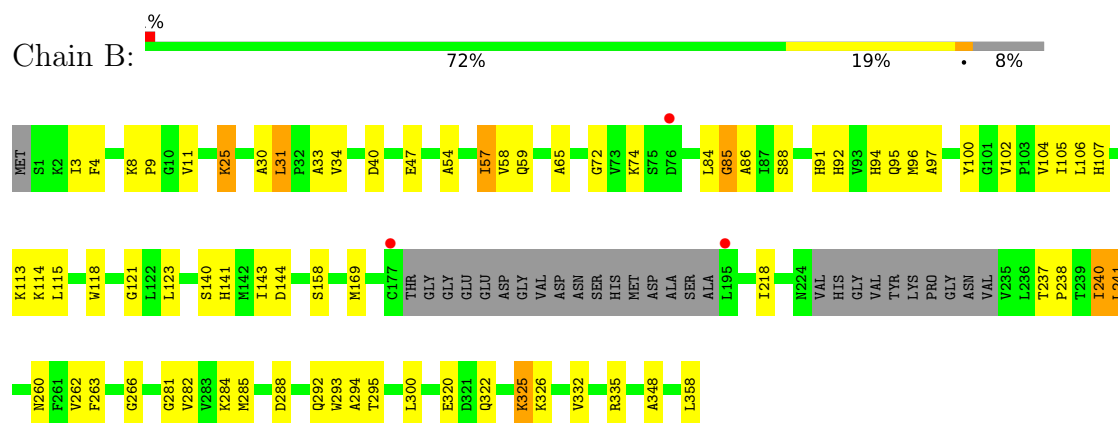
3 Residue-property plots [i](#)

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: Fructose-bisphosphate aldolase class 2



- Molecule 1: Fructose-bisphosphate aldolase class 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	72.03Å 73.00Å 73.04Å 90.00° 104.09° 90.00°	Depositor
Resolution (Å)	50.00 – 1.80 50.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.1 (50.00-1.80) 98.5 (50.00-1.80)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	52.89 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.157 , 0.194 0.172 , 0.204	Depositor DCC
R_{free} test set	3404 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	25.8	Xtriage
Anisotropy	0.033	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 37.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.025 for l,-k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5651	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.60% 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: CIT, ZN, PEG

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	1.68	37/2638 (1.4%)	1.18	11/3571 (0.3%)
1	B	1.74	43/2645 (1.6%)	1.20	9/3579 (0.3%)
All	All	1.71	80/5283 (1.5%)	1.19	20/7150 (0.3%)

