wwPDB X-ray Structure Validation Summary Report ⓘ

May 16, 2020 – 06:09 pm BST

PDB ID	:	5GK5
Title	:	Apo structure of fructose 1,6-bisphosphate aldolase from Escherichia coli at 1.9 angstrom resolution
Authors	:	Tran, T.H.; Huynh, K.H.; Ho, T.H.; Kang, L.W.
Deposited on	:	2016-07-03
Resolution	:	1.90 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:

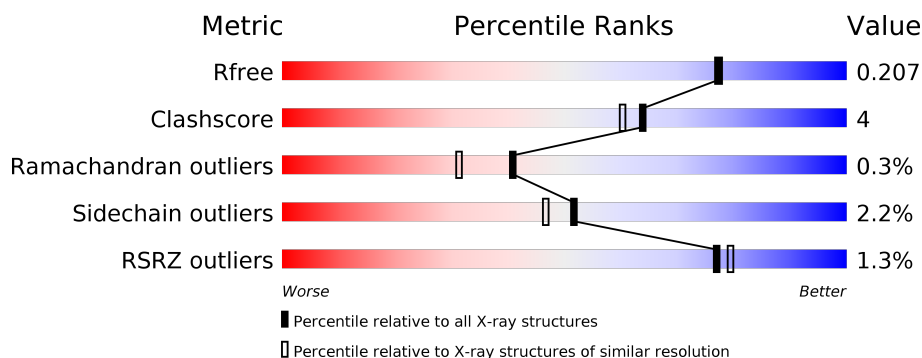|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 1.90 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}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 on 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 <=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	86% ... 7% 8%
1	B	359	86% ... 6% 8%
1	C	359	86% ... 7% 7%
1	D	359	82% ... 9% · 8%
1	E	359	85% ... 8% 7%
1	F	359	85% ... 7% · 8%

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Mol	Chain	Length	Quality of chain
1	G	359	85% 8% 7%
1	H	359	83% 9% 8%

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	402	-	-	X	-
4	PEG	C	402	-	-	X	-
4	PEG	D	402	-	-	X	-
4	PEG	E	402	-	-	X	-
4	PEG	G	402	-	-	X	-
4	PEG	G	403	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 21789 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	332	Total	C	N	O	S	0	0	0
			2568	1635	433	491	9			
1	B	331	Total	C	N	O	S	0	0	0
			2561	1630	432	490	9			
1	C	335	Total	C	N	O	S	0	0	0
			2581	1641	436	494	10			
1	D	331	Total	C	N	O	S	0	0	0
			2561	1630	432	490	9			
1	E	334	Total	C	N	O	S	0	0	0
			2574	1636	435	493	10			
1	F	332	Total	C	N	O	S	0	0	0
			2567	1633	433	491	10			
1	G	335	Total	C	N	O	S	0	0	0
			2581	1641	436	494	10			
1	H	331	Total	C	N	O	S	0	0	0
			2559	1628	432	490	9			

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

GOL

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

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	2	Total 2	Zn 2	0	0
3	D	2	Total 2	Zn 2	0	0
3	E	2	Total 2	Zn 2	0	0
3	H	2	Total 2	Zn 2	0	0
3	B	1	Total 1	Zn 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	2	Total 2	Zn 2	0	0
3	A	2	Total 2	Zn 2	0	0
3	F	1	Total 1	Zn 1	0	0

