



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 06:41 AM GMT

PDB ID : 3D7E  
Title : Enterococcus casseliflavus glycerol kinase mutant HIS232ALA complexed with glycerol  
Authors : Yeh, J.I.; Vahedi-Faridi, A.  
Deposited on : 2008-05-21  
Resolution : 2.03 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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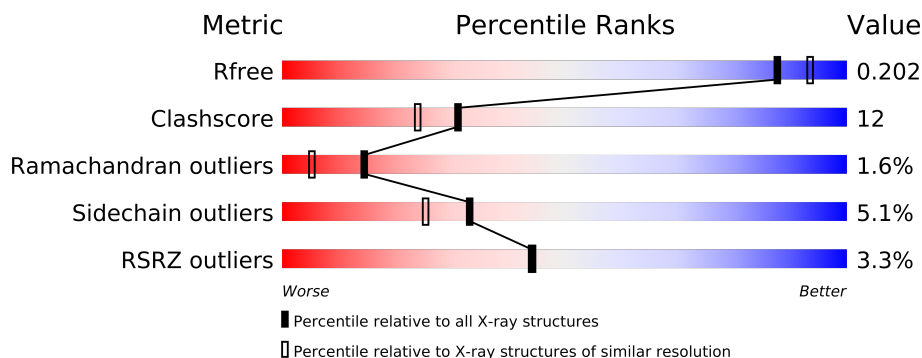
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.03 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))
$R_{free}$	66092	6003 (2.04-2.00)
Clashscore	79885	7467 (2.04-2.00)
Ramachandran outliers	78287	7370 (2.04-2.00)
Sidechain outliers	78261	7368 (2.04-2.00)
RSRZ outliers	66119	6006 (2.04-2.00)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	O	505	
1	X	505	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	GOL	O	507	-	X
2	GOL	X	507	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7995 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

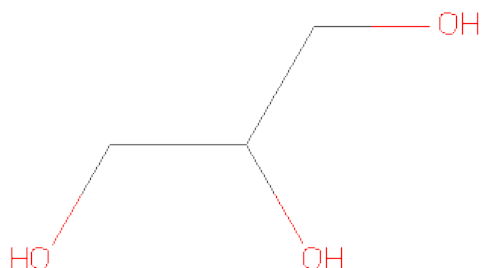
- Molecule 1 is a protein called Glycerol kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	O	495	Total	C	N	O	S	0	0	0
			3838	2433	638	753	14			
1	X	495	Total	C	N	O	S	0	0	0
			3838	2433	638	753	14			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	232	ALA	HIS	ENGINEERED MUTATION	UNP O34153
X	232	ALA	HIS	ENGINEERED MUTATION	UNP O34153

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

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

- Molecule 3 is water.

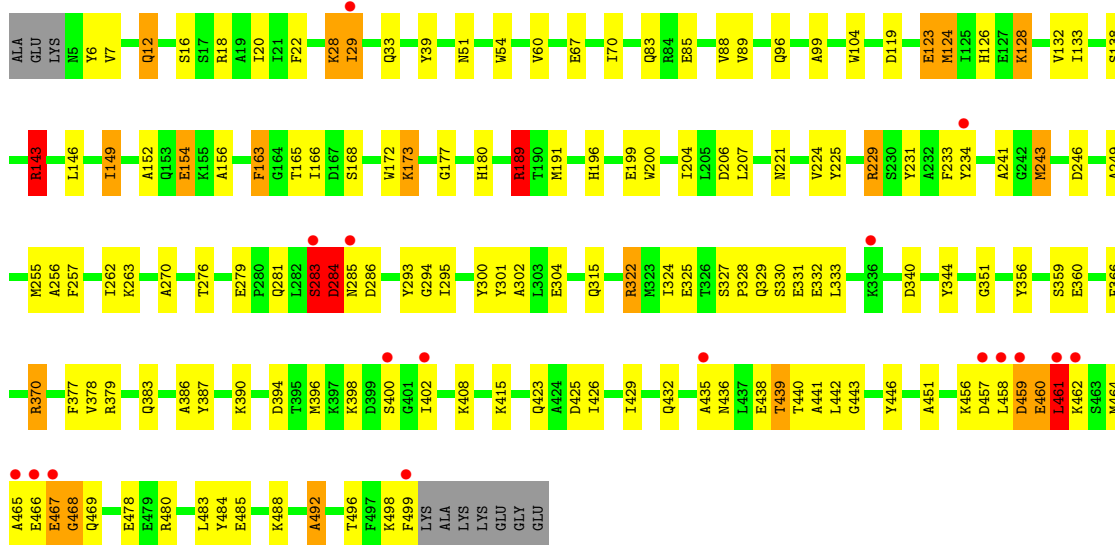
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	O	165	Total	O	0	0
			165	165		
3	X	142	Total	O	0	0
			142	142		

