



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 24, 2023 – 03:34 AM EDT

PDB ID : 3FLC  
Title : Crystal structure of the His-tagged H232R mutant of glycerol kinase from *Enterococcus casseliflavus* with glycerol  
Authors : Briozzo, P.  
Deposited on : 2008-12-18  
Resolution : 1.85 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

<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>.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

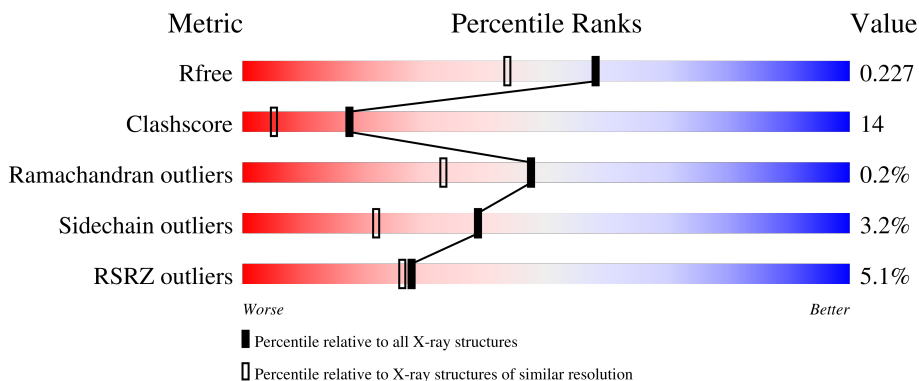
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.85 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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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  $\geq 3$ , 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	O	518	 6% 70% 23% . .
1	X	518	 4% 73% 21% . .

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8432 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 Glycerol kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	O	495	3849	2439	642	754	14	0	0	0
1	X	496	3853	2442	642	755	14	0	0	0

There are 26 discrepancies between the modelled and reference sequences:

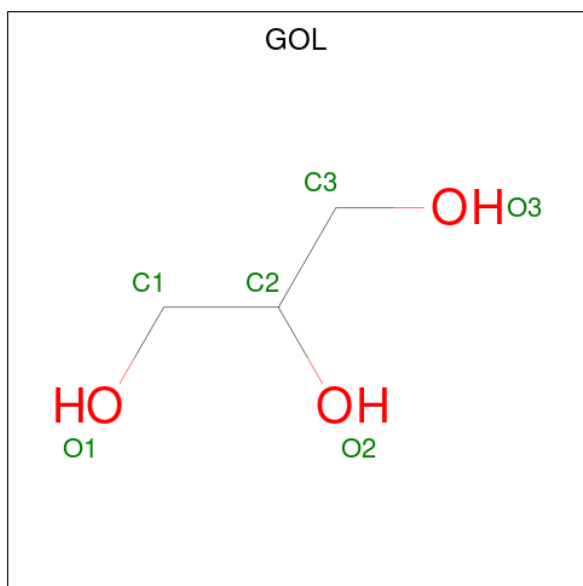
Chain	Residue	Modelled	Actual	Comment	Reference
O	-11	MET	-	expression tag	UNP O34153
O	-10	ARG	-	expression tag	UNP O34153
O	-9	GLY	-	expression tag	UNP O34153
O	-8	SER	-	expression tag	UNP O34153
O	-7	HIS	-	expression tag	UNP O34153
O	-6	HIS	-	expression tag	UNP O34153
O	-5	HIS	-	expression tag	UNP O34153
O	-4	HIS	-	expression tag	UNP O34153
O	-3	HIS	-	expression tag	UNP O34153
O	-2	HIS	-	expression tag	UNP O34153
O	-1	GLY	-	expression tag	UNP O34153
O	0	SER	-	expression tag	UNP O34153
O	232	ARG	HIS	engineered mutation	UNP O34153
X	-11	MET	-	expression tag	UNP O34153
X	-10	ARG	-	expression tag	UNP O34153
X	-9	GLY	-	expression tag	UNP O34153
X	-8	SER	-	expression tag	UNP O34153
X	-7	HIS	-	expression tag	UNP O34153
X	-6	HIS	-	expression tag	UNP O34153
X	-5	HIS	-	expression tag	UNP O34153
X	-4	HIS	-	expression tag	UNP O34153
X	-3	HIS	-	expression tag	UNP O34153
X	-2	HIS	-	expression tag	UNP O34153
X	-1	GLY	-	expression tag	UNP O34153
X	0	SER	-	expression tag	UNP O34153