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	136	Total 136	O 136	0	0
5	B	167	Total 167	O 167	0	0
5	C	128	Total 128	O 128	0	0
5	D	156	Total 156	O 156	0	0
5	E	129	Total 129	O 129	0	0
5	F	150	Total 150	O 150	0	0
5	G	130	Total 130	O 130	0	0
5	H	143	Total 143	O 143	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA 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 crit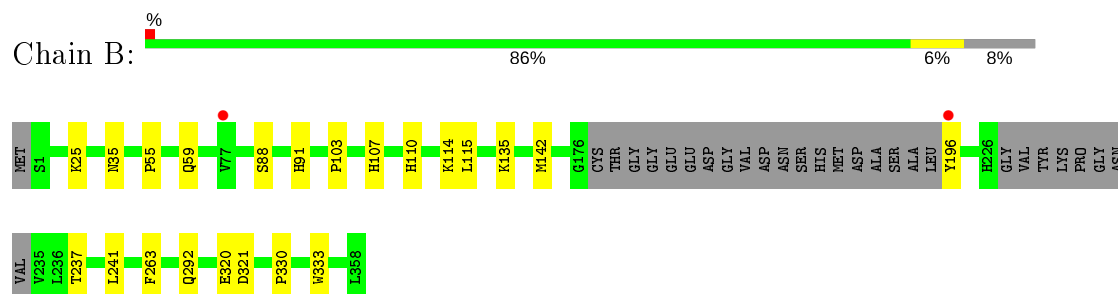eria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.
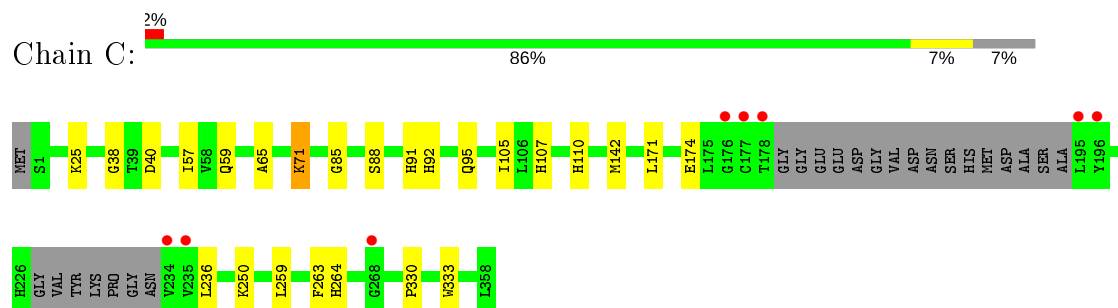
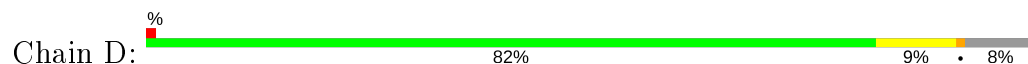- Molecule 1: Fructose-bisphosphate aldolase class 2

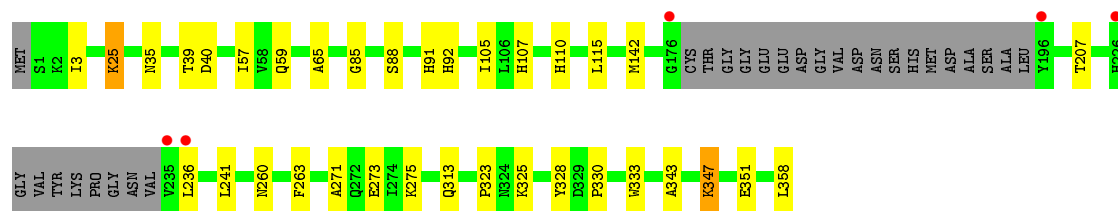- Molecule 1: Fructose-bisphosphate aldolase class 2

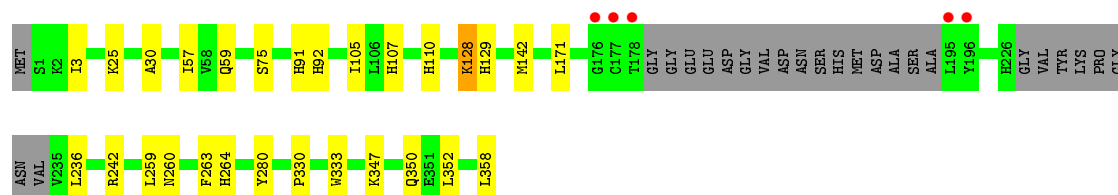- Molecule 1: Fructose-bisphosphate aldolase class 2

- Molecule 1: Fructose-bisphosphate aldolase class 2

MET S1 K2 I3 K25 N35 T39 D40 I57 V58 Q59 A65 G85 S88 H91 H92 I105 L106 H107 H110 L115 M142 G176 CYS THR GLY GLY GLU ASP GLY VAL ASP ASN SER HIS MET ASP ALA SER ALA LEU Y196 T207 H226

GLY VAL TYR LYS PRO GLY ASN VAL V235 L236 L241 N260 F263 A271 Q272 E273 I274 K275 Q313 P323 N324 K325 Y328 D329 P330 W333 A343 K347 E351 L358

• Molecule 1: Fructose-bisphosphate aldolase class 2

Chain E:

85%   8%   7%

MET S1 K2 I3 K25 A30 I57 V58 Q59 S75 H91 H92 I105 L106 H107 H110 K128 H129 M142 L171 G176 C177 T178 GLY GLU ASP GLY VAL ASP ASN SER HIS MET ASP ALA SER ALA L195 Y196 H226 GLY VAL TYR LYS PRO GLY

