



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 01:03 AM UTC

PDB ID : 5GK7 / pdb_00005gk7
Title : Structure of E.Coli fructose 1,6-bisphosphate aldolase bound to Tris
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

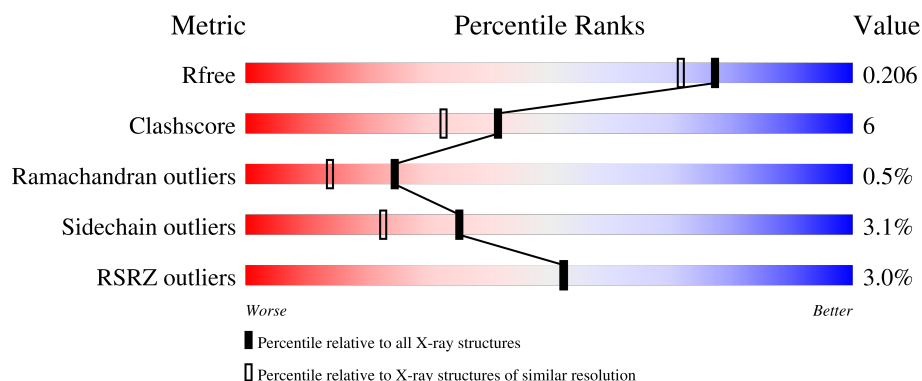
1 Overall quality at a glance

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	TRS	A	402	-	X	-	-
4	PEG	A	403	-	X	X	-

2 Entry composition [i](#)

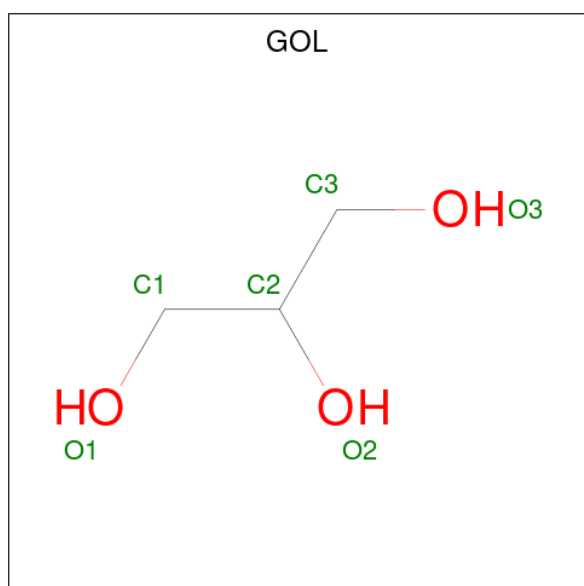
There are 6 unique types of molecules in this entry. The entry contains 5448 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

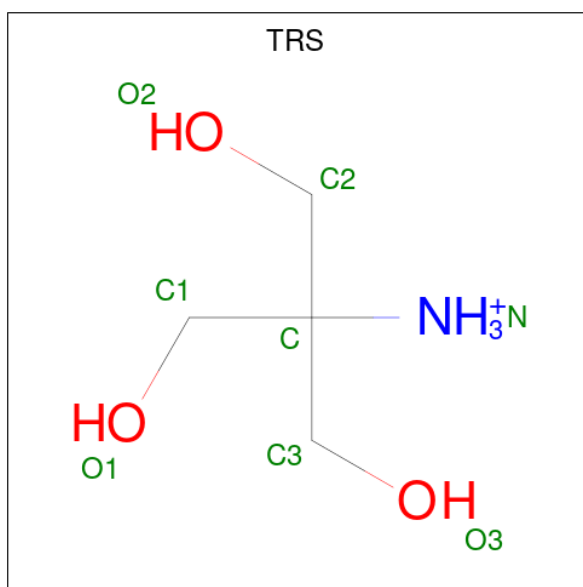
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	333	Total	C	N	O	S	0	0	0
			2566	1632	432	492	10			
1	B	331	Total	C	N	O	S	0	0	0
			2558	1628	430	490	10			

