WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Dec 14, 2024 – 09:52 PM EST

PDB ID	:	5PGM
Title	:	SACCHAROMYCES CEREVISIAE PHOSPHOGLYCERATE MUTASE
Authors	:	Rigden, D.J.; Phillips, S.E.V.; Fothergill-Gilmore, L.A.
Deposited on	:	1998-08-19
Resolution	:	2.12 Å(reported)

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

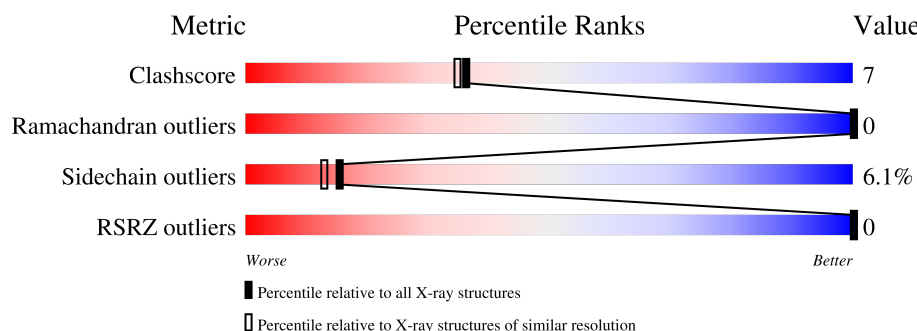|		
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 2.12 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	Percentile Ranks	Value
Clashscore		7
Ramachandran outliers		0
Sidechain outliers		6.1%
RSRZ outliers		0

Worse   *Better*

▌ Percentile relative to all X-ray structures

❙ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	180529	8431 (2.14-2.10)
Ramachandran outliers	177936	8366 (2.14-2.10)
Sidechain outliers	177891	8367 (2.14-2.10)
RSRZ outliers	164620	7689 (2.14-2.10)

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 <=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	246	76% 17% • 5%
1	B	246	78% 15% • •
1	C	246	75% 17% • •
1	D	246	74% 20% • •
1	E	246	73% 20% • 5%
1	F	246	75% 17% • •

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Mol	Chain	Length	Quality of chain
1	G	246	76% 17% 5%
1	H	246	78% 15%

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 16692 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 PHOSPHOGLYCERATE MUTASE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	235	Total	C	N	O	S	0	0	0
			1873	1199	323	350	1			
1	C	235	Total	C	N	O	S	0	0	0
			1873	1199	323	350	1			
1	A	234	Total	C	N	O	S	0	0	0
			1868	1196	322	349	1			
1	B	235	Total	C	N	O	S	0	0	0
			1873	1199	323	350	1			
1	E	234	Total	C	N	O	S	0	0	0
			1868	1196	322	349	1			
1	F	235	Total	C	N	O	S	0	0	0
			1873	1199	323	350	1			
1	G	234	Total	C	N	O	S	0	0	0
			1868	1196	322	349	1			
1	H	235	Total	C	N	O	S	0	0	0
			1873	1199	323	350	1			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

SO4

O1

O

O3 O⁻ — S — O⁻ O4

S

O

O2

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total 5	O 4	S 1	0	0
2	D	1	Total 5	O 4	S 1	0	0
2	C	1	Total 5	O 4	S 1	0	0
2	C	1	Total 5	O 4	S 1	0	0
2	A	1	Total 5	O 4	S 1	0	0
2	A	1	Total 5	O 4	S 1	0	0
2	B	1	Total 5	O 4	S 1	0	0
2	B	1	Total 5	O 4	S 1	0	0
2	E	1	Total 5	O 4	S 1	0	0
2	E	1	Total 5	O 4	S 1	0	0
2	F	1	Total 5	O 4	S 1	0	0
2	F	1	Total 5	O 4	S 1	0	0
2	G	1	Total 5	O 4	S 1	0	0
2	G	1	Total 5	O 4	S 1	0	0

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W O R L D W I D E
PDB
PROTEIN DATA BANK

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	H	1	Total 5	O 4	S 1	0	0
2	H	1	Total 5	O 4	S 1	0	0

