



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:56 PM UTC

PDB ID : 5GK3 / pdb_00005gk3
Title : Native structure of fructose 1,6-bisphosphate aldolase from Escherichia coli at 1.8 Angstrom resolution
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

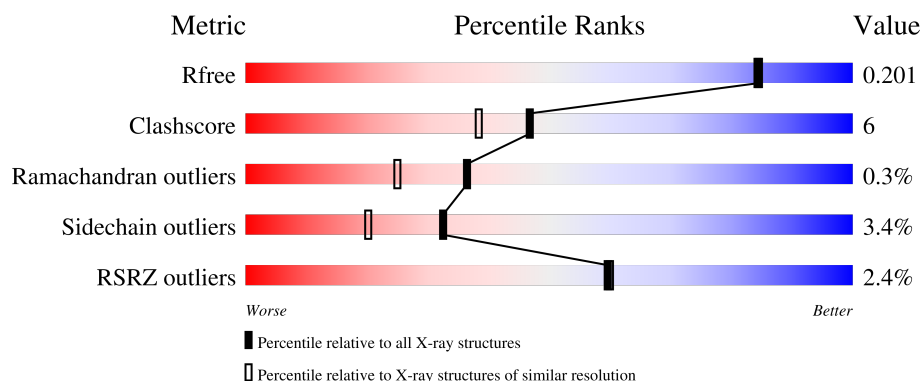
1 Overall quality at a glance

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
4	PEG	B	401	-	X	-	-

2 Entry composition [i](#)

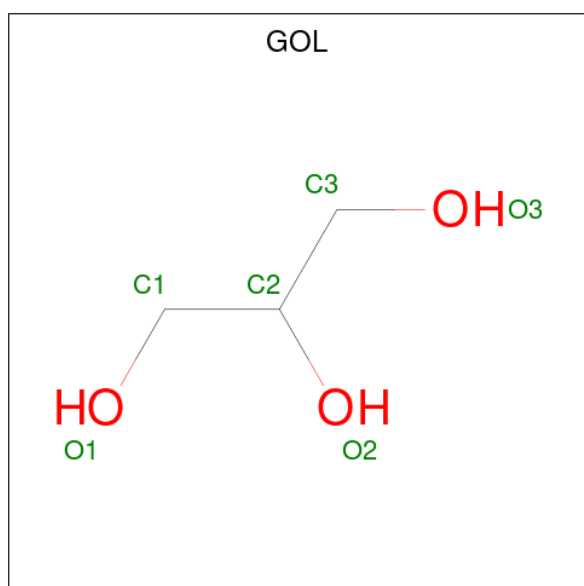
There are 5 unique types of molecules in this entry. The entry contains 5643 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	334	Total	C	N	O	S	0	1	0
			2587	1646	436	494	11			
1	B	332	Total	C	N	O	S	0	1	0
			2575	1638	434	492	11			

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).