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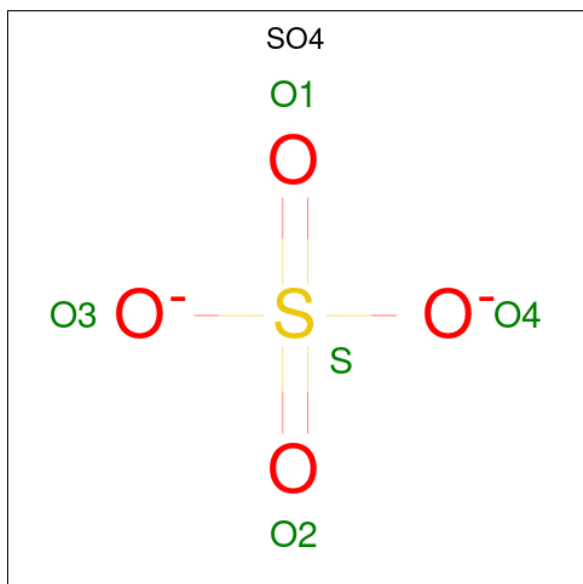
Chain	Residue	Modelled	Actual	Comment	Reference
X	232	ARG	HIS	engineered mutation	UNP O34153

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



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

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula:  $O_4S$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	O	1	Total	O	S	0	0
			5	4	1		
3	X	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	O	325	Total	O	0	0
			325	325		
4	X	383	Total	O	0	0
			383	383		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.56Å 192.23Å 57.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.85 29.57 – 1.85	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-1.85) 97.7 (29.57-1.85)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.88 (at 1.85Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.202 , 0.233 0.197 , 0.227	Depositor DCC
$R_{free}$ test set	8711 reflections (10.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.3	Xtrriage
Anisotropy	0.350	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 46.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8432	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.13% 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, 0.333 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, 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	O	0.31	0/3926	0.61	1/5318 (0.0%)
1	X	0.31	0/3932	0.61	1/5329 (0.0%)
All	All	0.31	0/7858	0.61	2/10647 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	240	ILE	N-CA-C	-5.56	95.98	111.00
1	X	240	ILE	N-CA-C	-5.29	96.72	111.00

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	O	3849	0	3748	116	0
1	X	3853	0	3753	92	0
2	O	6	0	8	0	0
2	X	6	0	8	0	0
3	O	5	0	0	0	0
3	X	5	0	0	0	0
4	O	325	0	0	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	X	383	0	0	6	0
All	All	8432	0	7517	208	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 14.