### 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 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.

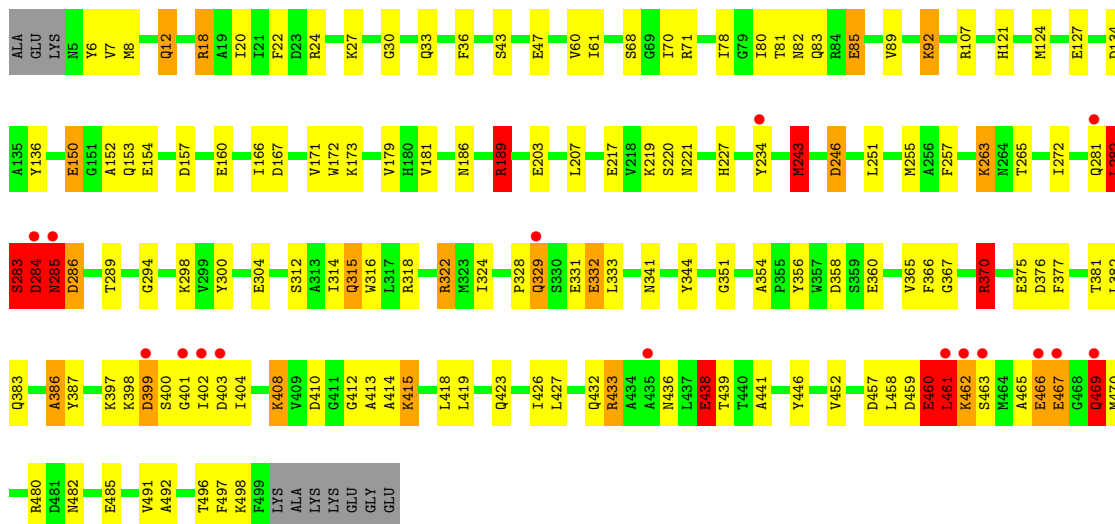
#### • Molecule 1: Glycerol kinase

Chain O: 



#### • Molecule 1: Glycerol kinase

Chain X: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	95.57Å 200.02Å 56.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.28 – 2.03 39.27 – 2.03	Depositor EDS
% Data completeness (in resolution range)	88.9 (39.28-2.03) 88.9 (39.27-2.03)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.45 (at 2.03Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.191 , 0.249 0.194 , 0.202	Depositor DCC
$R_{free}$ test set	3224 reflections (5.37%)	DCC
Wilson B-factor (Å <sup>2</sup> )	25.6	Xtriage
Anisotropy	0.721	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 33.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 63284 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7995	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.95% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

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

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	1.75	54/3918 (1.4%)	1.31	24/5314 (0.5%)
1	X	1.79	64/3918 (1.6%)	1.39	32/5314 (0.6%)
All	All	1.77	118/7836 (1.5%)	1.35	56/10628 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	O	0	5
1	X	0	6
All	All	0	11