ASN VAL V235 L236 R242 L259 N260 F263 H264 Y280 P330 W333 K347 Q350 E351 L352 L358

• Molecule 1: Fructose-bisphosphate aldolase class 2

Chain F: 85%   7% • 8%

MET S1 K25 P55 V56 I57 S88 H92 P103 V104 I105 H110 K114 L115 I119 K135 M142 I143 C177 THR GLY GLY GLU GLU ASP GLY VAL ASP ASN SER HIS MET ASP ALA SER ALA LEU Y196 H226 GLY VAL TYR LYS PRO GLY ASN VAL V235

L241 E246 K250 F263 A271 K275 E320 K325 Y328 D329 P330 W333 K347 E351 L358

• Molecule 1: Fructose-bisphosphate aldolase class 2

Chain G:

85%   8% • 7%

MET S1 G38 T39 P55 V56 I57 K71 H91 H92 V93 H94 P103 V104 I105 H110 D124 K128 K135 P136 M142 Q151 L171 E174 I175 G176 C177 T178 GLY GLY GLU GLU ASP GLY VAL ASP ASN SER HIS MET ASP ALA SER ALA L195 Y196 H226

H226 GLY VAL TYR LYS PRO GLY ASN V234 V235 Y247 K250 L259 F263 H264 I274 M285 P330 W333 L352 L358

• Molecule 1: Fructose-bisphosphate aldolase class 2

Chain H:

2%   83%   9%   8%

MET S1 K2 I3 T13 K25 D40 A65 K74 G85 S88 H91 H92 H110 C111 A112 K113 K114 L115 L123 G134 K135 M142 I143 D144 L145 G176 CYS THR GLY GLY GLU ASP GLY VAL ASP ASN SER HIS MET ASP ALA SER ALA LEU Y196

H226 GLY VAL TYR LYS PRO GLY ASN VAL V235 L241 N260 F263 G268 S269 T270 E273 Q313 D321 Q322 P323 N324 K325 Y328 D329 P330 W333 L358

4　Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	72.83Å　90.53Å　113.73Å 90.07°　90.01°　90.21°	Depositor
Resolution (Å)	22.05　–　1.90 22.05　–　1.90	Depositor EDS
% Data completeness (in resolution range)	95.6 (22.05-1.90) 95.4 (22.05-1.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.28 (at 1.90Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.172　,　0.207 0.172　,　0.207	Depositor DCC
R_{free} test set	10968 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	22.4	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 27.4	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.170 for h,-k,-l 0.170 for -h,k,-l 0.460 for -h,-k,l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	21789	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 3.84% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: 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	0.38	0/2624	0.53	0/3555
1	B	0.42	0/2617	0.52	0/3545
1	C	0.39	1/2637 (0.0%)	0.55	1/3572 (0.0%)
1	D	0.39	0/2617	0.54	0/3545
1	E	0.38	0/2630	0.54	0/3562
1	F	0.45	2/2623 (0.1%)	0.54	0/3553
1	G	0.38	0/2637	0.53	0/3572
1	H	0.42	0/2615	0.55	0/3542
All	All	0.40	3/21000 (0.0%)	0.54	1/28446 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	320	GLU	CD-OE1	-7.41	1.17	1.25
1	F	320	GLU	CD-OE2	-6.12	1.19	1.25
1	C	174	GLU	CD-OE1	-5.57	1.19	1.25

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	174	GLU	OE1-CD-OE2	-5.40	116.82	123.30

There are no chirality outliers.

There are no planarity outliers.

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	2568	0	2533	24	0
1	B	2561	0	2524	12	0
1	C	2581	0	2534	15	0
1	D	2561	0	2524	29	0
1	E	2574	0	2525	20	0
1	F	2567	0	2529	18	0
1	G	2581	0	2534	25	0
1	H	2559	0	2517	25	0
2	A	6	0	8	0	0
2	B	6	0	8	1	0
2	C	6	0	8	0	0
2	D	6	0	8	0	0
2	E	6	0	8	0	0
2	G	6	0	8	0	0
2	H	6	0	8	0	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	1	0	0	0	0
3	G	2	0	0	0	0
3	H	2	0	0	0	0
4	B	7	0	10	8	0
4	C	7	0	10	9	0
4	D	7	0	10	11	0
4	E	7	0	10	9	0
4	G	14	0	20	10	0
5	A	136	0	0	2	0
5	B	167	0	0	3	0
5	C	128	0	0	2	1
5	D	156	0	0	11	1
5	E	129	0	0	1	0
5	F	150	0	0	1	2
5	G	130	0	0	6	0
5	H	143	0	0	7	0
All	All	21789	0	20336	173	2

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 4.