All (208) 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:X:326:THR:HG22	1:X:328:PRO:HD2	1.32	1.06
1:O:80:ILE:HB	1:O:243:MET:HG2	1.52	0.92
1:O:5:ASN:HD22	1:O:5:ASN:H	0.95	0.90
1:X:255:MET:HE2	1:X:462:LYS:HA	1.54	0.88
1:O:5:ASN:HD22	1:O:5:ASN:N	1.72	0.83
1:O:400:SER:OG	1:O:402:ILE:HG22	1.79	0.83
1:O:38:GLN:HE22	1:O:48:HIS:HE1	1.27	0.82
1:X:325:GLU:HB2	1:X:329:GLN:HE22	1.48	0.79
1:O:38:GLN:NE2	1:O:48:HIS:HE1	1.82	0.77
1:O:5:ASN:H	1:O:5:ASN:ND2	1.78	0.76
1:X:255:MET:HE2	1:X:462:LYS:CA	2.15	0.75
1:O:390:LYS:HD2	1:O:426:ILE:HG22	1.68	0.75
1:X:438:GLU:HG3	1:X:441:ALA:HB3	1.71	0.73
1:O:315:GLN:HB2	4:O:547:HOH:O	1.89	0.72
1:O:143:ARG:HH22	1:O:153:GLN:HE21	1.37	0.72
1:O:254:GLN:HG2	1:O:439:THR:HG21	1.71	0.72
1:O:143:ARG:HH12	1:O:153:GLN:HE22	1.40	0.70
1:X:325:GLU:HB2	1:X:329:GLN:NE2	2.05	0.70
1:X:275:ASN:HD22	1:X:277:GLY:H	1.40	0.70
1:X:275:ASN:ND2	1:X:277:GLY:H	1.91	0.69
1:O:416:ASN:C	1:O:416:ASN:HD22	1.97	0.67
1:O:6:TYR:CE1	1:O:29:ILE:HD13	2.31	0.66
1:O:384:ALA:O	1:O:388:GLN:HG3	1.97	0.64
1:O:327:SER:HB3	1:O:328:PRO:HD3	1.79	0.64
1:X:478:GLU:H	1:X:478:GLU:CD	2.01	0.64
1:X:92:LYS:HE2	1:X:159:GLY:O	1.98	0.64
1:X:318:ARG:HD2	1:X:319:ASP:OD1	1.99	0.63
1:O:263:LYS:HD2	1:O:263:LYS:C	2.19	0.63
1:X:323:MET:O	1:X:374:LYS:HE3	2.00	0.62
1:X:263:LYS:HD2	1:X:263:LYS:C	2.19	0.62
1:O:275:ASN:ND2	1:O:277:GLY:H	1.98	0.61
1:X:172:TRP:CE3	1:X:177:GLY:HA2	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:341:ASN:HD21	1:O:383:GLN:HE22	1.48	0.61
1:O:415:LYS:HB3	1:O:437:LEU:HD21	1.83	0.61
1:O:219:LYS:HE3	4:O:660:HOH:O	2.00	0.60
1:X:107:ARG:NH2	1:X:135:ALA:HB3	2.17	0.60
1:O:475:MET:CE	1:O:480:ARG:HB2	2.30	0.60
1:O:379:ARG:O	1:O:383:GLN:HG3	2.02	0.60
1:O:276:THR:OG1	1:O:280:PRO:HG3	2.02	0.59
1:O:423:GLN:HE21	1:O:427:LEU:HD13	1.67	0.59
1:O:268:THR:HG23	1:O:312:SER:HB3	1.84	0.59
1:O:272:ILE:HD12	1:O:272:ILE:N	2.18	0.59
1:O:438:GLU:HG3	1:O:441:ALA:HB3	1.83	0.59
1:X:18:ARG:HG2	1:X:33:GLN:HG3	1.84	0.59
1:X:416:ASN:HD21	1:X:418:LEU:HB3	1.68	0.58
1:O:49:ASN:HD22	1:O:51:ASN:H	1.52	0.58
1:O:218:VAL:O	1:O:219:LYS:HD2	2.04	0.58
1:O:426:ILE:HD13	1:O:475:MET:HE3	1.85	0.58
1:O:143:ARG:HH22	1:O:153:GLN:NE2	2.01	0.58
1:X:38:GLN:OE1	1:X:48:HIS:HE1	1.87	0.58
1:O:475:MET:HE3	1:O:480:ARG:HB2	1.86	0.57
1:O:49:ASN:HD22	1:O:49:ASN:C	2.07	0.57
1:O:24:ARG:HG2	1:O:454:PHE:CZ	2.40	0.57