All (118) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	370	ARG	CG-CD	11.93	1.81	1.51
1	X	432	GLN	C-O	10.61	1.43	1.23
1	O	152	ALA	CA-CB	9.73	1.72	1.52
1	X	370	ARG	CZ-NH1	9.70	1.45	1.33
1	X	304	GLU	CB-CG	9.37	1.70	1.52
1	X	160	GLU	CD-OE2	9.27	1.35	1.25
1	X	452	VAL	CB-CG1	8.84	1.71	1.52
1	X	152	ALA	CA-CB	8.72	1.70	1.52
1	X	243	MET	CB-CG	8.09	1.77	1.51
1	O	67	GLU	CB-CG	8.07	1.67	1.52
1	O	99	ALA	CA-CB	8.02	1.69	1.52
1	X	127	GLU	CD-OE1	8.02	1.34	1.25
1	X	203	GLU	CD-OE1	7.94	1.34	1.25
1	X	399	ASP	CB-CG	7.82	1.68	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	256	ALA	CA-CB	7.72	1.68	1.52
1	O	301	TYR	CD2-CE2	7.70	1.50	1.39
1	O	189	ARG	CD-NE	-7.67	1.33	1.46
1	X	189	ARG	CD-NE	-7.50	1.33	1.46
1	O	88	VAL	CB-CG1	7.45	1.68	1.52
1	O	387	TYR	CD2-CE2	7.42	1.50	1.39
1	X	365	VAL	CB-CG1	7.28	1.68	1.52
1	O	128	LYS	CD-CE	7.24	1.69	1.51
1	O	293	TYR	CD2-CE2	7.17	1.50	1.39
1	X	136	TYR	CD1-CE1	7.09	1.50	1.39
1	X	387	TYR	CD1-CE1	7.08	1.50	1.39
1	X	497	PHE	CD2-CE2	7.03	1.53	1.39
1	X	469	GLN	C-O	6.97	1.36	1.23
1	X	89	VAL	CB-CG1	6.89	1.67	1.52
1	O	478	GLU	CG-CD	6.85	1.62	1.51
1	O	199	GLU	CD-OE2	6.75	1.33	1.25
1	X	203	GLU	CB-CG	-6.67	1.39	1.52
1	O	270	ALA	CA-CB	6.63	1.66	1.52
1	X	160	GLU	CB-CG	6.60	1.64	1.52
1	X	298	LYS	CE-NZ	6.50	1.65	1.49
1	O	302	ALA	CA-CB	6.50	1.66	1.52
1	X	107	ARG	CB-CG	6.48	1.70	1.52
1	O	315	GLN	CG-CD	6.48	1.66	1.51
1	X	446	TYR	CD1-CE1	6.47	1.49	1.39
1	O	377	PHE	CD2-CE2	6.44	1.52	1.39
1	X	387	TYR	CE2-CZ	6.42	1.46	1.38
1	X	344	TYR	CD1-CE1	6.42	1.49	1.39
1	X	414	ALA	CA-CB	6.41	1.66	1.52
1	O	16	SER	CB-OG	-6.37	1.33	1.42
1	X	360	GLU	CG-CD	6.33	1.61	1.51
1	O	7	VAL	CB-CG2	6.31	1.66	1.52
1	X	179	VAL	CB-CG2	6.29	1.66	1.52
1	O	295	ILE	CB-CG2	6.25	1.72	1.52
1	X	234	TYR	CG-CD2	6.21	1.47	1.39
1	X	92	LYS	CD-CE	6.18	1.66	1.51
1	O	39	TYR	CD1-CE1	6.15	1.48	1.39
1	X	217	GLU	CG-CD	6.10	1.61	1.51
1	O	224	VAL	CB-CG2	6.05	1.65	1.52
1	O	351	GLY	N-CA	6.05	1.55	1.46
1	O	344	TYR	CG-CD2	6.03	1.47	1.39
1	X	413	ALA	CA-CB	6.01	1.65	1.52
1	O	138	SER	CB-OG	5.97	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	60	VAL	CB-CG2	5.97	1.65	1.52
