



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:58 AM GMT

PDB ID : 3CWC  
Title : Crystal structure of putative glycerate kinase 2 from Salmonella typhimurium LT2  
Authors : Osipiuk, J.; Zhou, M.; Holzle, D.; Anderson, W.; Joachimiak, A.; Center for Structural Genomics of Infectious Diseases (CSGID)  
Deposited on : 2008-04-21  
Resolution : 2.23 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

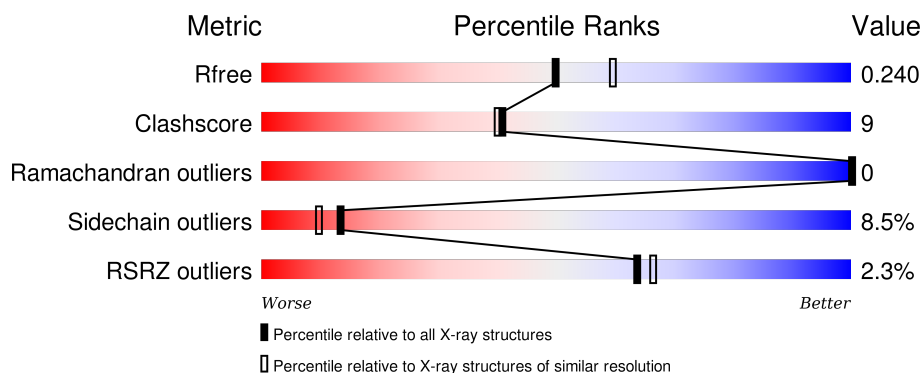
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

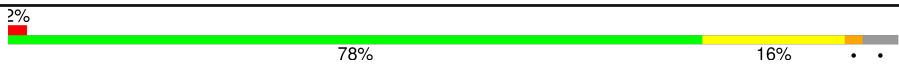

The reported resolution of this entry is 2.23 Å.

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))
$R_{free}$	91344	1611 (2.26-2.22)
Clashscore	102246	1764 (2.26-2.22)
Ramachandran outliers	100387	1724 (2.26-2.22)
Sidechain outliers	100360	1724 (2.26-2.22)
RSRZ outliers	91569	1616 (2.26-2.22)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	383	
1	B	383	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5567 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 Putative glycerate kinase 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	369	Total	C	N	O	S	Se	0	0	0
			2685	1673	477	523	5	7			
1	B	374	Total	C	N	O	S	Se	0	0	0
			2720	1695	483	530	5	7			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	EXPRESSION TAG	UNP Q8ZME0
A	-1	ASN	-	EXPRESSION TAG	UNP Q8ZME0
A	0	ALA	-	EXPRESSION TAG	UNP Q8ZME0
B	-2	SER	-	EXPRESSION TAG	UNP Q8ZME0
B	-1	ASN	-	EXPRESSION TAG	UNP Q8ZME0
B	0	ALA	-	EXPRESSION TAG	UNP Q8ZME0

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Cl	0	0
			1	1		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	70	Total	O	0	0
			70	70		
4	B	83	Total	O	0	0
			83	83		

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

- Chain A:
- 
- 78% 2% 16%
- SER ASN AO M1 K2 L14 D35 V53 E54 A55 G58 V63 N74 R84 M90 A93 S94 G95 L96 E97 D105 K108 T109 T110 L117 I129 I130 I131 S136 A137 T138 N139 G144 Q157 I166 G167 L168 L171 A172 S173 I176 L198 T199 G200 K201 F208 Q211 E217 N218 T227 Y229 R228 A230 H231 I233 L237 V238 V239 L242 D243 L244 A250 M253 Y258 A259 L276 H277 L278 E279 L282 E292 G293 R294 L295 D296 S297 GLN THR ILE HIS G302 I306 I311 R314 Y315 V319 L326 T327 ALA ASP VAL SER VAL HIS GLU H336 G337 L338 D339 V344 G349 T350 L351 E352 D353 A354 L355 N361 Q378 L379 R380