- Molecule 3 is ALANINE (three-letter code: ALA) (formula: $C_3H_7NO_2$).
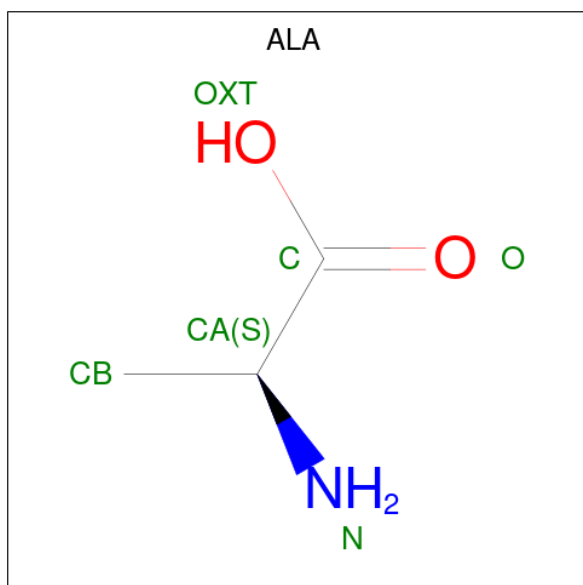
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	E	1	Total 5	C 3	N 1	O 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	201	Total 201	O 201	0	0
4	C	185	Total 185	O 185	0	0
4	A	223	Total 223	O 223	0	0
4	B	211	Total 211	O 211	0	0
4	E	201	Total 201	O 201	0	0
4	F	185	Total 185	O 185	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	221	Total O 221 221		0	0
4	H	211	Total O 211 211		0	0

3 Residue-property plots ⓘ

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.
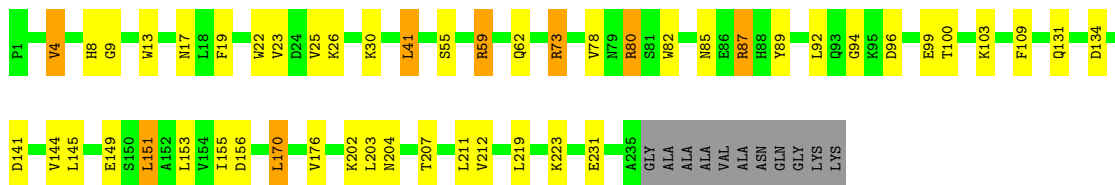
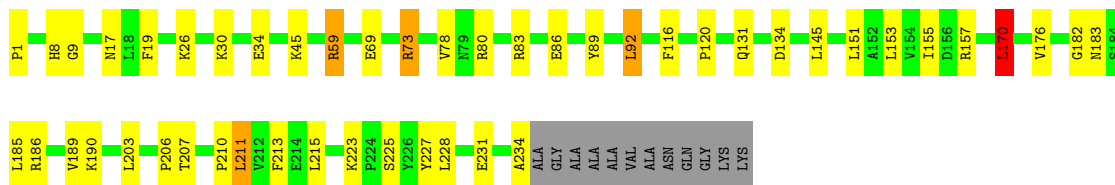- Molecule 1: PHOSPHOGLYCERATE MUTASE 1

Chain D:
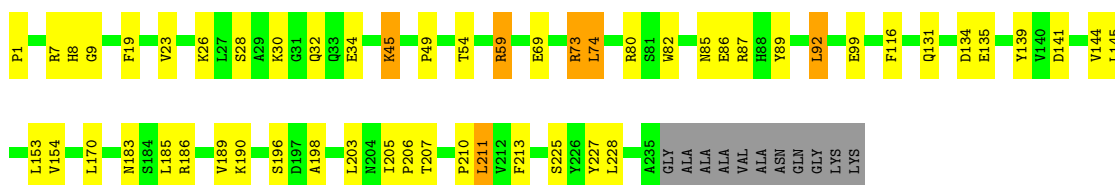
- Molecule 1: PHOSPHOGLYCERATE MUTASE 1

Chain C:

- Molecule 1: PHOSPHOGLYCERATE MUTASE 1

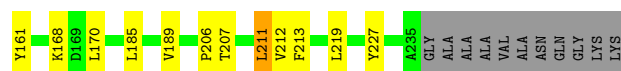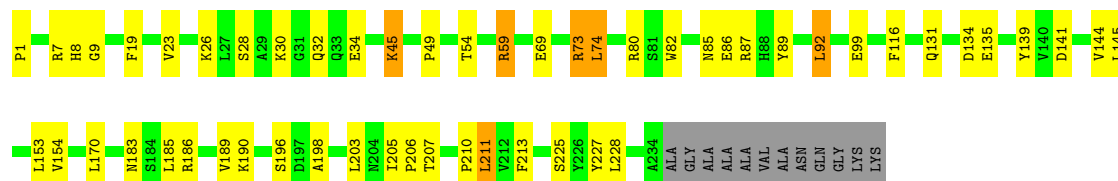Chain A:

- Molecule 1: PHOSPHOGLYCERATE MUTASE 1

Chain B:

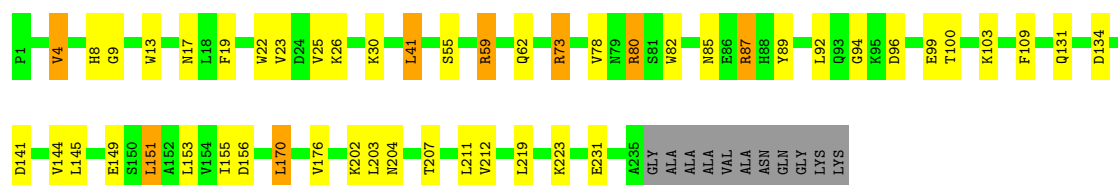Y161 K168 D169 L170 L185 V189 P206 T207 L211 V212 F213 L219 Y227 A235 GLY ALA ALA VAL ALA ASN GLN GLY LYS LYS

- Molecule 1: PHOSPHOGLYCERATE MUTASE 1

Chain E:

73%   20%   •   5%

P1 R7 H8 G9 F19 V23 K26 L27 S28 A29 K30 G31 Q32 Q33 E34 K45 P49 T54 R59 E69 R73 L74 R80 S81 W82 N85 E86 R87 H88 Y89 L92 E99 F116 Q131 D134 E135 Y139 V140 D141 V144 L145

L153 V154 L170 N183 S184 L185 R186 V189 K190 S196 D197 A198 L203 N204 I205 P206 T207 P210 L211 V212 F213 S225 Y226 Y227 L228 A234 ALA GLY ALA ALA VAL ALA ASN GLN GLY LYS LYS

- Molecule 1: PHOSPHOGLYCERATE MUTASE 1

Chain F:

75%   17%   •   •

P1 V4 H8 G9 W13 N17 L18 F19 W22 V23 D24 V25 K26 K30 L41 S55 R59 Q62 R73 V78 N79 R80 S81 W82 N85 E86 R87 H88 Y89 L92 Q93 G94 K95 D96 E99 T100 K103 F109 Q131 D134

D141 V144 L145 E149 S150 L151 A152 L153 V154 I155 D156 L170 V176 K202 L203 N204 T207 L211 V212 L219 K223 E231 A235 GLY ALA ALA ALA VAL ALA ASN GLN GLY LYS LYS

- Molecule 1: PHOSPHOGLYCERATE MUTASE 1

Chain G:

76%   17%   •   5%

P1 H8 G9 N17 L18 F19 K26 K30 E34 K45 R59 E69 R73 V78 N79 R80 R83 E86 Y89 L92 F116 P120 Q131 D134 L145 L151 A152 L153 V154 I155 D156 R157 L170 V176 G182 N183 S184

L185 R186 V189 K190 L203 P206 T207 P210 L211 V212 F213 E214 L215 K223 P224 S225 Y226 Y227 L228 E231 A234 ALA GLY ALA ALA VAL ALA ASN GLN GLY LYS LYS

- Molecule 1: PHOSPHOGLYCERATE MUTASE 1

Chain H:

78%   15%   •   •

P1 V4 R7 H8 G9 Q10 N14 E15 K16 N17 L18 F19 V23 K26 K30 E34 A35 A36 E40 L41 R59 R73 V78 N79 R80 R83 Y89 L92 F104 K108 P122 D134 E135 L145 T148 L151 A152 L153

Y161 K168 D169 L170 L185 V189 P206 T207 L211 V212 F213 L219 Y227 A235 GLY ALA ALA VAL ALA ASN GLN GLY LYS LYS

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	82.50Å 93.26Å 147.33Å 90.00° 90.15° 90.00°	Depositor
Resolution (Å)	30.00 – 2.12 30.00 – 2.12	Depositor EDS
% Data completeness (in resolution range)	89.5 (30.00-2.12) 89.6 (30.00-2.12)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$	-	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.196 , 0.228 0.200 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	19.2	Xtriage
Anisotropy	0.557	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 22.5	EDS
L-test for twinning[1]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.459 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	16692	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 3.59% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.76	0/1912	0.90	3/2592 (0.1%)
1	B	0.75	0/1917	0.97	6/2599 (0.2%)
1	C	0.71	0/1917	0.91	6/2599 (0.2%)
1	D	0.73	0/1917	0.90	4/2599 (0.2%)
1	E	0.73	0/1912	0.90	4/2592 (0.2%)
1	F	0.71	0/1917	0.91	6/2599 (0.2%)
1	G	0.76	0/1912	0.90	3/2592 (0.1%)
1	H	0.75	0/1917	0.97	6/2599 (0.2%)
All	All	0.74	0/15321	0.92	38/20771 (0.2%)