1	O	22	PHE	CE1-CZ	5.91	1.48	1.37
1	X	351	GLY	C-O	5.90	1.33	1.23
1	X	370	ARG	CZ-NH2	5.90	1.40	1.33
1	O	163	PHE	CD2-CE2	5.89	1.51	1.39
1	O	360	GLU	CB-CG	5.88	1.63	1.52
1	O	331	GLU	CD-OE1	-5.88	1.19	1.25
1	X	315	GLN	CG-CD	5.79	1.64	1.51
1	X	172	TRP	CZ3-CH2	5.79	1.49	1.40
1	O	344	TYR	CE1-CZ	5.77	1.46	1.38
1	X	381	THR	CB-CG2	5.76	1.71	1.52
1	O	89	VAL	CB-CG1	5.73	1.64	1.52
1	O	154	GLU	CB-CG	5.71	1.62	1.52
1	X	377	PHE	CE1-CZ	5.70	1.48	1.37
1	X	331	GLU	CD-OE1	-5.66	1.19	1.25
1	O	332	GLU	CG-CD	5.65	1.60	1.51
1	X	300	TYR	CE2-CZ	5.65	1.45	1.38
1	O	300	TYR	CD1-CE1	5.63	1.47	1.39
1	X	220	SER	CB-OG	5.62	1.49	1.42
1	X	386	ALA	CA-CB	5.59	1.64	1.52
1	O	304	GLU	CB-CG	5.59	1.62	1.52
1	X	286	ASP	N-CA	5.58	1.57	1.46
1	X	36	PHE	CE1-CZ	5.58	1.48	1.37
1	O	485	GLU	CB-CG	-5.55	1.41	1.52
1	O	460	GLU	CB-CG	5.53	1.62	1.52
1	X	285	ASN	C-O	5.51	1.33	1.23
1	X	43	SER	CB-OG	5.46	1.49	1.42
1	X	47	GLU	CG-CD	5.44	1.60	1.51
1	O	492	ALA	CA-CB	5.41	1.63	1.52
1	X	438	GLU	CG-CD	5.40	1.60	1.51
1	X	485	GLU	CG-CD	5.40	1.60	1.51
1	O	279	GLU	CB-CG	5.39	1.62	1.52
1	O	168	SER	CB-OG	5.38	1.49	1.42
1	O	173	LYS	CD-CE	5.38	1.64	1.51
1	O	200	TRP	CE3-CZ3	5.38	1.47	1.38
1	X	153	GLN	C-O	5.38	1.33	1.23
1	O	123	GLU	CD-OE2	5.36	1.31	1.25
1	O	156	ALA	CA-CB	5.32	1.63	1.52
1	X	408	LYS	CD-CE	5.28	1.64	1.51
1	O	262	ILE	CB-CG2	5.27	1.69	1.52
1	O	356	TYR	CZ-OH	5.25	1.46	1.37
1	O	206	ASP	N-CA	5.20	1.56	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	150	GLU	CD-OE1	5.17	1.31	1.25
1	X	366	PHE	CB-CG	-5.15	1.42	1.51
1	O	446	TYR	CB-CG	-5.15	1.44	1.51
1	X	136	TYR	CE2-CZ	5.14	1.45	1.38
1	O	322	ARG	CB-CG	5.13	1.66	1.52
1	X	173	LYS	CE-NZ	5.13	1.61	1.49
1	X	354	ALA	CA-CB	5.13	1.63	1.52
1	X	85	GLU	C-O	5.12	1.33	1.23
1	X	376	ASP	C-O	-5.10	1.13	1.23
1	X	322	ARG	CD-NE	-5.09	1.37	1.46
1	X	60	VAL	CB-CG1	5.08	1.63	1.52
1	X	154	GLU	CB-CG	5.08	1.61	1.52
1	X	367	GLY	N-CA	5.08	1.53	1.46
1	O	483	LEU	C-O	5.07	1.32	1.23
1	X	251	LEU	CG-CD1	5.06	1.70	1.51
1	X	171	VAL	CB-CG1	5.05	1.63	1.52
1	O	359	SER	CA-CB	5.04	1.60	1.52
1	X	398	LYS	CD-CE	5.04	1.63	1.51
1	O	28	LYS	CE-NZ	5.03	1.61	1.49
1	O	366	PHE	CE1-CZ	5.02	1.46	1.37