All (80) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	35	ASN	N-CA	-7.51	1.36	1.46
1	B	292	GLN	C-O	-7.12	1.16	1.24
1	A	218	ILE	C-O	-6.97	1.16	1.24
1	B	57	ILE	C-O	-6.93	1.16	1.24
1	A	106	LEU	C-O	-6.72	1.16	1.24
1	A	33	ALA	C-O	-6.70	1.16	1.24
1	A	104	VAL	C-O	-6.56	1.17	1.24
1	B	218	ILE	C-O	-6.56	1.17	1.24
1	B	106	LEU	C-O	-6.53	1.16	1.24
1	A	292	GLN	C-O	-6.50	1.16	1.24
1	A	100	TYR	C-O	-6.44	1.15	1.24
1	B	84	LEU	N-CA	-6.43	1.38	1.46
1	B	140	SER	C-O	-6.43	1.16	1.23
1	A	335	ARG	C-O	-6.37	1.16	1.24
1	B	85	GLY	C-O	-6.34	1.16	1.23
1	B	123	LEU	C-O	-6.30	1.16	1.24
1	B	294	ALA	C-O	-6.18	1.16	1.24
1	B	30	ALA	CA-CB	-6.14	1.43	1.54
1	B	95	GLN	C-O	-6.12	1.16	1.24
1	A	240	ILE	C-O	-6.10	1.17	1.24
1	A	34	VAL	C-O	-6.02	1.17	1.24
1	A	49	ALA	N-CA	-6.02	1.39	1.46
1	B	40	ASP	N-CA	6.00	1.53	1.46
1	A	344	ARG	C-O	5.97	1.31	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	118	TRP	C-O	-5.92	1.17	1.24
1	A	81	ALA	C-O	-5.86	1.17	1.24
1	B	240	ILE	C-O	-5.84	1.17	1.24
1	A	57	ILE	C-O	-5.83	1.17	1.24
1	B	102	VAL	C-O	-5.80	1.17	1.24
1	A	102	VAL	C-O	-5.73	1.17	1.24
1	A	105	ILE	C-O	-5.73	1.17	1.24
1	B	300	LEU	C-O	-5.70	1.17	1.24
1	A	331	ARG	CA-CB	-5.69	1.44	1.53
1	B	158	SER	CA-CB	5.68	1.62	1.53
1	B	262	VAL	C-O	-5.68	1.18	1.24
1	B	86	ALA	C-O	-5.67	1.17	1.24
1	A	46	LEU	N-CA	5.61	1.53	1.46
1	B	47	GLU	C-O	5.57	1.30	1.24
1	B	59	GLN	C-O	-5.57	1.16	1.23
1	B	143	ILE	C-O	-5.54	1.18	1.24
1	B	104	VAL	C-O	-5.47	1.18	1.24
1	B	113	LYS	C-O	-5.44	1.17	1.24
1	B	97	ALA	C-O	-5.42	1.17	1.24
1	A	222	PHE	C-O	-5.41	1.18	1.24
1	B	322	GLN	CA-C	5.39	1.59	1.53
1	B	282	VAL	C-O	-5.37	1.18	1.24
1	A	138	PHE	C-O	-5.35	1.17	1.23
1	A	172	GLU	C-O	-5.34	1.17	1.24
1	A	3	ILE	C-O	-5.34	1.18	1.24
1	A	260	ASN	C-O	-5.33	1.17	1.24
1	A	262	VAL	C-O	-5.32	1.18	1.24
1	A	140	SER	C-O	-5.32	1.17	1.23
1	B	33	ALA	C-O	-5.31	1.18	1.24
1	B	34	VAL	C-O	-5.30	1.18	1.24
1	B	295	THR	C-O	-5.30	1.18	1.24
1	A	93	VAL	C-O	5.30	1.30	1.24
1	B	144	ASP	C-O	-5.30	1.17	1.23
1	A	50	ALA	C-O	-5.28	1.17	1.24
1	B	3	ILE	C-O	-5.27	1.18	1.24
1	A	55	PRO	C-O	-5.26	1.17	1.23
1	B	58	VAL	C-O	-5.25	1.18	1.24
1	A	305	ALA	C-O	-5.24	1.17	1.24
1	B	284	LYS	N-CA	5.22	1.52	1.46
1	A	52	VAL	C-O	-5.21	1.18	1.24
1	B	293	TRP	C-O	-5.20	1.18	1.24
1	B	288	ASP	N-CA	5.20	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	142	MET	C-O	-5.19	1.17	1.24
1	A	126	GLY	CA-C	5.17	1.58	1.51
1	A	263	PHE	C-O	-5.17	1.17	1.24
1	B	121	GLY	C-O	-5.09	1.17	1.23
1	A	30	ALA	C-O	-5.08	1.17	1.23
1	A	83	ILE	CA-CB	5.08	1.59	1.54
1	B	94	HIS	C-O	-5.08	1.18	1.24
1	B	348	ALA	C-O	-5.08	1.18	1.24
1	B	11	VAL	C-O	5.06	1.29	1.24
1	B	332	VAL	C-O	-5.05	1.18	1.24
1	A	291	THR	C-O	-5.04	1.17	1.24
1	B	281	GLY	C-O	-5.04	1.17	1.24
1	B	31	LEU	C-O	-5.02	1.17	1.24
1	A	124	ASP	C-O	-5.02	1.18	1.24