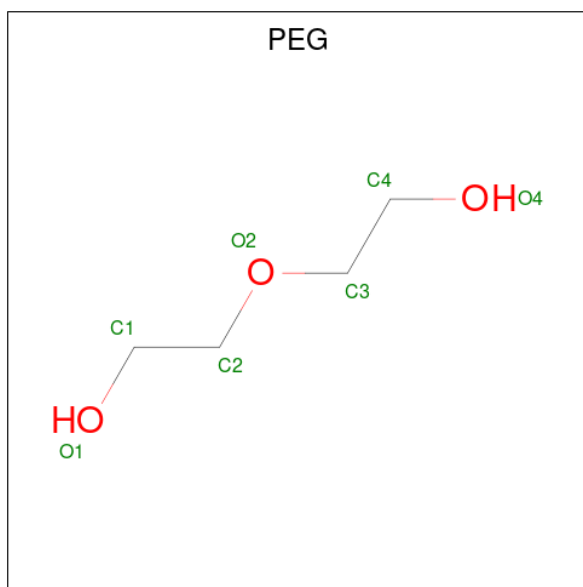


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

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



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

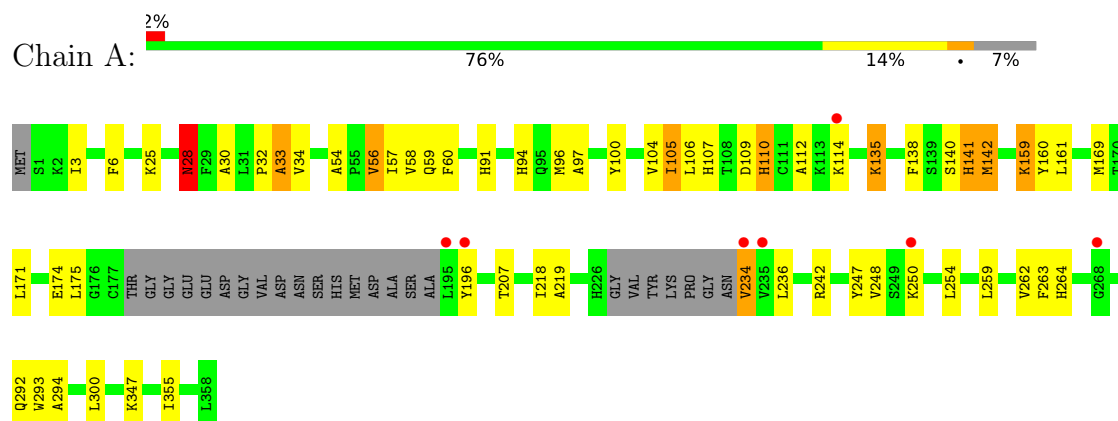
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	218	Total	O	0	0
			218	218		
5	B	236	Total	O	0	0
			236	236		

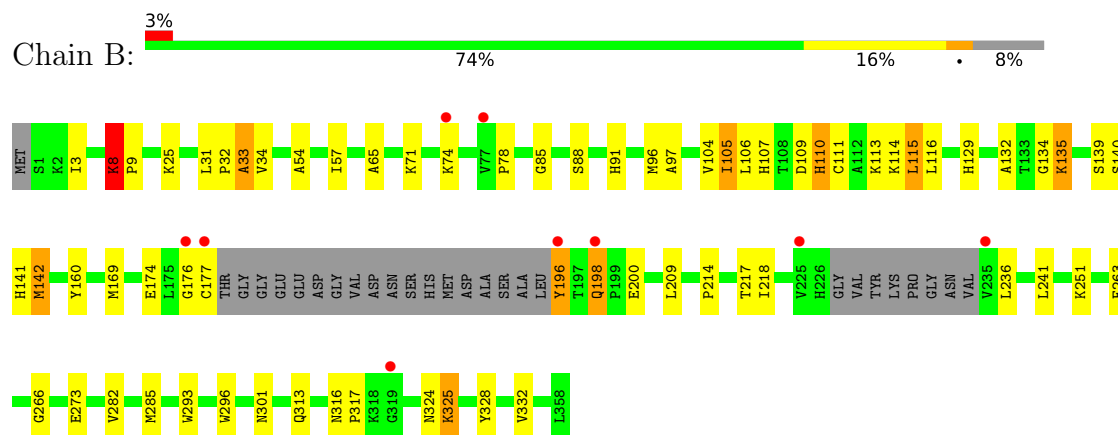
3 Residue-property plots [i](#)

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	72.25Å 72.84Å 73.36Å 90.00° 103.09° 90.00°	Depositor
Resolution (Å)	50.00 – 1.80 50.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (50.00-1.80) 99.7 (50.00-1.80)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.14 (at 1.81Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.155 , 0.189 0.169 , 0.201	Depositor DCC
R_{free} test set	3458 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	20.7	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 41.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.014 for l,-k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5643	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.52% 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: GOL, 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	1.59	35/2643 (1.3%)	1.05	9/3580 (0.3%)
1	B	1.60	30/2631 (1.1%)	1.09	6/3563 (0.2%)
All	All	1.59	65/5274 (1.2%)	1.07	15/7143 (0.2%)