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	189	ARG	NE-CZ-NH2	-18.55	111.02	120.30
1	O	189	ARG	NE-CZ-NH2	-16.87	111.86	120.30
1	X	370	ARG	NE-CZ-NH2	-15.68	112.46	120.30
1	O	189	ARG	NE-CZ-NH1	14.62	127.61	120.30
1	X	322	ARG	NE-CZ-NH2	-14.22	113.19	120.30
1	X	189	ARG	NE-CZ-NH1	13.08	126.84	120.30
1	O	143	ARG	NE-CZ-NH2	-12.49	114.06	120.30
1	X	322	ARG	NE-CZ-NH1	10.06	125.33	120.30
1	X	433	ARG	NE-CZ-NH1	9.94	125.27	120.30
1	X	246	ASP	CB-CG-OD1	9.88	127.19	118.30
1	X	243	MET	CA-CB-CG	8.97	128.55	113.30
1	X	71	ARG	NE-CZ-NH1	8.92	124.76	120.30
1	O	460	GLU	N-CA-C	-8.63	87.70	111.00
1	X	286	ASP	CB-CG-OD1	8.16	125.64	118.30
1	X	418	LEU	CB-CG-CD2	-8.08	97.26	111.00
1	X	286	ASP	CB-CG-OD2	-8.07	111.04	118.30
1	X	461	LEU	CA-CB-CG	8.03	133.76	115.30
1	O	189	ARG	CB-CG-CD	-7.89	91.07	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	189	ARG	CB-CG-CD	-7.73	91.51	111.60
1	O	243	MET	CG-SD-CE	-7.67	87.92	100.20
1	O	283	SER	N-CA-C	7.67	131.70	111.00
1	O	149	ILE	CG1-CB-CG2	-7.58	94.73	111.40
1	X	134	ASP	CB-CG-OD1	7.52	125.07	118.30
1	X	460	GLU	N-CA-C	-7.21	91.53	111.00
1	X	71	ARG	NE-CZ-NH2	-6.86	116.87	120.30
1	O	284	ASP	CB-CG-OD2	-6.74	112.24	118.30
1	O	143	ARG	NE-CZ-NH1	6.67	123.64	120.30
1	O	199	GLU	OE1-CD-OE2	6.64	131.27	123.30
1	X	358	ASP	CB-CG-OD2	-6.54	112.41	118.30
1	X	419	LEU	CB-CG-CD2	-6.45	100.04	111.00
1	O	29	ILE	CG1-CB-CG2	-6.37	97.39	111.40
1	X	136	TYR	CB-CG-CD2	-6.26	117.24	121.00
1	X	480	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	O	461	LEU	CA-CB-CG	6.14	129.42	115.30
1	O	143	ARG	CD-NE-CZ	6.14	132.19	123.60
1	O	146	LEU	CB-CG-CD2	6.04	121.27	111.00
1	O	246	ASP	CB-CG-OD1	5.83	123.55	118.30
1	X	157	ASP	CB-CG-OD1	5.81	123.53	118.30
1	X	370	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	O	442	LEU	CB-CG-CD1	5.72	120.73	111.00
1	X	283	SER	N-CA-C	5.58	126.06	111.00
1	O	283	SER	C-N-CA	5.35	135.07	121.70
1	O	88	VAL	CA-CB-CG1	-5.33	102.90	110.90
1	O	119	ASP	CB-CG-OD1	5.23	123.01	118.30
1	O	283	SER	CB-CA-C	-5.23	100.16	110.10
1	X	18	ARG	NE-CZ-NH2	5.23	122.91	120.30
1	O	207	LEU	CB-CG-CD2	-5.21	102.14	111.00
1	X	24	ARG	NE-CZ-NH2	5.18	122.89	120.30
1	X	107	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	X	438	GLU	CA-CB-CG	5.16	124.75	113.40
1	X	134	ASP	CB-CG-OD2	-5.12	113.69	118.30
1	O	283	SER	N-CA-CB	-5.09	102.86	110.50
1	X	7	VAL	CA-CB-CG2	-5.09	103.27	110.90
1	X	322	ARG	CG-CD-NE	-5.08	101.13	111.80
1	X	461	LEU	CA-C-N	-5.08	106.03	117.20
1	O	370	ARG	CB-CG-CD	5.07	124.79	111.60