- Chain B:
- 
- | Amino Acid | Count |
|------------|-------|
| SER        | 1     |
| R1         | 1     |
| L14        | 1     |
| Q25        | 1     |
| V49        | 1     |
| M52        | 1     |
| R64        | 1     |
| R72        | 1     |
| D82        | 1     |
| A83        | 1     |
| E89        | 1     |
| M90        | 1     |
| A102       | 1     |
| Q103       | 1     |
| R104       | 1     |
| R119       | 1     |
| E127       | 1     |
| I130       | 1     |
| A137       | 1     |
| T138       | 1     |
| N139       | 1     |
| M145       | 1     |
| R154       | 1     |
| D155       | 1     |
| A156       | 1     |
| Q157       | 1     |
| Q163       | 1     |
| A166       | 1     |
| V167       | 1     |
| E168       | 1     |
| T170       | 1     |
| L171       | 1     |
| V190       | 1     |
| L198       | 1     |
| R201       | 1     |
| E202       | 1     |
| R228       | 1     |
| V236       | 1     |
| A230       | 1     |
| H231       | 1     |
| L232       | 1     |
| L233       | 1     |
| A234       | 1     |
| R235       | 1     |
| V239       | 1     |
| D240       | 1     |
| V241       | 1     |
| L242       | 1     |
| D243       | 1     |
| L244       | 1     |
| M253       | 1     |
| D254       | 1     |
| A255       | 1     |
| A256       | 1     |
| L257       | 1     |
| I269       | 1     |
| T273       | 1     |
| H277       | 1     |
| G283       | 1     |
| R294       | 1     |
| L295       | 1     |
| D296       | 1     |
| S297       | 1     |
| I300       | 1     |
| V304       | 1     |
| A309       | 1     |
| R313       | 1     |
| R314       | 1     |
| V319       | 1     |
| A328       | 1     |
| ASP        | 1     |
| VAL        | 1     |
| SER        | 1     |
| VAL        | 1     |
| VAL        | 1     |
| HIS        | 1     |
| GLU        | 1     |
| H336       | 1     |
| G337       | 1     |
| L338       | 1     |
| T350       | 1     |
| L351       | 1     |
| E352       | 1     |
| L355       | 1     |

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.73Å 59.55Å 103.61Å 90.00° 106.01° 90.00°	Depositor
Resolution (Å)	49.81 – 2.23 49.79 – 2.23	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.81-2.23) 99.6 (49.79-2.23)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.04 (at 2.22Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.188 , 0.237 0.192 , 0.240	Depositor DCC
$R_{free}$ test set	1827 reflections (5.25%)	DCC
Wilson B-factor (Å <sup>2</sup> )	46.4	Xtriage
Anisotropy	0.211	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 54.1	EDS
Estimated twinning fraction	0.021 for h,-k,-h-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 36722 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5567	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.95% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: EDO, CL

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	0.72	0/2713	0.78	2/3663 (0.1%)
1	B	0.79	0/2750	0.80	2/3718 (0.1%)
All	All	0.76	0/5463	0.79	4/7381 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	110	THR	CB-CA-C	-5.46	96.86	111.60
1	A	351	LEU	CA-CB-CG	5.45	127.84	115.30
1	B	367	ARG	NE-CZ-NH2	5.14	122.87	120.30
1	B	294	ARG	NE-CZ-NH1	5.05	122.82	120.30

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	2685	0	2699	45	0
1	B	2720	0	2731	48	0
2	B	1	0	0	0	0
3	A	4	0	6	0	0
3	B	4	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	70	0	0	3	0
4	B	83	0	0	3	0
All	All	5567	0	5442	93	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 9.