All (65) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	3	ILE	C-O	-7.99	1.15	1.24
1	A	104	VAL	C-O	-7.12	1.16	1.24
1	B	33	ALA	C-O	-7.08	1.15	1.23
1	A	33	ALA	C-O	-7.04	1.16	1.24
1	A	58	VAL	C-O	-6.93	1.16	1.24
1	B	106	LEU	C-O	-6.83	1.15	1.24
1	B	109	ASP	C-O	-6.64	1.15	1.23
1	B	104	VAL	C-O	-6.63	1.17	1.24
1	B	209	LEU	C-O	-6.63	1.16	1.24
1	A	300	LEU	C-O	-6.53	1.16	1.24
1	B	296	TRP	C-O	-6.40	1.16	1.24
1	A	263	PHE	C-O	-6.37	1.16	1.23
1	B	3	ILE	C-O	-6.30	1.17	1.24
1	A	292	GLN	C-O	-6.29	1.16	1.24
1	B	218	ILE	C-O	-6.26	1.17	1.24
1	B	54	ALA	C-O	-6.19	1.17	1.24
1	A	109	ASP	C-O	-6.17	1.15	1.23
1	A	97	ALA	C-O	-6.08	1.17	1.24
1	B	160	TYR	C-O	-6.05	1.17	1.24
1	A	32	PRO	C-O	-6.02	1.17	1.23
1	A	59	GLN	C-O	-5.96	1.16	1.23
1	A	355	ILE	C-O	5.93	1.30	1.24
1	B	31	LEU	C-O	-5.91	1.16	1.24
1	B	8	LYS	C-O	-5.87	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	140	SER	C-O	-5.86	1.17	1.23
1	B	293	TRP	C-O	-5.85	1.17	1.24
1	A	140	SER	C-O	-5.83	1.17	1.23
1	B	282	VAL	C-O	-5.81	1.17	1.24
1	A	138	PHE	C-O	-5.74	1.16	1.23
1	B	105	ILE	C-O	-5.72	1.17	1.24
1	B	78	PRO	CA-C	5.69	1.59	1.52
1	B	32	PRO	C-O	-5.66	1.17	1.23
1	A	56	VAL	C-O	-5.60	1.16	1.23
1	A	135	LYS	CA-C	5.58	1.58	1.52
1	A	96	MET	C-O	-5.57	1.16	1.24
1	B	301	ASN	C-O	-5.54	1.17	1.24
1	B	111	CYS	C-O	-5.54	1.17	1.23
1	A	100	TYR	C-O	-5.51	1.16	1.24
1	A	6	PHE	C-O	-5.50	1.16	1.24
1	A	105	ILE	C-O	-5.47	1.17	1.24
1	A	106	LEU	C-O	-5.44	1.17	1.24
1	A	262	VAL	C-O	-5.42	1.18	1.24
1	B	263	PHE	C-O	-5.38	1.17	1.23
1	B	139	SER	C-O	-5.33	1.17	1.24
1	B	113	LYS	C-O	-5.33	1.17	1.24
1	B	251	LYS	N-CA	-5.32	1.39	1.46
1	A	94	HIS	C-O	-5.31	1.18	1.24
1	A	242	ARG	CA-C	5.27	1.59	1.52
1	A	294	ALA	C-O	-5.26	1.18	1.24
1	A	30	ALA	C-O	-5.25	1.17	1.23
1	A	171	LEU	C-O	-5.21	1.17	1.24
1	B	107	HIS	C-O	-5.19	1.17	1.23
1	A	161	LEU	C-O	-5.17	1.18	1.24
1	A	219	ALA	C-O	-5.17	1.17	1.23
1	A	34	VAL	C-O	-5.16	1.18	1.24
1	B	97	ALA	C-O	-5.15	1.17	1.24
1	A	160	TYR	C-O	-5.13	1.18	1.24
1	B	217	THR	C-O	-5.11	1.17	1.23
1	A	141	HIS	C-O	-5.11	1.17	1.23
1	A	293	TRP	C-O	-5.08	1.18	1.24
1	B	214	PRO	C-O	-5.08	1.18	1.24
1	A	207	THR	N-CA	5.07	1.52	1.46
1	B	116	LEU	C-O	-5.05	1.17	1.24
1	A	60	PHE	C-O	-5.02	1.18	1.24
1	B	332	VAL	C-O	-5.01	1.18	1.24

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	34	VAL	N-CA-C	6.89	117.80	107.80
1	B	107	HIS	N-CA-CB	-6.49	100.41	111.69
1	A	34	VAL	N-CA-C	6.25	116.93	108.17
1	A	218	ILE	N-CA-C	6.20	117.05	108.12
1	B	132	ALA	N-CA-C	5.88	117.49	111.14
1	B	96	MET	N-CA-C	5.79	120.47	113.41
1	B	218	ILE	N-CA-C	5.73	116.25	107.77
1	A	107	HIS	N-CA-CB	-5.71	101.75	111.69
1	B	54	ALA	O-C-N	5.53	125.68	121.65
1	A	54	ALA	CA-C-N	-5.49	115.08	120.52
1	A	54	ALA	C-N-CA	-5.49	115.08	120.52
1	A	54	ALA	N-CA-C	5.23	112.93	108.22
1	A	107	HIS	N-CA-C	5.12	116.97	109.24
1	A	96	MET	N-CA-C	5.04	119.56	113.41
1	A	28	ASN	N-CA-C	5.01	118.30	111.39

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	2587	0	2548	20	0
1	B	2575	0	2537	39	0
2	A	6	0	8	0	0
2	B	12	0	16	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	B	7	0	10	3	0
5	A	218	0	0	5	0
5	B	236	0	0	8	0
All	All	5643	0	5119	59	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 6.