The worst 5 of 173 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)
4:G:403:PEG:H11	1:H:88:SER:HA	1.39	1.04
1:D:88:SER:HA	4:D:402:PEG:H11	1.47	0.96
1:D:347:LYS:NZ	5:D:501:HOH:O	1.98	0.95
1:G:136:PRO:O	5:G:501:HOH:O	1.85	0.94
4:E:402:PEG:H11	1:F:88:SER:HA	1.54	0.89

All (2) 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)
5:D:639:HOH:O	5:F:522:HOH:O[1_465]	1.97	0.23
5:C:1314:HOH:O	5:F:511:HOH:O[1_565]	2.06	0.14

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	326/359 (91%)	318 (98%)	7 (2%)	1 (0%)	41	31
1	B	325/359 (90%)	317 (98%)	7 (2%)	1 (0%)	41	31
1	C	329/359 (92%)	323 (98%)	5 (2%)	1 (0%)	41	31
1	D	325/359 (90%)	318 (98%)	6 (2%)	1 (0%)	41	31
1	E	328/359 (91%)	320 (98%)	7 (2%)	1 (0%)	41	31
1	F	326/359 (91%)	318 (98%)	7 (2%)	1 (0%)	41	31
1	G	329/359 (92%)	322 (98%)	6 (2%)	1 (0%)	41	31
1	H	325/359 (90%)	318 (98%)	6 (2%)	1 (0%)	41	31
All	All	2613/2872 (91%)	2554 (98%)	51 (2%)	8 (0%)	41	31

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	110	HIS
1	C	110	HIS
1	E	110	HIS
1	H	110	HIS
1	A	110	HIS

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	277/297 (93%)	272 (98%)	5 (2%)	59	55
1	B	276/297 (93%)	271 (98%)	5 (2%)	59	55
1	C	277/297 (93%)	270 (98%)	7 (2%)	47	41
1	D	276/297 (93%)	270 (98%)	6 (2%)	52	47
1	E	276/297 (93%)	271 (98%)	5 (2%)	59	55
1	F	277/297 (93%)	269 (97%)	8 (3%)	42	35
1	G	277/297 (93%)	270 (98%)	7 (2%)	47	41
1	H	275/297 (93%)	270 (98%)	5 (2%)	59	55
All	All	2211/2376 (93%)	2163 (98%)	48 (2%)	52	47

5 of 48 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	263	PHE
1	E	259	LEU
1	H	142	MET
1	D	347	LYS
1	E	171	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	129	HIS

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Mol	Chain	Res	Type
1	H	272	GLN
1	E	264	HIS
1	D	272	GLN
1	G	264	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 27 ligands modelled in this entry, 14 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	#$|Z| > 2$
4	PEG	G	403	-	6,6,6	0.51	0	5,5,5	1.27	1 (20%)
2	GOL	D	401	-	5,5,5	0.40	0	5,5,5	0.49	0
2	GOL	G	401	-	5,5,5	0.38	0	5,5,5	0.31	0
2	GOL	B	401	-	5,5,5	0.39	0	5,5,5	0.82	0
2	GOL	E	401	-	5,5,5	0.36	0	5,5,5	0.38	0
2	GOL	C	401	-	5,5,5	0.38	0	5,5,5	0.47	0
2	GOL	A	401	-	5,5,5	0.40	0	5,5,5	0.17	0
4	PEG	B	402	-	6,6,6	0.55	0	5,5,5	0.96	0
2	GOL	H	401	-	5,5,5	0.38	0	5,5,5	0.23	0
4	PEG	G	402	-	6,6,6	0.56	0	5,5,5	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
4	PEG	D	402	-	6,6,6	0.51	0	5,5,5	1.13	0
4	PEG	E	402	-	6,6,6	0.48	0	5,5,5	1.27	1 (20%)
4	PEG	C	402	-	6,6,6	0.46	0	5,5,5	0.71	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
4	PEG	G	403	-	-	2/4/4/4	-
2	GOL	D	401	-	-	0/4/4/4	-
2	GOL	G	401	-	-	2/4/4/4	-
2	GOL	B	401	-	-	4/4/4/4	-
2	GOL	E	401	-	-	2/4/4/4	-
2	GOL	C	401	-	-	0/4/4/4	-
2	GOL	A	401	-	-	2/4/4/4	-
4	PEG	B	402	-	-	4/4/4/4	-
2	GOL	H	401	-	-	2/4/4/4	-
4	PEG	G	402	-	-	3/4/4/4	-
4	PEG	D	402	-	-	1/4/4/4	-
4	PEG	E	402	-	-	3/4/4/4	-
4	PEG	C	402	-	-	2/4/4/4	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	G	403	PEG	O2-C2-C1	2.15	119.51	110.07
4	E	402	PEG	O2-C2-C1	2.01	118.91	110.07