1:O:181:VAL:HG22	1:O:182:THR:N	2.19	0.57
1:O:275:ASN:HD22	1:O:277:GLY:H	1.53	0.56
1:O:38:GLN:HE22	1:O:48:HIS:CE1	2.15	0.56
1:X:416:ASN:C	1:X:416:ASN:HD22	2.08	0.56
1:O:49:ASN:ND2	1:O:51:ASN:H	2.03	0.56
1:O:29:ILE:CD1	1:O:70:ILE:HG13	2.36	0.56
1:X:324:ILE:O	1:X:325:GLU:HB2	2.06	0.55
1:X:326:THR:CG2	1:X:328:PRO:HD2	2.22	0.55
1:X:329:GLN:O	1:X:333:LEU:HD13	2.07	0.55
1:O:48:HIS:HD2	1:O:83:GLN:HE22	1.55	0.55
1:O:326:THR:OG1	1:O:328:PRO:HD2	2.06	0.55
1:O:390:LYS:HD2	1:O:426:ILE:CG2	2.37	0.55
1:X:72:PRO:HG2	1:X:234:TYR:HB2	1.88	0.55
1:X:326:THR:HG22	1:X:328:PRO:CD	2.22	0.54
1:X:400:SER:OG	1:X:402:ILE:HG12	2.07	0.54
1:O:280:PRO:CG	1:O:301:TYR:HB2	2.38	0.54
1:X:274:MET:SD	1:X:402:ILE:HD11	2.46	0.54
1:O:48:HIS:CD2	1:O:83:GLN:HE22	2.25	0.54
1:X:107:ARG:NH2	1:X:134:ASP:OD2	2.40	0.54
1:O:478:GLU:H	1:O:478:GLU:CD	2.11	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:426:ILE:HD13	1:O:475:MET:CE	2.39	0.53
1:O:82:ASN:ND2	1:O:167:ASP:HB3	2.24	0.53
1:O:85:GLU:HB2	1:O:104:TRP:HB3	1.91	0.53
1:O:29:ILE:HD12	1:O:70:ILE:HG13	1.91	0.52
1:X:194:ASN:CG	1:X:197:LYS:HG2	2.30	0.52
1:O:279:GLU:N	1:O:280:PRO:HD3	2.25	0.52
1:X:348:ALA:HB2	1:X:352:LEU:HD13	1.91	0.52
1:O:20:ILE:CD1	1:O:438:GLU:HG2	2.40	0.52
1:O:282:LEU:HD21	1:O:285:ASN:HB2	1.92	0.52
1:X:48:HIS:CD2	1:X:83:GLN:HE22	2.27	0.52
1:X:110:SER:OG	1:X:111:PRO:HD3	2.10	0.52
1:X:327:SER:HB2	1:X:328:PRO:HD3	1.92	0.52
1:O:49:ASN:HD21	1:O:51:ASN:HB2	1.74	0.52
1:X:282:LEU:HD22	1:X:282:LEU:N	2.25	0.52
1:O:81:THR:HG21	1:O:440:THR:HG22	1.92	0.51
1:O:485:GLU:HB2	4:O:752:HOH:O	2.11	0.51
1:X:390:LYS:HG3	1:X:427:LEU:HD23	1.91	0.51
1:X:81:THR:OG1	1:X:246:ASP:HA	2.11	0.51
1:X:196:HIS:HE1	4:X:607:HOH:O	1.94	0.51
1:X:197:LYS:HG3	1:X:199:GLU:HG2	1.92	0.51
1:X:194:ASN:ND2	1:X:197:LYS:HE3	2.25	0.51
1:X:155:LYS:HB3	1:X:161:LEU:HD13	1.93	0.51
1:O:326:THR:HG22	1:O:329:GLN:HB2	1.93	0.50
1:X:260:GLY:HA2	1:X:402:ILE:CD1	2.41	0.50
1:O:54:TRP:CD1	1:O:173:LYS:HE2	2.45	0.50
1:X:234:TYR:N	1:X:234:TYR:CD2	2.76	0.50
1:O:128:LYS:HD3	1:O:201:ASP:OD2	2.12	0.50
1:O:181:VAL:HG22	1:O:182:THR:H	1.77	0.50
1:O:284:ASP:HB3	4:O:614:HOH:O	2.10	0.50
1:O:180:HIS:HD2	4:O:605:HOH:O	1.96	0.49
1:O:275:ASN:HD22	1:O:276:THR:N	2.09	0.49
1:O:81:THR:OG1	1:O:246:ASP:HA	2.13	0.49
1:X:456:LYS:HG2	1:X:460:GLU:OE1	2.13	0.49