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	O	233	PHE	Peptide
1	O	283	SER	Peptide
1	O	459	ASP	Peptide
1	O	461	LEU	Peptide
1	O	468	GLY	Peptide
1	X	282	LEU	Peptide
1	X	283	SER	Peptide
1	X	284	ASP	Peptide
1	X	461	LEU	Peptide
1	X	466	GLU	Peptide
1	X	467	GLU	Peptide

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	O	3838	0	3735	102	0
1	X	3838	0	3735	81	0
2	O	6	0	8	0	0
2	X	6	0	8	0	0
3	O	165	0	0	5	0
3	X	142	0	0	4	0
All	All	7995	0	7486	178	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 12.

All (178) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:X:243:MET:CB	1:X:243:MET:CG	1.77	1.56
1:O:370:ARG:CG	1:O:370:ARG:CD	1.81	1.52
1:O:229:ARG:HG3	1:O:229:ARG:HH11	1.09	1.11
1:X:459:ASP:C	1:X:461:LEU:N	2.11	1.02
1:X:466:GLU:HG2	1:X:466:GLU:O	1.60	1.01
1:O:18:ARG:HD2	3:O:600:HOH:O	1.61	0.99
1:O:284:ASP:OD1	1:O:286:ASP:HB2	1.64	0.98