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



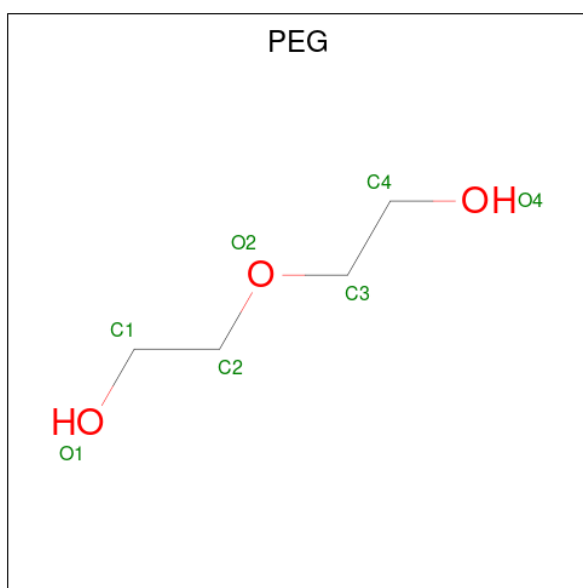
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			8	4	1	3		
3	B	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



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

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

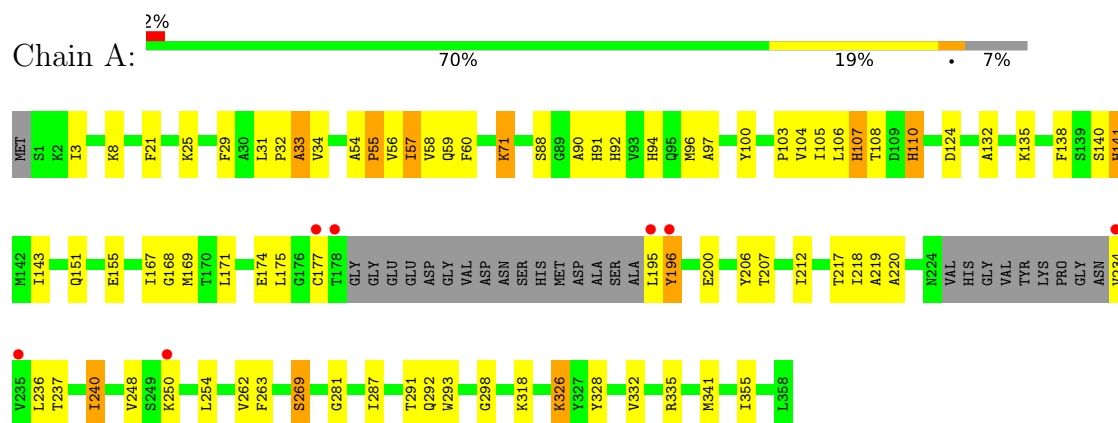
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	137	Total 137	O 137	0	0
6	B	156	Total 156	O 156	0	0

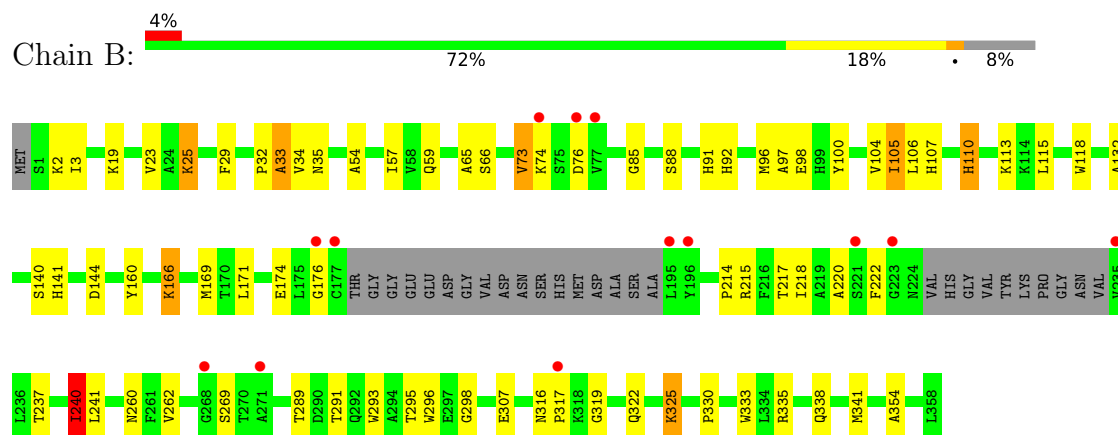
3 Residue-property plots [i](#)

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: 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	72.42Å 72.67Å 73.05Å 90.00° 103.16° 90.00°	Depositor
Resolution (Å)	50.00 – 1.80 50.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	97.4 (50.00-1.80) 97.7 (50.00-1.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.80 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.163 , 0.197 0.177 , 0.206	Depositor DCC
R_{free} test set	3408 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	19.2	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 36.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.015 for l,-k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5448	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.55% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: TRS, 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	1.66	46/2621 (1.8%)	1.20	10/3550 (0.3%)
1	B	1.69	41/2613 (1.6%)	1.21	11/3539 (0.3%)
All	All	1.68	87/5234 (1.7%)	1.21	21/7089 (0.3%)