1:X:180:HIS:HD2	4:X:596:HOH:O	1.95	0.49
1:X:255:MET:HE2	1:X:462:LYS:N	2.27	0.49
1:O:275:ASN:HD22	1:O:275:ASN:C	2.16	0.49
1:X:20:ILE:CD1	1:X:438:GLU:HG2	2.42	0.49
1:X:403:ASP:C	1:X:405:PRO:HD3	2.33	0.48
1:X:82:ASN:ND2	1:X:167:ASP:HB3	2.29	0.48
1:X:3:GLU:HB3	1:X:5:ASN:ND2	2.28	0.48
1:O:326:THR:HG23	1:O:329:GLN:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:241:ALA:HB1	1:X:451:ALA:HB3	1.95	0.48
1:O:345:VAL:O	1:O:347:PRO:HD3	2.13	0.47
1:X:116:LEU:HB3	1:X:133:ILE:HD13	1.96	0.47
1:X:325:GLU:CB	1:X:329:GLN:HE22	2.23	0.47
1:O:326:THR:CG2	1:O:329:GLN:HB2	2.43	0.47
1:O:123:GLU:O	1:O:127:GLU:HG3	2.14	0.47
1:O:120:GLY:HA2	4:O:663:HOH:O	2.15	0.47
1:O:416:ASN:C	1:O:416:ASN:ND2	2.67	0.47
1:O:482:ASN:O	1:O:485:GLU:HG2	2.15	0.47
1:O:18:ARG:HE	1:O:33:GLN:CD	2.19	0.47
1:X:72:PRO:HD2	4:X:740:HOH:O	2.15	0.46
1:X:181:VAL:HG22	1:X:182:THR:N	2.30	0.46
1:X:356:TYR:CZ	1:X:491:VAL:HG11	2.50	0.46
1:O:427:LEU:HB3	1:O:429:ILE:HG12	1.97	0.46
1:O:49:ASN:HD22	1:O:51:ASN:N	2.13	0.46
1:O:329:GLN:NE2	1:O:332:GLU:HB2	2.30	0.46
1:O:198:LEU:HD21	1:O:299:VAL:HG21	1.98	0.46
1:X:275:ASN:HD22	1:X:276:THR:N	2.14	0.46
1:X:85:GLU:HB2	1:X:104:TRP:HB3	1.98	0.45
1:X:272:ILE:HD12	1:X:272:ILE:N	2.30	0.45
1:O:423:GLN:NE2	1:O:427:LEU:HD13	2.32	0.45
1:O:433:ARG:HD3	4:O:668:HOH:O	2.15	0.45
1:X:336:LYS:HG2	1:X:336:LYS:O	2.16	0.45
1:X:180:HIS:CE1	1:X:216:PRO:HB3	2.50	0.45
1:X:68:SER:OG	1:X:70:ILE:HG12	2.17	0.45
1:O:6:TYR:CE2	1:O:70:ILE:HD12	2.51	0.45
1:X:20:ILE:HG23	1:X:28:LYS:HG3	1.98	0.45
1:O:412:GLY:O	1:O:415:LYS:HG2	2.17	0.45
1:X:83:GLN:O	1:X:83:GLN:HG3	2.16	0.45
1:O:334:ALA:HB2	1:O:382:LEU:HD12	1.99	0.44
1:X:48:HIS:HD2	1:X:83:GLN:HE22	1.63	0.44
1:X:379:ARG:O	1:X:383:GLN:HG3	2.17	0.44
1:X:402:ILE:O	1:X:402:ILE:HG13	2.17	0.44
1:O:280:PRO:HG3	1:O:301:TYR:HB2	1.99	0.44
1:X:255:MET:HE1	1:X:461:LEU:HB2	1.99	0.44
1:O:121:HIS:CD2	1:O:207:LEU:HD21	2.53	0.44
1:X:81:THR:HG21	1:X:440:THR:HG22	1.98	0.44
1:X:314:ILE:HD11	1:X:382:LEU:HD23	2.00	0.44
1:X:263:LYS:HA	1:X:408:LYS:O	2.17	0.44
1:O:38:GLN:NE2	1:O:48:HIS:CE1	2.73	0.44
1:X:461:LEU:HA	1:X:464:MET:HE3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:314:ILE:HD11	1:O:382:LEU:HD23	2.00	0.44
1:X:475:MET:HA	1:X:476:PRO:HD3	1.83	0.44
1:O:388:GLN:HG2	1:O:487:TRP:CZ2	2.53	0.43
1:O:263:LYS:HA	1:O:408:LYS:O	2.19	0.43
1:X:254:GLN:HG2	1:X:439:THR:HG21	1.99	0.43