All (93) 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:295:ILE:HG22	1:A:326:LEU:HD21	1.31	1.10
1:A:295:ILE:HA	1:A:326:LEU:HD23	1.58	0.83
1:B:309:ALA:HB2	1:B:338:LEU:HD23	1.65	0.77
1:B:155:ASP:HB2	1:B:170:THR:HG22	1.71	0.72
1:A:242:LEU:H	1:A:242:LEU:CD1	2.03	0.71
1:A:242:LEU:N	1:A:242:LEU:HD12	2.08	0.69
1:A:295:ILE:HG22	1:A:326:LEU:CD2	2.16	0.68
1:A:90:MSE:HE2	1:A:94:SER:HB2	1.75	0.68
1:A:242:LEU:HD12	1:A:242:LEU:H	1.58	0.68
1:B:269:ILE:HD13	1:B:304:VAL:HG22	1.76	0.67
1:B:350:THR:O	1:B:350:THR:HG22	1.95	0.66
1:B:52:MSE:CE	1:B:130:ILE:HD13	2.25	0.66
1:B:25:GLN:HG2	4:B:460:HOH:O	1.95	0.66
1:B:64:GLU:OE1	1:B:72:ARG:HB3	1.96	0.66
1:B:309:ALA:HB2	1:B:338:LEU:CD2	2.25	0.66
1:B:232:LEU:HD22	1:B:235:ARG:HH21	1.61	0.65
1:A:294:ARG:HD3	4:A:448:HOH:O	1.98	0.62
1:A:244:LEU:HD11	1:A:258:TYR:CG	2.35	0.62
1:A:278:LEU:HD13	1:A:311:ILE:HD12	1.80	0.62
1:A:208:PHE:O	1:A:211:GLN:HG2	1.99	0.61
1:A:319:VAL:HG22	1:A:338:LEU:CD2	2.32	0.59
1:A:230:ALA:HB1	1:A:242:LEU:HG	1.84	0.59
1:B:297:SER:O	1:B:300:ILE:HG22	2.02	0.58
1:B:49:VAL:HG23	1:B:89:GLU:HG3	1.84	0.57
1:B:171:LEU:HD13	1:B:232:LEU:HD12	1.86	0.57
1:A:279:GLU:OE2	1:A:315:TYR:OH	2.20	0.57
1:B:232:LEU:HD22	1:B:235:ARG:NH2	2.21	0.56
1:A:105:ASP:OD1	1:A:218:MSE:HE2	2.06	0.56
1:A:242:LEU:N	1:A:242:LEU:CD1	2.67	0.56
1:B:14:LEU:HD23	1:B:355:LEU:HD22	1.89	0.55
1:B:351:LEU:O	1:B:352:GLU:HB3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:ILE:HG23	1:A:239:VAL:HG13	1.90	0.54
1:A:176:ILE:HD12	1:A:176:ILE:O	2.09	0.53
1:B:350:THR:O	1:B:350:THR:CG2	2.58	0.52
1:A:250:ALA:HB3	1:A:253:MSE:HB3	1.90	0.52
1:A:108:LYS:CE	1:A:166:ILE:HG21	2.40	0.52
1:B:374:LYS:O	1:B:378:GLN:HG2	2.09	0.52
1:B:52:MSE:CE	1:B:130:ILE:CD1	2.87	0.52
1:A:344:VAL:HG13	1:A:361:ASN:HB3	1.91	0.52
1:A:349:CYS:HA	1:A:354:ALA:HB3	1.92	0.51
1:A:353:ASP:HB2	4:A:419:HOH:O	2.09	0.51
1:B:356:LYS:NZ	1:B:360:GLU:OE1	2.42	0.51
1:B:155:ASP:CB	1:B:170:THR:HG22	2.40	0.51
1:A:110:THR:HG23	4:A:424:HOH:O	2.11	0.51
1:A:129:ILE:HG22	1:A:131:ILE:HG13	1.93	0.51
1:B:166:ILE:HG22	1:B:167:GLY:N	2.25	0.51
1:B:294:ARG:HB2	1:B:300:ILE:HD13	1.93	0.50
1:B:52:MSE:HE3	1:B:130:ILE:CD1	2.41	0.50
1:A:0:ALA:HB3	1:A:35:ASP:OD2	2.11	0.50
1:A:319:VAL:HG22	1:A:338:LEU:HD22	1.94	0.49
1:A:295:ILE:HA	1:A:326:LEU:CD2	2.37	0.49
1:B:313:LYS:HG2	1:B:314:ARG:N	2.27	0.49
1:B:230:ALA:HB1	1:B:242:LEU:HG	1.94	0.49
1:A:311:ILE:O	1:A:314:ARG:HB3	2.13	0.48
1:B:277:HIS:HD2	4:B:511:HOH:O	1.96	0.48
1:A:278:LEU:HD22	1:A:282:LEU:HD22	1.96	0.48
1:B:230:ALA:HB3	1:B:242:LEU:HD21	1.95	0.48
1:B:269:ILE:O	1:B:273:THR:HB	2.14	0.48
1:A:53:VAL:HG13	1:A:58:GLY:C	2.33	0.48
1:A:237:LEU:HB3	1:A:239:VAL:HG12	1.96	0.48
1:B:241:VAL:HG22	1:B:255:ALA:HB1	1.94	0.48
1:A:93:ALA:HB2	1:A:117:LEU:HD22	1.96	0.47
1:B:295:ILE:CG2	1:B:296:ASP:N	2.77	0.47
1:A:96:LEU:HD13	1:A:137:ALA:HA	1.96	0.47
1:A:176:ILE:HG12	1:A:237:LEU:HD11	1.96	0.47
1:B:293:GLY:O	1:B:294:ARG:HD3	2.14	0.47
1:B:230:ALA:CB	1:B:242:LEU:CD2	2.94	0.46
1:B:295:ILE:HG22	1:B:296:ASP:N	2.31	0.46
1:A:105:ASP:OD1	1:A:218:MSE:CE	2.63	0.46
1:B:241:VAL:CG2	1:B:255:ALA:HB1	2.46	0.46
1:A:237:LEU:HD13	1:A:237:LEU:HA	1.73	0.46
1:B:90:MSE:HE2	1:B:253:MSE:HE1	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:ARG:HB2	1:B:228:ARG:CZ	2.47	0.45
1:B:14:LEU:HD23	1:B:355:LEU:CD2	2.47	0.45
1:B:104:ARG:HB2	4:B:468:HOH:O	2.16	0.44
1:B:145:MSE:HE1	1:B:257:LEU:HG	2.00	0.44
1:A:326:LEU:HD22	1:A:326:LEU:N	2.33	0.43
1:B:102:ALA:C	1:B:103:GLN:HG2	2.39	0.43
1:B:319:VAL:HG22	1:B:338:LEU:HD22	2.00	0.43
1:A:292:GLU:OE1	1:A:302:GLY:HA2	2.18	0.43
1:A:90:MSE:HE1	1:A:136:SER:HB2	2.02	0.42
1:B:234:ALA:HA	1:B:239:VAL:O	2.20	0.42
1:A:14:LEU:HD23	1:A:355:LEU:HD22	2.02	0.42
1:B:82:ASP:O	1:B:83:ALA:HB3	2.20	0.41
1:A:55:ALA:HB1	1:A:276:LEU:HD22	2.02	0.41
1:B:309:ALA:CB	1:B:338:LEU:HD23	2.43	0.41
1:B:228:ARG:HB2	1:B:228:ARG:NH2	2.36	0.41
1:B:154:ARG:O	1:B:171:LEU:HD23	2.21	0.41
1:A:110:THR:HG22	1:A:144:GLY:HA3	2.01	0.41
1:B:253:MSE:HG2	1:B:257:LEU:HD12	2.02	0.41
1:A:344:VAL:CG1	1:A:361:ASN:HB3	2.51	0.41
1:B:295:ILE:HD12	1:B:295:ILE:HA	1.97	0.41
1:A:199:THR:HG21	1:A:227:THR:HA	2.03	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	363/383 (95%)	353 (97%)	10 (3%)	0	100	100
1	B	370/383 (97%)	357 (96%)	13 (4%)	0	100	100
All	All	733/766 (96%)	710 (97%)	23 (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	269/275 (98%)	244 (91%)	25 (9%)	11	7
1	B	273/275 (99%)	252 (92%)	21 (8%)	16	13
All	All	542/550 (98%)	496 (92%)	46 (8%)	13	10