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	269	SER	N-CA-C	8.23	122.10	110.50
1	A	96	MET	N-CA-C	7.60	122.68	113.41
1	A	218	ILE	N-CA-C	7.22	118.52	108.12
1	B	100	TYR	N-CA-C	-7.10	104.65	113.38
1	B	34	VAL	N-CA-C	6.67	117.51	108.17
1	B	218	ILE	N-CA-C	6.55	117.55	108.12
1	A	34	VAL	N-CA-C	6.52	117.68	108.36
1	B	96	MET	N-CA-C	6.19	121.06	112.45
1	A	54	ALA	CA-C-N	-5.94	114.49	120.31
1	A	54	ALA	C-N-CA	-5.94	114.49	120.31
1	B	107	HIS	N-CA-CB	-5.90	101.42	111.69
1	B	54	ALA	N-CA-C	5.77	113.41	108.22
1	A	251	LYS	N-CA-C	5.76	117.56	111.28
1	A	107	HIS	N-CA-CB	-5.74	102.33	111.62
1	B	107	HIS	N-CA-C	5.53	117.59	109.24
1	B	54	ALA	CA-C-N	-5.47	115.10	120.52
1	B	54	ALA	C-N-CA	-5.47	115.10	120.52
1	A	215	ARG	N-CA-C	5.47	118.09	109.39
1	A	268	GLY	N-CA-C	5.13	123.89	115.73
1	A	168	GLY	N-CA-C	5.02	122.63	114.90

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	2583	0	2545	31	0
1	B	2590	0	2560	26	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	13	0	4	0	0
3	B	13	0	4	0	0
4	A	7	0	10	9	0
5	A	228	0	0	6	0
5	B	215	0	0	4	0
All	All	5651	0	5123	54	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 5.

All (54) 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:8:LYS:HE2	5:A:668:HOH:O	1.53	1.07
1:A:8:LYS:HG2	1:A:9:PRO:HD2	1.38	1.03
1:A:74:LYS:NZ	5:A:502:HOH:O	1.91	0.99
1:A:159:LYS:NZ	1:A:162:GLU:OE1	1.96	0.98
1:A:91:HIS:HD1	4:A:403:PEG:HO1	1.01	0.90
1:A:8:LYS:HG2	1:A:9:PRO:CD	2.07	0.83
1:A:8:LYS:CE	5:A:668:HOH:O	2.18	0.79
1:A:91:HIS:ND1	4:A:403:PEG:O1	2.15	0.78
1:B:8:LYS:HE2	1:B:9:PRO:O	1.88	0.73
4:A:403:PEG:H41	1:B:88:SER:OG	1.92	0.69
1:B:237:THR:HB	1:B:240:ILE:HD12	1.75	0.67
1:A:8:LYS:HD3	1:A:9:PRO:O	1.94	0.67
1:A:322:GLN:OE1	5:A:504:HOH:O	2.14	0.65
1:A:71:LYS:HE3	1:B:335:ARG:HD3	1.79	0.62
1:A:292:GLN:OE1	1:B:325:LYS:HE3	2.00	0.61
1:A:263:PHE:CD2	1:A:285[B]:MET:HE2	2.37	0.59
1:A:55:PRO:HB3	1:A:103:PRO:HG2	1.86	0.57
1:A:151:GLN:NE2	5:A:503:HOH:O	2.13	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:266:GLY:HA3	1:B:285[A]:MET:HE3	1.88	0.56
1:B:141:HIS:CD2	1:B:169:MET:HE1	2.42	0.54
1:B:74:LYS:HE3	5:B:650:HOH:O	2.07	0.54
1:A:71:LYS:H	1:A:71:LYS:CE	2.21	0.54
1:B:326:LYS:HG2	5:B:641:HOH:O	2.10	0.52
4:A:403:PEG:H21	1:B:92:HIS:N	2.25	0.51
4:A:403:PEG:H42	1:B:91:HIS:HB2	1.92	0.51
1:B:8:LYS:NZ	5:B:503:HOH:O	2.43	0.50
4:A:403:PEG:H21	1:B:91:HIS:C	2.36	0.50
1:A:8:LYS:NZ	5:A:510:HOH:O	2.46	0.48
1:A:57:ILE:HG12	1:A:105:ILE:HB	1.96	0.48
1:A:15:ASP:OD1	1:A:215:ARG:NH2	2.37	0.47
1:A:8:LYS:CD	1:A:9:PRO:O	2.62	0.47
1:B:320:GLU:H	1:B:320:GLU:CD	2.23	0.46
1:B:263:PHE:CD2	1:B:285[B]:MET:CE	2.99	0.46
1:B:114:LYS:HG2	5:B:643:HOH:O	2.16	0.45
1:A:71:LYS:CE	1:B:335:ARG:HD3	2.44	0.45
1:A:71:LYS:H	1:A:71:LYS:NZ	2.15	0.45
1:A:92:HIS:HB2	4:A:403:PEG:H31	1.99	0.44
1:B:65:ALA:O	1:B:85:GLY:HA3	2.18	0.44
1:A:8:LYS:CE	1:A:9:PRO:O	2.65	0.44
1:B:57:ILE:HG12	1:B:105:ILE:HB	2.00	0.43
1:A:88:SER:HA	4:A:403:PEG:H11	1.99	0.43
1:B:74:LYS:HA	1:B:74:LYS:HD3	1.90	0.43
1:A:71:LYS:HB2	1:A:71:LYS:HE2	1.64	0.43
4:A:403:PEG:H12	1:B:91:HIS:O	2.19	0.43
1:B:25:LYS:HD3	1:B:260:ASN:OD1	2.18	0.43
1:A:65:ALA:O	1:A:85:GLY:HA3	2.20	0.42
1:A:8:LYS:HG2	1:A:9:PRO:N	2.32	0.41
1:B:4:PHE:HB2	1:B:358:LEU:OXT	2.21	0.41
1:B:72:GLY:O	1:B:74:LYS:HE2	2.20	0.41
1:B:31:LEU:HD12	1:B:31:LEU:N	2.36	0.41
1:A:330:PRO:HA	1:A:333:TRP:CE2	2.56	0.41
1:B:238:PRO:O	1:B:241:LEU:HB2	2.20	0.41
1:A:285[B]:MET:HE3	1:A:285[B]:MET:HB2	1.58	0.41
1:A:3:ILE:HB	1:A:358:LEU:HA	2.02	0.41