1:O:143:ARG:HH12	1:O:153:GLN:NE2	2.11	0.43
1:X:295:ILE:HD11	1:X:450:LEU:HD23	2.01	0.43
1:X:478:GLU:CD	1:X:478:GLU:N	2.70	0.43
1:X:20:ILE:HD11	1:X:438:GLU:HG2	1.99	0.43
1:X:403:ASP:O	1:X:405:PRO:HD3	2.18	0.43
1:O:348:ALA:O	1:O:362:ARG:HA	2.19	0.43
1:O:45:TRP:CD2	1:O:108:GLN:HB3	2.54	0.43
1:O:80:ILE:O	1:O:243:MET:HA	2.18	0.43
1:O:287:LEU:HD13	1:O:396:MET:HG2	2.00	0.43
1:O:262:ILE:HD11	1:O:272:ILE:CG2	2.49	0.42
1:O:382:LEU:O	1:O:385:VAL:HG12	2.19	0.42
1:O:449:GLY:HA3	1:O:455:TRP:CE3	2.54	0.42
1:X:275:ASN:HD22	1:X:275:ASN:C	2.22	0.42
1:O:150:GLU:HG3	4:O:587:HOH:O	2.18	0.42
1:O:458:LEU:O	1:O:461:LEU:HB2	2.19	0.42
1:O:5:ASN:N	1:O:5:ASN:ND2	2.45	0.42
1:O:278:GLU:OE2	1:O:298:LYS:HD2	2.18	0.42
1:O:438:GLU:OE2	1:O:440:THR:HB	2.20	0.42
1:X:387:TYR:HB3	1:X:487:TRP:CD2	2.54	0.42
1:X:345:VAL:HG12	1:X:347:PRO:HD3	2.02	0.42
1:O:124:MET:SD	1:O:128:LYS:HD2	2.59	0.42
1:O:178:GLN:HG3	1:O:229:ARG:HH21	1.83	0.42
1:O:180:HIS:CE1	1:O:216:PRO:HB3	2.54	0.42
1:X:124:MET:HG2	1:X:125:ILE:N	2.35	0.42
1:X:138:SER:HB2	1:X:190:THR:HA	2.02	0.42
1:X:120:GLY:HA2	4:X:732:HOH:O	2.19	0.42
1:O:92:LYS:HB3	1:O:162:LEU:HG	2.01	0.41
1:O:318:ARG:O	1:O:322:ARG:HA	2.20	0.41
1:X:326:THR:O	1:X:329:GLN:HB2	2.21	0.41
1:O:6:TYR:CD1	1:O:29:ILE:HD13	2.56	0.41
1:O:305:GLY:HA3	1:O:392:VAL:CG1	2.51	0.41
1:O:266:TYR:HB3	1:O:413:ALA:HB3	2.01	0.41
1:O:85:GLU:O	1:O:86:THR:C	2.58	0.41
1:O:390:LYS:HD3	1:O:484:TYR:CE1	2.55	0.41
1:X:348:ALA:CB	1:X:352:LEU:HD13	2.50	0.41
1:O:276:THR:OG1	1:O:280:PRO:CG	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:283:SER:O	1:X:399:ASP:HB3	2.20	0.41
1:X:407:LEU:HD13	1:X:409:VAL:CG1	2.50	0.41
1:X:172:TRP:HZ3	4:X:799:HOH:O	2.04	0.41
1:X:263:LYS:HD2	1:X:264:ASN:N	2.36	0.40
1:O:103:VAL:HG12	1:O:104:TRP:N	2.37	0.40
1:X:110:SER:N	1:X:111:PRO:CD	2.85	0.40
1:X:390:LYS:HA	1:X:427:LEU:HD21	2.02	0.40
1:O:185:SER:O	1:O:189:ARG:HG2	2.22	0.40
1:X:159:GLY:HA2	4:X:581:HOH:O	2.20	0.40
1:O:29:ILE:HD11	1:O:70:ILE:HG13	2.04	0.40
1:O:425:ASP:HB3	1:O:475:MET:HB3	2.04	0.40
1:X:181:VAL:HG22	1:X:182:THR:H	1.86	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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	O	489/518 (94%)	473 (97%)	14 (3%)	2 (0%)	34	19
1	X	492/518 (95%)	478 (97%)	14 (3%)	0	100	100
All	All	981/1036 (95%)	951 (97%)	28 (3%)	2 (0%)	47	33