All (87) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	287	ILE	C-O	8.12	1.32	1.24
1	B	140	SER	C-O	-7.96	1.14	1.23
1	B	33	ALA	C-O	-7.92	1.14	1.23
1	B	215	ARG	C-O	-7.53	1.15	1.23
1	A	143	ILE	C-O	-7.43	1.16	1.24
1	B	106	LEU	C-O	-7.30	1.15	1.24
1	B	35	ASN	C-O	-7.28	1.15	1.23
1	B	3	ILE	C-O	-7.07	1.16	1.24
1	B	218	ILE	C-O	-7.07	1.16	1.24
1	B	217	THR	C-O	-6.73	1.15	1.23
1	A	207	THR	C-O	-6.66	1.16	1.24
1	A	32	PRO	C-O	-6.65	1.16	1.23
1	A	105	ILE	C-O	-6.62	1.16	1.24
1	B	23	VAL	C-O	6.55	1.31	1.24
1	B	298	GLY	C-O	6.53	1.31	1.23
1	A	97	ALA	C-O	-6.50	1.16	1.24
1	B	289	THR	C-O	-6.49	1.16	1.24
1	A	58	VAL	C-O	-6.38	1.16	1.24
1	A	8	LYS	C-O	-6.37	1.17	1.24
1	A	262	VAL	C-O	-6.36	1.17	1.24
1	B	160	TYR	C-O	-6.34	1.16	1.24
1	A	124	ASP	C-O	-6.31	1.16	1.24
1	A	140	SER	C-O	-6.20	1.16	1.23
1	A	3	ILE	C-O	-6.20	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	104	VAL	C-O	-6.07	1.17	1.24
1	A	90	ALA	C-O	6.06	1.31	1.24
1	A	104	VAL	C-O	-6.05	1.17	1.24
1	B	32	PRO	C-O	-6.00	1.17	1.23
1	B	118	TRP	C-O	-5.97	1.17	1.24
1	A	141	HIS	C-O	-5.97	1.16	1.23
1	B	307	GLU	C-O	-5.96	1.17	1.24
1	B	97	ALA	C-O	-5.95	1.17	1.24
1	B	171	LEU	C-O	-5.94	1.16	1.24
1	A	55	PRO	C-O	-5.84	1.16	1.23
1	B	105	ILE	C-O	-5.83	1.17	1.24
1	A	106	LEU	C-O	-5.81	1.17	1.24
1	B	295	THR	C-O	-5.81	1.17	1.24
1	A	21	PHE	C-O	-5.72	1.16	1.24
1	A	219	ALA	C-O	-5.67	1.17	1.23
1	A	29	PHE	C-O	-5.65	1.16	1.23
1	B	354	ALA	CA-C	-5.65	1.47	1.53
1	A	263	PHE	C-O	-5.65	1.17	1.24
1	A	138	PHE	C-O	-5.64	1.17	1.23
1	A	56	VAL	C-O	-5.62	1.16	1.23
1	A	94	HIS	C-O	-5.61	1.17	1.24
1	B	73	VAL	C-O	-5.60	1.16	1.24
1	B	220	ALA	N-CA	5.56	1.52	1.45
1	B	66	SER	C-O	-5.53	1.17	1.24
1	B	293	TRP	C-O	-5.53	1.17	1.24
1	A	318	LYS	N-CA	-5.53	1.39	1.46
1	A	108	THR	C-O	-5.50	1.17	1.24
1	A	220	ALA	C-O	-5.49	1.17	1.23
1	B	29	PHE	C-O	-5.47	1.17	1.23
1	A	57	ILE	C-O	-5.45	1.18	1.24
1	A	328	TYR	C-O	-5.43	1.17	1.24
1	B	98	GLU	C-O	-5.43	1.17	1.24
1	A	298	GLY	C-O	-5.43	1.17	1.23
1	A	206	TYR	C-O	-5.42	1.17	1.24
1	A	217	THR	C-O	-5.39	1.17	1.23
1	B	34	VAL	C-O	-5.39	1.18	1.24
1	A	96	MET	C-O	-5.38	1.17	1.24
1	B	107	HIS	C-O	-5.31	1.17	1.23
1	B	144	ASP	C-O	-5.29	1.17	1.23
1	B	296	TRP	C-O	-5.29	1.18	1.24
1	B	113	LYS	C-O	-5.28	1.18	1.24
1	A	34	VAL	C-O	-5.24	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	214	PRO	C-O	-5.24	1.17	1.24
1	A	293	TRP	C-O	-5.24	1.18	1.24
1	B	100	TYR	C-O	-5.24	1.17	1.24
1	A	33	ALA	C-O	-5.22	1.18	1.24
1	A	167	ILE	C-O	-5.21	1.17	1.24
1	A	31	LEU	C-O	-5.20	1.17	1.24
1	B	54	ALA	C-O	-5.20	1.17	1.24
1	A	168	GLY	C-O	-5.16	1.16	1.23
1	B	222	PHE	C-O	-5.13	1.18	1.23
1	A	281	GLY	C-O	-5.12	1.17	1.24
1	B	262	VAL	C-O	-5.11	1.18	1.24
1	B	59	GLN	C-O	-5.08	1.17	1.23
1	B	240	ILE	C-O	-5.07	1.18	1.24
1	A	60	PHE	C-O	-5.07	1.18	1.24
1	A	335	ARG	C-O	-5.04	1.18	1.24
1	B	2	LYS	C-O	-5.03	1.17	1.23
1	A	100	TYR	C-O	-5.03	1.17	1.24
1	A	355	ILE	C-O	5.03	1.29	1.24
1	B	269	SER	C-O	-5.02	1.17	1.23
1	A	171	LEU	C-O	-5.02	1.18	1.24
1	A	135	LYS	CA-C	5.01	1.57	1.52