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	329/359 (92%)	320 (97%)	8 (2%)	1 (0%)	36	25
1	B	329/359 (92%)	322 (98%)	7 (2%)	0	100	100
All	All	658/718 (92%)	642 (98%)	15 (2%)	1 (0%)	43	31

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	110	HIS

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	278/297 (94%)	271 (98%)	7 (2%)	42	30
1	B	280/297 (94%)	276 (99%)	4 (1%)	59	52
All	All	558/594 (94%)	547 (98%)	11 (2%)	48	38

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	LYS
1	A	159	LYS
1	A	162	GLU
1	A	171	LEU
1	A	175	LEU

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Mol	Chain	Res	Type
1	A	236	LEU
1	A	259	LEU
1	B	25	LYS
1	B	115	LEU
1	B	241	LEU
1	B	325	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	256	HIS
1	B	18	GLN
1	B	95	GLN
1	B	151	GLN
1	B	198	GLN
1	B	256	HIS

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 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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
4	PEG	A	403	-	6,6,6	0.29	0	5,5,5	1.60	2 (40%)
3	CIT	B	402	2	12,12,12	2.77	5 (41%)	17,17,17	2.81	12 (70%)
3	CIT	A	402	2	12,12,12	3.86	7 (58%)	17,17,17	3.31	8 (47%)

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
4	PEG	A	403	-	-	3/4/4/4	-
3	CIT	B	402	2	-	8/16/16/16	-
3	CIT	A	402	2	-	2/16/16/16	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	CIT	C3-C6	7.83	1.61	1.53
3	A	402	CIT	C2-C3	-6.95	1.45	1.54
3	B	402	CIT	C3-C6	6.54	1.60	1.53
3	A	402	CIT	C4-C3	-6.19	1.46	1.54
3	B	402	CIT	O7-C3	-3.76	1.36	1.43
3	B	402	CIT	C4-C3	-3.55	1.49	1.54
3	B	402	CIT	C2-C3	-3.07	1.50	1.54
3	A	402	CIT	O5-C6	2.75	1.30	1.22
3	A	402	CIT	O7-C3	-2.66	1.38	1.43
3	B	402	CIT	O1-C1	2.61	1.30	1.22
3	A	402	CIT	O6-C6	-2.46	1.21	1.30
3	A	402	CIT	O3-C5	2.04	1.28	1.22