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:O:126:HIS:NE2	1:O:283:SER:HB3	1.80	0.96
1:O:435:ALA:H	1:O:467:GLU:HB2	1.32	0.94
1:X:85:GLU:OE2	1:X:189:ARG:HD2	1.69	0.91
1:O:435:ALA:HB2	1:O:467:GLU:HA	1.51	0.90
1:X:459:ASP:C	1:X:461:LEU:H	1.70	0.89
1:O:132:VAL:O	1:O:191:MET:HE1	1.73	0.88
1:O:12:GLN:HE22	1:O:83:GLN:HE21	1.21	0.87
1:O:370:ARG:HG2	3:O:627:HOH:O	1.74	0.87
1:X:312:SER:HA	1:X:315:GLN:HG2	1.60	0.82
1:O:370:ARG:HG3	1:O:370:ARG:NH1	1.94	0.82
1:X:85:GLU:OE2	1:X:189:ARG:CD	2.29	0.81
1:O:124:MET:HE3	1:O:128:LYS:HE3	1.61	0.81
1:X:243:MET:CB	1:X:243:MET:SD	2.71	0.79
1:O:322:ARG:NH2	1:X:375:GLU:OE2	2.15	0.79
1:X:221:ASN:HD22	1:X:294:GLY:H	1.27	0.79
1:O:435:ALA:H	1:O:467:GLU:CB	1.97	0.77
1:X:284:ASP:HB3	1:X:286:ASP:H	1.49	0.77
1:O:126:HIS:NE2	1:O:283:SER:CB	2.48	0.76
1:O:229:ARG:HH11	1:O:229:ARG:CG	1.96	0.76
1:O:229:ARG:HG3	1:O:229:ARG:NH1	1.88	0.76
1:O:221:ASN:HD22	1:O:294:GLY:H	1.32	0.75
1:O:370:ARG:CG	3:O:627:HOH:O	2.33	0.74
1:O:283:SER:OG	1:O:284:ASP:N	2.21	0.74
1:O:126:HIS:CE1	1:O:283:SER:HB3	2.23	0.73
1:O:12:GLN:HE21	1:O:166:ILE:HG21	1.51	0.73
1:O:457:ASP:H	1:O:460:GLU:HG3	1.54	0.73
1:X:227:HIS:HB2	3:X:519:HOH:O	1.89	0.72
1:O:379:ARG:O	1:O:383:GLN:HG3	1.90	0.71
1:X:12:GLN:HE21	1:X:166:ILE:HG21	1.56	0.71
1:X:466:GLU:CG	1:X:466:GLU:O	2.39	0.70
1:O:370:ARG:CG	1:O:370:ARG:NE	2.54	0.69
1:X:221:ASN:ND2	1:X:294:GLY:H	1.90	0.69
1:O:457:ASP:OD1	1:O:460:GLU:N	2.26	0.68
1:X:458:LEU:O	1:X:461:LEU:HA	1.93	0.68
1:X:18:ARG:HD2	1:X:438:GLU:OE1	1.94	0.67
1:O:462:LYS:HB3	1:O:465:ALA:HB2	1.77	0.66
1:O:370:ARG:HG3	1:O:370:ARG:HH11	1.59	0.66
1:X:412:GLY:O	1:X:415:LYS:HG2	1.95	0.66
1:O:276:THR:HB	1:O:281:GLN:HE21	1.61	0.64
1:O:124:MET:HE2	1:O:128:LYS:HD2	1.79	0.64
1:O:85:GLU:OE2	1:O:189:ARG:CD	2.46	0.64
1:O:459:ASP:C	1:O:461:LEU:N	2.50	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:O:143:ARG:HD3	1:O:143:ARG:O	1.98	0.62
1:O:438:GLU:HG3	1:O:441:ALA:HB3	1.82	0.62
1:X:12:GLN:HE22	1:X:83:GLN:HE21	1.48	0.61
1:O:492:ALA:O	1:O:496:THR:HG23	2.00	0.61
1:O:285:ASN:O	1:O:285:ASN:CG	2.39	0.61
1:O:370:ARG:HD3	3:X:532:HOH:O	2.01	0.61
1:O:438:GLU:OE1	1:O:440:THR:HB	2.02	0.60
1:O:124:MET:CE	1:O:204:ILE:HG13	2.32	0.60
1:O:221:ASN:ND2	1:O:294:GLY:H	1.99	0.60
1:X:324:ILE:HG22	1:X:333:LEU:CD1	2.32	0.59
1:O:436:ASN:O	1:O:439:THR:HG22	2.01	0.59
1:O:133:ILE:HA	1:O:191:MET:CE	2.34	0.58
1:X:461:LEU:C	1:X:463:SER:H	2.07	0.57
1:O:325:GLU:HB2	1:O:329:GLN:OE1	2.04	0.57