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	34	VAL	N-CA-C	7.02	118.00	108.17
1	B	107	HIS	N-CA-CB	-6.78	99.89	111.69
1	A	132	ALA	N-CA-C	6.56	118.51	111.36
1	A	107	HIS	N-CA-CB	-6.50	100.38	111.69
1	B	96	MET	N-CA-C	6.44	121.27	113.41
1	A	34	VAL	N-CA-C	6.16	116.80	108.17
1	A	269	SER	N-CA-C	-6.07	100.40	110.17
1	A	54	ALA	CA-C-N	-5.87	114.71	120.52
1	A	54	ALA	C-N-CA	-5.87	114.71	120.52
1	B	176	GLY	CA-C-N	5.51	131.61	121.70
1	B	176	GLY	C-N-CA	5.51	131.61	121.70
1	B	107	HIS	N-CA-C	5.44	117.45	109.24
1	A	218	ILE	N-CA-C	5.40	115.90	108.12
1	B	54	ALA	CA-C-N	-5.40	115.18	120.52
1	B	54	ALA	C-N-CA	-5.40	115.18	120.52
1	B	218	ILE	N-CA-C	5.38	115.87	108.12
1	B	100	TYR	N-CA-C	-5.33	106.83	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	132	ALA	N-CA-C	5.29	118.19	111.69
1	A	332	VAL	N-CA-C	5.24	115.45	110.53
1	A	54	ALA	N-CA-C	5.17	112.87	108.22
1	A	212	ILE	CB-CA-C	-5.13	105.74	111.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2566	0	2523	33	0
1	B	2558	0	2524	33	0
2	A	6	0	8	0	0
3	A	8	0	9	3	0
3	B	8	0	9	0	0
4	A	7	0	10	13	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	137	0	0	6	0
6	B	156	0	0	5	0
All	All	5448	0	5083	65	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 (65) 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)
3:A:402:TRS:C1	6:A:502:HOH:O	1.92	1.16
1:A:110:HIS:HE1	6:A:501:HOH:O	1.35	1.07
1:A:196:TYR:OH	1:A:234:VAL:HB	1.58	1.03
1:B:110:HIS:HE1	6:B:501:HOH:O	1.42	1.01
4:A:403:PEG:H12	1:B:91:HIS:HB3	1.57	0.87
1:B:174:GLU:OE1	6:B:501:HOH:O	1.98	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:402:TRS:H11	6:A:502:HOH:O	1.65	0.77
1:A:177:CYS:HB3	1:A:195:LEU:O	1.85	0.75
4:A:403:PEG:H32	1:B:91:HIS:HB2	1.68	0.75
1:A:237:THR:HG22	1:A:240:ILE:HD12	1.70	0.72
1:A:177:CYS:CB	1:A:195:LEU:O	2.39	0.70
1:B:338:GLN:NE2	6:B:502:HOH:O	2.25	0.69
1:A:88:SER:OG	4:A:403:PEG:H21	1.94	0.67
1:A:91:HIS:ND1	4:A:403:PEG:O1	2.25	0.67
1:B:73:VAL:O	1:B:74:LYS:HE2	1.93	0.67
1:A:196:TYR:OH	1:A:234:VAL:CB	2.40	0.66
1:A:174:GLU:OE1	6:A:501:HOH:O	2.12	0.66