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	401	GOL	O1-C1-C2-C3
2	B	401	GOL	O1-C1-C2-C3
2	B	401	GOL	C1-C2-C3-O3
2	A	401	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
2	A	401	GOL	O1-C1-C2-C3

There are no ring outliers.

7 monomers are involved in 48 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	403	PEG	6	0
2	B	401	GOL	1	0
4	B	402	PEG	8	0
4	G	402	PEG	4	0
4	D	402	PEG	11	0
4	E	402	PEG	9	0
4	C	402	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 ⓘ

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	332/359 (92%)	-0.06	3 (0%)	84	85	13, 21, 40, 75	0
1	B	331/359 (92%)	-0.13	2 (0%)	89	90	13, 19, 37, 59	0
1	C	335/359 (93%)	0.05	8 (2%)	59	62	15, 23, 42, 80	0
1	D	331/359 (92%)	-0.09	5 (1%)	73	76	12, 21, 42, 64	0
1	E	334/359 (93%)	-0.07	5 (1%)	73	76	14, 22, 41, 78	0
1	F	332/359 (92%)	-0.11	1 (0%)	94	94	13, 19, 38, 63	0
1	G	335/359 (93%)	0.01	5 (1%)	73	76	15, 23, 43, 76	0
1	H	331/359 (92%)	-0.06	6 (1%)	68	71	12, 21, 41, 59	0
All	All	2661/2872 (92%)	-0.06	35 (1%)	77	79	12, 21, 41, 80	0

The worst 5 of 35 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	178	THR	9.2
1	C	195	LEU	9.1
1	C	234	VAL	7.3
1	A	234	VAL	7.2
1	A	196	TYR	6.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates 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	D	402	7/7	0.77	0.36	25,27,32,35	0
2	GOL	B	401	6/6	0.81	0.22	30,36,42,43	0
4	PEG	G	403	7/7	0.82	0.29	26,31,33,35	0
4	PEG	C	402	7/7	0.82	0.34	28,32,38,39	0
4	PEG	B	402	7/7	0.84	0.28	23,24,35,36	0
4	PEG	E	402	7/7	0.84	0.48	25,30,33,40	0
4	PEG	G	402	7/7	0.85	0.26	27,36,41,41	0
2	GOL	D	401	6/6	0.89	0.28	30,37,41,49	0
2	GOL	G	401	6/6	0.91	0.18	28,34,38,40	0
2	GOL	H	401	6/6	0.92	0.13	35,48,55,55	0
2	GOL	E	401	6/6	0.92	0.13	24,30,35,35	0
2	GOL	C	401	6/6	0.94	0.11	27,34,36,37	0
2	GOL	A	401	6/6	0.94	0.22	22,28,33,34	0
3	ZN	A	403	1/1	0.97	0.07	34,34,34,34	1
3	ZN	C	403	1/1	0.98	0.05	27,27,27,27	1
3	ZN	E	404	1/1	0.98	0.10	33,33,33,33	1
3	ZN	D	404	1/1	0.98	0.04	35,35,35,35	1
3	ZN	B	403	1/1	0.99	0.09	22,22,22,22	1
3	ZN	D	403	1/1	0.99	0.06	26,26,26,26	1
3	ZN	H	402	1/1	0.99	0.08	26,26,26,26	1
3	ZN	G	404	1/1	0.99	0.07	28,28,28,28	1
3	ZN	G	405	1/1	0.99	0.06	33,33,33,33	1
3	ZN	C	404	1/1	0.99	0.05	33,33,33,33	1
3	ZN	H	403	1/1	0.99	0.05	33,33,33,33	1
3	ZN	E	403	1/1	0.99	0.04	26,26,26,26	1
3	ZN	F	401	1/1	1.00	0.05	22,22,22,22	1
3	ZN	A	402	1/1	1.00	0.09	26,26,26,26	1

6.5 Other polymers (i)

There are no such residues in this entry.