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	74	ASN
1	A	97	GLU
1	A	110	THR
1	A	117	LEU
1	A	139	ASN
1	A	157	GLN
1	A	168	LEU
1	A	171	LEU
1	A	173	SER
1	A	198	LEU
1	A	201	LYS
1	A	217	GLU
1	A	228	ARG
1	A	233	ILE
1	A	237	LEU
1	A	239	VAL
1	A	242	LEU
1	A	278	LEU
1	A	282	LEU
1	A	306	ILE
1	A	327	THR
1	A	339	ASP
1	A	351	LEU
1	A	378	GLN

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Mol	Chain	Res	Type
1	B	64	GLU
1	B	72	ARG
1	B	103	GLN
1	B	119	ARG
1	B	127	GLU
1	B	139	ASN
1	B	157	GLN
1	B	163	GLN
1	B	166	ILE
1	B	170	THR
1	B	171	LEU
1	B	190	VAL
1	B	198	LEU
1	B	202	GLU
1	B	241	VAL
1	B	244	LEU
1	B	273	THR
1	B	295	ILE
1	B	351	LEU
1	B	367	ARG
1	B	378	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	ASN
1	B	74	ASN
1	B	120	HIS
1	B	159	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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	$\# Z  > 2$
3	EDO	A	402	-	3,3,3	0.58	0	2,2,2	0.74	0
3	EDO	B	401	-	3,3,3	0.54	0	2,2,2	0.40	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	EDO	A	402	-	-	0/1/1/1	0/0/0/0
3	EDO	B	401	-	-	0/1/1/1	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

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

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	362/383 (94%)	0.26	8 (2%) 65 68	28, 47, 62, 67	0
1	B	367/383 (95%)	0.25	9 (2%) 61 64	29, 45, 62, 69	0
All	All	729/766 (95%)	0.26	17 (2%) 64 66	28, 46, 62, 69	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	336	HIS	4.1
1	A	63	VAL	3.6
1	A	327	THR	3.5
1	A	258	TYR	3.2
1	B	232	LEU	3.1
1	B	300	ILE	3.0
1	B	242	LEU	3.0
1	B	201	LYS	2.6
1	B	352	GLU	2.6
1	A	231	HIS	2.4
1	B	137	ALA	2.4
1	B	168	LEU	2.3
1	A	84	ARG	2.2
1	A	259	ALA	2.2
1	A	380	ARG	2.2
1	B	202	GLU	2.1
1	A	326	LEU	2.1

### 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 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CL	B	403	1/1	0.99	0.07	-4.01	45,45,45,45	0
3	EDO	A	402	4/4	0.92	0.13	-	65,66,66,66	0
3	EDO	B	401	4/4	0.88	0.14	-	63,65,65,65	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.