1:B:73:VAL:C	1:B:74:LYS:HE2	2.22	0.65
4:A:403:PEG:H11	1:B:91:HIS:O	1.96	0.64
1:A:91:HIS:C	4:A:403:PEG:H41	2.23	0.62
1:A:237:THR:CG2	1:A:240:ILE:HD12	2.33	0.59
1:A:196:TYR:HH	1:A:234:VAL:HB	1.63	0.58
1:A:110:HIS:CE1	6:A:501:HOH:O	2.26	0.57
1:A:71:LYS:HE3	1:B:335:ARG:HD3	1.87	0.57
1:A:237:THR:CG2	1:A:240:ILE:CD1	2.82	0.57
3:A:402:TRS:H12	6:A:502:HOH:O	1.83	0.56
4:A:403:PEG:H11	1:B:91:HIS:C	2.30	0.56
1:A:71:LYS:CE	1:B:335:ARG:HD3	2.36	0.55
1:A:92:HIS:N	4:A:403:PEG:H41	2.20	0.55
1:A:141:HIS:CD2	1:A:169:MET:HE1	2.42	0.54
1:A:151:GLN:NE2	1:A:155:GLU:OE2	2.36	0.54
1:B:174:GLU:CD	6:B:501:HOH:O	2.50	0.53
1:B:237:THR:CG2	1:B:240:ILE:HD12	2.40	0.51
1:B:73:VAL:O	1:B:74:LYS:CE	2.58	0.50
1:B:338:GLN:CD	6:B:502:HOH:O	2.54	0.50
1:A:177:CYS:CA	1:A:195:LEU:O	2.59	0.50
1:B:141:HIS:CD2	1:B:169:MET:HE1	2.48	0.49
1:B:316:ASN:HB2	1:B:317:PRO:HD2	1.95	0.48
1:A:55:PRO:HB3	1:A:103:PRO:HG2	1.95	0.48
1:B:25:LYS:HD3	1:B:260:ASN:OD1	2.13	0.48
4:A:403:PEG:H22	1:B:92:HIS:HA	1.96	0.47
1:B:65:ALA:O	1:B:85:GLY:HA3	2.16	0.46
1:B:237:THR:HG22	1:B:240:ILE:HD12	1.97	0.45
1:B:237:THR:HB	1:B:240:ILE:HD12	1.98	0.45
1:B:291:THR:HB	1:B:341:MET:HE3	1.98	0.44
1:A:92:HIS:HA	4:A:403:PEG:H42	1.99	0.44
1:A:326:LYS:H	1:A:326:LYS:CE	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:ILE:HG12	1:B:105:ILE:HB	1.99	0.44
1:A:248:VAL:HG12	1:A:254:LEU:HD12	2.00	0.42
4:A:403:PEG:H22	1:B:92:HIS:CA	2.49	0.42
1:A:92:HIS:HA	4:A:403:PEG:C4	2.48	0.42
4:A:403:PEG:H31	1:B:88:SER:OG	2.19	0.42
1:B:319:GLY:HA3	1:B:322:GLN:HG2	2.02	0.42
1:A:237:THR:HB	1:A:240:ILE:CD1	2.50	0.42
1:A:33:ALA:HA	1:A:57:ILE:HB	2.01	0.42
1:A:71:LYS:HB2	1:A:71:LYS:HE2	1.62	0.42
1:A:177:CYS:HA	1:A:195:LEU:O	2.20	0.41
1:B:166:LYS:HB2	1:B:166:LYS:HE2	1.87	0.41
1:A:59:GLN:HA	1:A:107:HIS:O	2.20	0.41
1:A:292:GLN:OE1	1:B:325:LYS:HE3	2.20	0.41
1:B:33:ALA:HA	1:B:57:ILE:HB	2.02	0.41
1:B:330:PRO:HA	1:B:333:TRP:CE2	2.55	0.41
1:A:71:LYS:HE2	1:B:335:ARG:HD3	2.03	0.41
1:A:291:THR:HB	1:A:341:MET:HE3	2.03	0.40
1:B:316:ASN:HB2	1:B:317:PRO:CD	2.52	0.40