There are no bond length outliers.

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	80	ARG	NE-CZ-NH2	-12.38	114.11	120.30
1	H	80	ARG	NE-CZ-NH2	-12.33	114.14	120.30
1	B	80	ARG	NE-CZ-NH1	8.84	124.72	120.30
1	H	80	ARG	NE-CZ-NH1	8.75	124.67	120.30
1	E	73	ARG	NE-CZ-NH2	-8.59	116.01	120.30

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	1868	0	1889	29	0
1	B	1873	0	1894	25	0
1	C	1873	0	1894	27	0
1	D	1873	0	1894	34	0
1	E	1868	0	1889	34	0
1	F	1873	0	1894	27	0
1	G	1868	0	1889	29	0
1	H	1873	0	1894	25	0
2	A	10	0	0	0	0
2	B	10	0	0	0	0
2	C	10	0	0	0	0
2	D	10	0	0	0	0
2	E	10	0	0	0	0
2	F	10	0	0	0	0
2	G	10	0	0	0	0
2	H	10	0	0	0	0
3	E	5	0	4	0	0
4	A	223	0	0	4	1
4	B	211	0	0	2	3
4	C	185	0	0	2	2
4	D	201	0	0	2	0
4	E	201	0	0	2	0
4	F	185	0	0	2	2
4	G	221	0	0	4	1
4	H	211	0	0	2	3
All	All	16692	0	15141	215	6

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 7.

The worst 5 of 215 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:234:ALA:O	1:G:234:ALA:O	2.01	0.79
1:G:231:GLU:HG2	4:G:773:HOH:O	1.82	0.79
1:A:231:GLU:HG2	4:A:610:HOH:O	1.82	0.79
1:H:10:GLN:NE2	1:H:15:GLU:HG2	2.00	0.76
1:B:10:GLN:NE2	1:B:15:GLU:HG2	2.00	0.76

The worst 5 of 6 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)
4:F:681:HOH:O	4:H:510:HOH:O[1_655]	1.68	0.52
4:C:681:HOH:O	4:B:510:HOH:O[1_655]	1.88	0.32
4:A:585:HOH:O	4:H:594:HOH:O[2_555]	1.95	0.25
4:F:687:HOH:O	4:H:593:HOH:O[1_655]	2.04	0.16
4:C:687:HOH:O	4:B:593:HOH:O[1_655]	2.07	0.13

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	232/246 (94%)	228 (98%)	4 (2%)	0	100	100
1	B	233/246 (95%)	229 (98%)	4 (2%)	0	100	100
1	C	233/246 (95%)	226 (97%)	7 (3%)	0	100	100
1	D	233/246 (95%)	224 (96%)	9 (4%)	0	100	100
1	E	232/246 (94%)	223 (96%)	9 (4%)	0	100	100
1	F	233/246 (95%)	226 (97%)	7 (3%)	0	100	100
1	G	232/246 (94%)	228 (98%)	4 (2%)	0	100	100
1	H	233/246 (95%)	229 (98%)	4 (2%)	0	100	100
All	All	1861/1968 (95%)	1813 (97%)	48 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	202/207 (98%)	193 (96%)	9 (4%)	23	22
1	B	202/207 (98%)	188 (93%)	14 (7%)	13	10
1	C	202/207 (98%)	186 (92%)	16 (8%)	10	7
1	D	202/207 (98%)	192 (95%)	10 (5%)	20	19
1	E	202/207 (98%)	192 (95%)	10 (5%)	20	19
1	F	202/207 (98%)	186 (92%)	16 (8%)	10	7
1	G	202/207 (98%)	193 (96%)	9 (4%)	23	22
1	H	202/207 (98%)	188 (93%)	14 (7%)	13	10
All	All	1616/1656 (98%)	1518 (94%)	98 (6%)	15	13

5 of 98 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	170	LEU
1	F	202	LYS
1	F	4	VAL
1	F	87	ARG
1	G	17	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	65	ASN
1	G	10	GLN
1	F	65	ASN
1	G	17	ASN
1	A	17	ASN

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 ⓘ

17 ligands are modelled in this entry.