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	O	280	PRO
1	O	476	PRO

### 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	O	402/420 (96%)	391 (97%)	11 (3%)	44	29
1	X	403/420 (96%)	388 (96%)	15 (4%)	34	17
All	All	805/840 (96%)	779 (97%)	26 (3%)	39	22

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	5	ASN
1	O	12	GLN
1	O	49	ASN
1	O	198	LEU
1	O	263	LYS
1	O	275	ASN
1	O	280	PRO
1	O	329	GLN
1	O	407	LEU
1	O	416	ASN
1	O	461	LEU
1	X	3	GLU
1	X	12	GLN
1	X	116	LEU
1	X	146	LEU
1	X	150	GLU
1	X	165	THR
1	X	233	PHE
1	X	263	LYS
1	X	275	ASN
1	X	352	LEU
1	X	407	LEU
1	X	416	ASN
1	X	419	LEU
1	X	447	LEU
1	X	450	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	O	5	ASN
1	O	38	GLN
1	O	48	HIS
1	O	49	ASN
1	O	82	ASN
1	O	153	GLN
1	O	180	HIS
1	O	186	ASN
1	O	275	ASN
1	O	285	ASN
1	O	383	GLN
1	O	416	ASN
1	O	432	GLN
1	X	25	ASN
1	X	48	HIS
1	X	82	ASN
1	X	121	HIS
1	X	180	HIS
1	X	186	ASN
1	X	196	HIS
1	X	275	ASN
1	X	329	GLN
1	X	383	GLN
1	X	416	ASN

### 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 monosaccharides in this entry.



## 5.6 Ligand geometry [i](#)

4 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
3	SO4	O	508	-	4,4,4	0.31	0	6,6,6	0.16	0
2	GOL	X	507	-	5,5,5	0.60	0	5,5,5	0.47	0
3	SO4	X	508	-	4,4,4	0.33	0	6,6,6	0.12	0
2	GOL	O	507	-	5,5,5	0.47	0	5,5,5	0.39	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	X	507	-	-	0/4/4/4	-
2	GOL	O	507	-	-	0/4/4/4	-

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 [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, 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	O	495/518 (95%)	0.36	29 (5%) 22 22	14, 22, 41, 70	0
1	X	496/518 (95%)	0.29	22 (4%) 34 33	14, 22, 39, 50	0
All	All	991/1036 (95%)	0.33	51 (5%) 28 26	14, 22, 40, 70	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	281	GLN	12.3
1	O	282	LEU	9.5
1	X	282	LEU	7.4
1	O	402	ILE	5.5
1	O	280	PRO	5.3
1	X	280	PRO	5.0
1	O	476	PRO	4.5
1	X	325	GLU	4.4
1	O	332	GLU	4.2
1	X	324	ILE	4.1
1	O	279	GLU	4.1
1	X	402	ILE	4.0
1	O	329	GLN	3.8
1	X	338	LYS	3.7
1	X	403	ASP	3.4
1	X	401	GLY	3.3
1	X	478	GLU	3.2
1	O	478	GLU	3.2
1	O	325	GLU	3.2
1	O	436	ASN	3.1
1	X	476	PRO	3.1
1	X	326	THR	3.0
1	O	499	PHE	3.0
1	O	403	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	O	336	LYS	2.9
1	O	466	GLU	2.9
1	X	466	GLU	2.9
1	O	474	GLU	2.8
1	O	27	LYS	2.7
1	X	418	LEU	2.7
1	O	326	THR	2.6
1	O	71	ARG	2.6
1	X	332	GLU	2.6
1	X	336	LYS	2.5
1	O	340	ASP	2.5
1	O	338	LYS	2.5
1	O	178	GLN	2.4
1	O	335	ALA	2.4
1	O	3	GLU	2.3
1	X	279	GLU	2.2
1	O	10	ILE	2.2
1	X	337	ALA	2.1
1	X	328	PRO	2.1
1	X	339	GLY	2.1
1	O	327	SER	2.1
1	X	463	SER	2.1
1	X	329	GLN	2.1
1	O	365	VAL	2.1
1	X	340	ASP	2.0
1	O	477	ALA	2.0
1	O	80	ILE	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 monosaccharides 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, 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	B-factors(Å <sup>2</sup> )	Q<0.9
3	SO4	X	508	5/5	0.94	0.12	42,42,43,43	0
2	GOL	O	507	6/6	0.95	0.17	15,15,18,18	0
3	SO4	O	508	5/5	0.97	0.08	25,26,27,28	0
2	GOL	X	507	6/6	0.97	0.16	15,16,18,18	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.