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	327/359 (91%)	319 (98%)	6 (2%)	2 (1%)	21	11
1	B	325/359 (90%)	319 (98%)	5 (2%)	1 (0%)	36	25
All	All	652/718 (91%)	638 (98%)	11 (2%)	3 (0%)	24	14

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	110	HIS
1	A	196	TYR
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	276/297 (93%)	267 (97%)	9 (3%)	33	21
1	B	276/297 (93%)	268 (97%)	8 (3%)	37	25
All	All	552/594 (93%)	535 (97%)	17 (3%)	35	23

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	LYS
1	A	71	LYS
1	A	175	LEU
1	A	200	GLU
1	A	236	LEU
1	A	240	ILE
1	A	250	LYS
1	A	269	SER
1	A	326	LYS
1	B	19	LYS
1	B	25	LYS
1	B	76	ASP
1	B	115	LEU
1	B	166	LYS
1	B	240	ILE
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	322	GLN
1	B	62	ASN
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	A	401	-	5,5,5	0.49	0	5,5,5	1.19	0
4	PEG	A	403	-	6,6,6	0.57	0	5,5,5	2.38	2 (40%)
3	TRS	B	401	5	7,7,7	1.07	0	9,9,9	1.63	1 (11%)
3	TRS	A	402	5	7,7,7	1.48	1 (14%)	9,9,9	1.90	4 (44%)

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	A	401	-	-	2/4/4/4	-
4	PEG	A	403	-	-	4/4/4/4	-
3	TRS	B	401	5	-	2/9/9/9	-
3	TRS	A	402	5	-	5/9/9/9	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	TRS	O1-C1	3.06	1.52	1.42

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	TRS	O3-C3-C	-3.77	100.36	110.88
3	B	401	TRS	O2-C2-C	-3.70	100.56	110.88
4	A	403	PEG	C3-O2-C2	3.23	127.39	113.26
4	A	403	PEG	O2-C2-C1	3.11	123.84	110.11
3	A	402	TRS	O2-C2-C	-2.37	104.26	110.88
3	A	402	TRS	C3-C-N	2.26	113.94	108.17
3	A	402	TRS	C1-C-N	-2.24	102.46	108.17

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	GOL	O1-C1-C2-O2
2	A	401	GOL	O1-C1-C2-C3
4	A	403	PEG	O2-C3-C4-O4
4	A	403	PEG	O1-C1-C2-O2
3	A	402	TRS	N-C-C3-O3
4	A	403	PEG	C1-C2-O2-C3
4	A	403	PEG	C4-C3-O2-C2
3	A	402	TRS	C2-C-C1-O1
3	A	402	TRS	C3-C-C1-O1
3	A	402	TRS	C1-C-C3-O3
3	A	402	TRS	C2-C-C3-O3
3	B	401	TRS	C3-C-C1-O1
3	B	401	TRS	C2-C-C1-O1

There are no ring outliers.

2 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	403	PEG	13	0
3	A	402	TRS	3	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

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	333/359 (92%)	-0.02	7 (2%) 63 64	11, 20, 40, 101	0
1	B	331/359 (92%)	-0.12	13 (3%) 43 43	10, 18, 39, 80	0
All	All	664/718 (92%)	-0.07	20 (3%) 52 52	10, 19, 40, 101	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	195	LEU	9.8
1	A	178	THR	6.2
1	A	235	VAL	6.1
1	A	195	LEU	5.8
1	A	234	VAL	5.1
1	A	196	TYR	4.7
1	B	196	TYR	4.1
1	B	177	CYS	4.0
1	A	177	CYS	3.6
1	B	176	GLY	2.7
1	A	250	LYS	2.7
1	B	74	LYS	2.7
1	B	76	ASP	2.6
1	B	235	VAL	2.6
1	B	271	ALA	2.5
1	B	77	VAL	2.5
1	B	223	GLY	2.4
1	B	268	GLY	2.3
1	B	221	SER	2.1
1	B	317	PRO	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
3	TRS	B	401	8/8	0.83	0.14	18,26,35,38	0
3	TRS	A	402	8/8	0.85	0.14	24,32,37,44	0
4	PEG	A	403	7/7	0.87	0.16	23,24,31,34	0
2	GOL	A	401	6/6	0.90	0.10	27,33,37,40	0
5	ZN	A	404	1/1	1.00	0.02	18,18,18,18	1
5	ZN	B	402	1/1	1.00	0.02	17,17,17,17	1

6.5 Other polymers [i](#)

There are no such residues in this entry.