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	SO4	C	301	-	4,4,4	0.48	0	6,6,6	0.26	0
2	SO4	E	301	-	4,4,4	0.51	0	6,6,6	0.18	0
2	SO4	F	301	-	4,4,4	0.48	0	6,6,6	0.26	0
2	SO4	G	300	-	4,4,4	0.30	0	6,6,6	0.89	0
2	SO4	A	300	-	4,4,4	0.30	0	6,6,6	0.89	0
2	SO4	G	301	-	4,4,4	0.44	0	6,6,6	0.50	0
2	SO4	H	300	-	4,4,4	0.30	0	6,6,6	0.62	0
2	SO4	D	301	-	4,4,4	0.51	0	6,6,6	0.18	0
2	SO4	B	300	-	4,4,4	0.30	0	6,6,6	0.62	0
2	SO4	B	301	-	4,4,4	0.39	0	6,6,6	0.31	0
2	SO4	E	300	-	4,4,4	0.37	0	6,6,6	0.28	0
3	ALA	E	302	-	3,4,5	0.87	0	2,4,6	1.71	<mark>1 (50%)</mark>
2	SO4	D	300	-	4,4,4	0.37	0	6,6,6	0.28	0
2	SO4	C	300	-	4,4,4	0.35	0	6,6,6	0.65	0
2	SO4	A	301	-	4,4,4	0.44	0	6,6,6	0.50	0
2	SO4	F	300	-	4,4,4	0.34	0	6,6,6	0.65	0
2	SO4	H	301	-	4,4,4	0.39	0	6,6,6	0.32	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	ALA	E	302	-	-	0/1/2/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	302	ALA	O-C-CA	-2.42	116.49	124.23

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	234/246 (95%)	-1.87	0	100	100	4, 15, 44, 90	0
1	B	235/246 (95%)	-1.82	0	100	100	6, 18, 43, 79	0
1	C	235/246 (95%)	-1.76	0	100	100	8, 22, 57, 86	0
1	D	235/246 (95%)	-1.78	0	100	100	8, 19, 51, 92	0
1	E	234/246 (95%)	-1.78	0	100	100	8, 19, 51, 92	0
1	F	235/246 (95%)	-1.75	0	100	100	8, 22, 57, 86	0
1	G	234/246 (95%)	-1.87	0	100	100	4, 15, 44, 90	0
1	H	235/246 (95%)	-1.81	0	100	100	6, 18, 43, 79	0
All	All	1877/1968 (95%)	-1.81	0	100	100	4, 19, 50, 92	0

There are no RSRZ outliers to report.

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 monosaccharides in this entry.

6.4 Ligands ⓘ

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
3	ALA	E	302	5/6	0.95	0.06	74,82,88,91	0
2	SO4	F	301	5/5	0.97	0.08	89,91,95,98	0
2	SO4	C	301	5/5	0.97	0.09	89,91,95,98	0
2	SO4	E	301	5/5	0.98	0.07	75,83,86,87	0
2	SO4	B	301	5/5	0.99	0.04	51,53,56,60	0
2	SO4	H	301	5/5	0.99	0.04	51,53,56,60	0
2	SO4	D	301	5/5	0.99	0.06	75,83,86,87	0
2	SO4	C	300	5/5	1.00	0.01	24,29,34,35	0
2	SO4	E	300	5/5	1.00	0.04	38,42,47,48	0
2	SO4	D	300	5/5	1.00	0.04	38,42,47,48	0
2	SO4	F	300	5/5	1.00	0.02	24,29,34,35	0
2	SO4	A	300	5/5	1.00	0.02	24,28,33,35	0
2	SO4	G	300	5/5	1.00	0.02	24,28,33,35	0
2	SO4	G	301	5/5	1.00	0.02	25,33,36,37	0
2	SO4	H	300	5/5	1.00	0.02	17,22,27,28	0
2	SO4	A	301	5/5	1.00	0.02	25,33,36,37	0
2	SO4	B	300	5/5	1.00	0.01	17,22,27,28	0

6.5 Other polymers (i)

There are no such residues in this entry.