All (59) 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:110:HIS:HE1	5:B:687:HOH:O	1.28	1.15
1:B:313:GLN:O	5:B:503:HOH:O	1.66	1.13
1:A:110:HIS:HE1	5:A:686:HOH:O	1.40	1.02
1:B:198:GLN:HE21	1:B:200:GLU:H	1.19	0.88
1:B:88:SER:HA	4:B:401:PEG:H42	1.56	0.85
1:A:110:HIS:CE1	5:A:686:HOH:O	2.23	0.77
1:B:110:HIS:CE1	5:B:687:HOH:O	2.14	0.76
1:A:196:TYR:CE1	1:A:234:VAL:HG12	2.24	0.72
1:A:114:LYS:NZ	5:A:501:HOH:O	2.02	0.70
1:B:266:GLY:HA3	1:B:285[A]:MET:HE3	1.75	0.68
1:B:198:GLN:NE2	1:B:200:GLU:H	1.91	0.67
1:B:198:GLN:HE21	1:B:200:GLU:N	1.92	0.66
1:B:135:LYS:NZ	5:B:502:HOH:O	1.63	0.65
1:B:176:GLY:O	1:B:177:CYS:HB2	1.95	0.65
1:B:325:LYS:CE	5:B:503:HOH:O	2.45	0.64
1:B:325:LYS:CE	1:B:325:LYS:H	2.11	0.64
1:B:325:LYS:N	1:B:325:LYS:HE2	2.13	0.63
1:B:135:LYS:HA	1:B:135:LYS:HE3	1.83	0.60
1:B:196:TYR:CD1	1:B:196:TYR:N	2.70	0.60
1:B:328:TYR:HE2	5:B:503:HOH:O	1.85	0.59
1:B:196:TYR:N	1:B:196:TYR:HD1	1.99	0.59
1:B:91:HIS:C	4:B:401:PEG:H12	2.30	0.57
1:A:141:HIS:CD2	1:A:169:MET:HE1	2.43	0.53
1:A:28:ASN:OD1	5:A:503:HOH:O	2.20	0.50
1:A:114:LYS:H	1:A:114:LYS:HE2	1.78	0.49
1:A:112:ALA:HB1	5:A:501:HOH:O	2.12	0.49
1:A:247:TYR:O	1:A:250:LYS:HG3	2.13	0.49
1:B:141:HIS:CD2	1:B:169:MET:HE1	2.48	0.48
1:A:142:MET:HE3	1:A:264:HIS:HE1	1.78	0.48
1:B:236:LEU:HD23	1:B:273:GLU:HB3	1.94	0.48
1:B:129:HIS:HD1	2:B:403:GOL:C1	2.26	0.48
1:B:324:ASN:N	5:B:503:HOH:O	2.24	0.47
1:B:135:LYS:HA	1:B:135:LYS:CE	2.45	0.47
1:A:91:HIS:HB2	4:B:401:PEG:H21	1.97	0.46
1:B:65:ALA:O	1:B:85:GLY:HA3	2.16	0.46
1:A:196:TYR:HE1	1:A:234:VAL:HG12	1.77	0.45
1:A:57:ILE:HG12	1:A:105:ILE:HB	1.99	0.45
1:B:316:ASN:HB2	1:B:317:PRO:CD	2.47	0.44
1:A:159:LYS:HD2	1:A:159:LYS:HA	1.53	0.44
1:B:324:ASN:HB2	5:B:503:HOH:O	2.17	0.44
1:B:33:ALA:HA	1:B:57:ILE:HB	1.99	0.43
1:B:74:LYS:HE3	1:B:74:LYS:HB2	1.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:ILE:HG12	1:B:105:ILE:HB	2.00	0.43
1:A:33:ALA:HA	1:A:57:ILE:HB	2.00	0.43
1:A:142:MET:CE	1:A:264:HIS:HE1	2.32	0.43
1:B:142:MET:HE1	1:B:174:GLU:HB2	2.00	0.43
1:A:135:LYS:HB2	1:A:135:LYS:HE3	1.89	0.43
1:B:134:GLY:O	1:B:135:LYS:HD2	2.19	0.43
1:B:324:ASN:N	1:B:325:LYS:HE3	2.34	0.42
1:A:142:MET:CE	1:A:174:GLU:HB2	2.50	0.42
1:B:198:GLN:HE21	1:B:200:GLU:CB	2.32	0.42
1:B:114:LYS:HG3	1:B:115:LEU:HD13	2.02	0.41
1:B:8:LYS:HB2	1:B:8:LYS:HE2	1.56	0.41
1:A:56:VAL:HG22	1:A:57:ILE:N	2.35	0.41
1:B:285[B]:MET:HB2	1:B:285[B]:MET:HE3	1.82	0.41
1:B:325:LYS:CE	1:B:325:LYS:N	2.72	0.41
1:A:248:VAL:HG12	1:A:254:LEU:HD12	2.02	0.41
1:B:8:LYS:HB2	1:B:9:PRO:HD2	2.03	0.41
1:B:198:GLN:NE2	1:B:200:GLU:HB2	2.36	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%)	321 (98%)	7 (2%)	1 (0%)	36	25
1	B	327/359 (91%)	322 (98%)	4 (1%)	1 (0%)	36	25
All	All	656/718 (91%)	643 (98%)	11 (2%)	2 (0%)	36	25