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	CIT	O7-C3-C6	-10.44	94.16	108.96
3	B	402	CIT	O7-C3-C6	-6.13	100.26	108.96
3	B	402	CIT	O6-C6-C3	5.13	122.98	113.14
3	A	402	CIT	O6-C6-C3	4.10	121.01	113.14
3	A	402	CIT	O7-C3-C2	3.43	117.20	109.38
3	A	402	CIT	O7-C3-C4	3.24	116.77	109.38
3	B	402	CIT	O7-C3-C4	3.10	116.45	109.38
3	B	402	CIT	O2-C1-O1	2.95	130.92	123.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	402	CIT	O7-C3-C2	2.91	116.02	109.38
3	A	402	CIT	C2-C3-C6	-2.85	103.73	110.03
3	B	402	CIT	C2-C3-C6	-2.69	104.08	110.03
3	B	402	CIT	O4-C5-C4	2.67	122.80	114.35
3	A	402	CIT	O2-C1-C2	2.67	122.79	114.35
3	B	402	CIT	O6-C6-O5	-2.50	115.85	123.86
3	A	402	CIT	O1-C1-C2	-2.33	116.36	122.95
4	A	403	PEG	O4-C4-C3	2.30	125.35	111.82
3	B	402	CIT	C4-C3-C6	-2.19	105.20	110.03
3	B	402	CIT	O3-C5-C4	-2.14	116.89	122.95
3	B	402	CIT	C3-C2-C1	2.11	119.69	113.92
3	A	402	CIT	O6-C6-O5	-2.10	117.14	123.86
4	A	403	PEG	O2-C2-C1	2.09	119.32	110.11
3	B	402	CIT	O1-C1-C2	-2.04	117.17	122.95

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	403	PEG	C4-C3-O2-C2
4	A	403	PEG	O1-C1-C2-O2
3	A	402	CIT	O2-C1-C2-C3
3	B	402	CIT	C2-C3-C6-O5
3	B	402	CIT	C2-C3-C6-O6
3	B	402	CIT	C4-C3-C6-O5
3	B	402	CIT	C4-C3-C6-O6
3	B	402	CIT	C3-C4-C5-O4
3	B	402	CIT	C3-C4-C5-O3
3	B	402	CIT	O7-C3-C6-O6
3	A	402	CIT	O1-C1-C2-C3
4	A	403	PEG	O2-C3-C4-O4
3	B	402	CIT	O7-C3-C6-O5

There are no ring outliers.

1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	403	PEG	9	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	333/359 (92%)	0.05	9 (2%) 56 56	12, 26, 43, 72	2 (0%)
1	B	331/359 (92%)	0.05	3 (0%) 81 81	12, 26, 44, 67	4 (1%)
All	All	664/718 (92%)	0.05	12 (1%) 67 68	12, 26, 44, 72	6 (0%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	178	THR	4.7
1	B	195	LEU	3.9
1	A	195	LEU	3.7
1	A	151	GLN	3.1
1	B	177	CYS	3.1
1	A	196	TYR	2.8
1	A	234	VAL	2.8
1	A	71	LYS	2.6
1	A	268	GLY	2.3
1	B	76	ASP	2.2
1	A	235	VAL	2.1
1	A	177	CYS	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	PEG	A	403	7/7	0.88	0.12	38,41,46,49	0
3	CIT	A	402	13/13	0.92	0.10	31,39,50,52	0
3	CIT	B	402	13/13	0.94	0.10	29,34,46,52	0
2	ZN	A	401	1/1	0.99	0.09	30,30,30,30	1
2	ZN	B	401	1/1	1.00	0.15	29,29,29,29	1

6.5 Other polymers [i](#)

There are no such residues in this entry.