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	110	HIS

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Mol	Chain	Res	Type
1	B	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	279/297 (94%)	270 (97%)	9 (3%)	34	22
1	B	278/297 (94%)	268 (96%)	10 (4%)	31	18
All	All	557/594 (94%)	538 (97%)	19 (3%)	32	20

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

Mol	Chain	Res	Type
1	A	25	LYS
1	A	28	ASN
1	A	142	MET
1	A	159	LYS
1	A	175	LEU
1	A	234	VAL
1	A	236	LEU
1	A	259	LEU
1	A	347	LYS
1	B	8	LYS
1	B	25	LYS
1	B	71	LYS
1	B	115	LEU
1	B	135	LYS
1	B	142	MET
1	B	196	TYR
1	B	198	GLN
1	B	241	LEU
1	B	325	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	HIS
1	A	256	HIS
1	B	18	GLN
1	B	198	GLN
1	B	313	GLN

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 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	$\# Z > 2$
2	GOL	B	402	-	5,5,5	0.36	0	5,5,5	1.70	2 (40%)
2	GOL	A	401	-	5,5,5	0.63	0	5,5,5	0.85	0
4	PEG	B	401	-	6,6,6	0.99	0	5,5,5	3.10	3 (60%)
2	GOL	B	403	-	5,5,5	0.52	0	5,5,5	1.01	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
2	GOL	B	402	-	-	0/4/4/4	-
2	GOL	A	401	-	-	0/4/4/4	-
4	PEG	B	401	-	-	4/4/4/4	-
2	GOL	B	403	-	-	2/4/4/4	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	401	PEG	O2-C3-C4	4.62	130.47	110.11
4	B	401	PEG	O1-C1-C2	3.75	133.88	111.82
4	B	401	PEG	O4-C4-C3	3.10	130.05	111.82
2	B	402	GOL	O3-C3-C2	2.51	121.66	110.38
2	B	402	GOL	O2-C2-C1	-2.10	100.49	109.18

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	403	GOL	O1-C1-C2-O2
2	B	403	GOL	O1-C1-C2-C3
4	B	401	PEG	O1-C1-C2-O2
4	B	401	PEG	C1-C2-O2-C3
4	B	401	PEG	C4-C3-O2-C2
4	B	401	PEG	O2-C3-C4-O4

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	401	PEG	3	0
2	B	403	GOL	1	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	334/359 (93%)	-0.14	7 (2%) 63 64	9, 22, 39, 74	1 (0%)
1	B	332/359 (92%)	-0.20	9 (2%) 56 56	9, 19, 39, 58	1 (0%)
All	All	666/718 (92%)	-0.17	16 (2%) 59 60	9, 21, 39, 74	2 (0%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	177	CYS	5.4
1	A	195	LEU	5.0
1	A	234	VAL	3.1
1	A	235	VAL	3.0
1	B	196	TYR	2.9
1	B	176	GLY	2.7
1	B	235	VAL	2.5
1	A	250	LYS	2.5
1	B	198	GLN	2.4
1	B	77	VAL	2.4
1	B	319	GLY	2.3
1	A	268	GLY	2.2
1	B	74	LYS	2.1
1	A	196	TYR	2.1
1	A	114	LYS	2.1
1	B	225	VAL	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
2	GOL	B	403	6/6	0.84	0.13	38,48,54,55	0
4	PEG	B	401	7/7	0.87	0.15	20,22,34,35	0
2	GOL	B	402	6/6	0.88	0.13	31,37,42,42	0
2	GOL	A	401	6/6	0.92	0.10	26,30,37,39	0
3	ZN	B	404	1/1	0.99	0.01	17,17,17,17	1
3	ZN	A	402	1/1	1.00	0.03	22,22,22,22	1

6.5 Other polymers [i](#)

There are no such residues in this entry.