1:O:85:GLU:OE2	1:O:189:ARG:HD3	2.04	0.57
1:O:370:ARG:CG	1:O:370:ARG:HH11	2.17	0.57
1:O:126:HIS:CE1	1:O:283:SER:CB	2.86	0.57
1:O:132:VAL:O	1:O:191:MET:CE	2.50	0.56
1:O:124:MET:HE3	1:O:128:LYS:CE	2.32	0.56
1:O:370:ARG:HE	1:X:315:GLN:HG3	1.69	0.56
1:X:436:ASN:O	1:X:439:THR:HG22	2.05	0.56
1:O:18:ARG:HG2	1:O:33:GLN:HG3	1.87	0.56
1:X:18:ARG:HG3	1:X:33:GLN:HB3	1.87	0.56
1:X:82:ASN:HD21	1:X:186:ASN:ND2	2.04	0.56
1:O:435:ALA:N	1:O:467:GLU:HB2	2.13	0.56
1:O:124:MET:HE1	1:O:204:ILE:HG13	1.87	0.56
1:X:82:ASN:HD21	1:X:186:ASN:HD21	1.53	0.55
1:O:85:GLU:OE2	1:O:189:ARG:HD2	2.07	0.55
1:O:370:ARG:NH1	1:O:370:ARG:CG	2.67	0.55
1:X:426:ILE:HD12	1:X:426:ILE:C	2.28	0.55
1:O:370:ARG:HG3	1:O:370:ARG:CZ	2.36	0.54
1:X:457:ASP:OD1	1:X:460:GLU:N	2.41	0.54
1:X:461:LEU:HB2	1:X:463:SER:H	1.73	0.53
1:O:123:GLU:HG2	3:O:660:HOH:O	2.07	0.53
1:O:386:ALA:HA	1:O:423:GLN:NE2	2.23	0.53
1:O:154:GLU:CD	1:O:154:GLU:H	2.12	0.53
1:X:397:LYS:HG2	1:X:404:ILE:HD12	1.90	0.53
1:X:85:GLU:OE2	1:X:189:ARG:HD3	2.09	0.53
1:X:438:GLU:HB3	3:X:587:HOH:O	2.08	0.53
1:X:461:LEU:C	1:X:463:SER:N	2.61	0.52
1:X:436:ASN:O	1:X:439:THR:CG2	2.57	0.52
1:X:400:SER:O	1:X:402:ILE:N	2.42	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:X:282:LEU:HD22	1:X:282:LEU:N	2.25	0.52
1:O:196:HIS:HE1	3:O:561:HOH:O	1.92	0.52
1:O:400:SER:C	1:O:402:ILE:H	2.14	0.52
1:O:322:ARG:HH21	1:X:375:GLU:CD	2.14	0.51
1:O:408:LYS:HZ3	1:O:432:GLN:NE2	2.08	0.51
1:X:282:LEU:C	1:X:399:ASP:OD2	2.49	0.51
1:O:85:GLU:HB2	1:O:104:TRP:HB3	1.93	0.51
1:O:370:ARG:CG	1:O:370:ARG:CZ	2.89	0.50
1:O:124:MET:CE	1:O:128:LYS:HD2	2.41	0.50
1:X:282:LEU:CD2	1:X:282:LEU:N	2.74	0.50
1:X:492:ALA:O	1:X:496:THR:HG23	2.12	0.50
1:X:281:GLN:OE1	1:X:400:SER:CB	2.60	0.49
1:X:255:MET:HA	1:X:257:PHE:CZ	2.48	0.49
1:X:121:HIS:HB3	1:X:124:MET:HE2	1.95	0.49
1:X:167:ASP:HB2	1:X:243:MET:HG2	1.95	0.48
1:X:462:LYS:HG2	1:X:465:ALA:CB	2.42	0.48
1:X:386:ALA:HA	1:X:423:GLN:HE22	1.78	0.48
1:O:390:LYS:HE3	1:O:484:TYR:CD2	2.49	0.48
1:X:80:ILE:O	1:X:243:MET:HA	2.14	0.47
1:O:396:MET:O	1:O:400:SER:HB2	2.14	0.47
1:O:241:ALA:HB1	1:O:451:ALA:HB3	1.96	0.47
1:X:341:ASN:HD21	1:X:383:GLN:HE22	1.61	0.47
1:X:314:ILE:HD11	1:X:382:LEU:HD23	1.97	0.47
1:X:272:ILE:N	1:X:272:ILE:HD12	2.29	0.47
1:O:124:MET:HE1	1:O:204:ILE:CG1	2.45	0.47
1:O:458:LEU:O	1:O:461:LEU:HA	2.14	0.47
1:X:356:TYR:CZ	1:X:491:VAL:HG11	2.50	0.47
1:O:459:ASP:HA	1:O:461:LEU:HA	1.96	0.47
1:X:20:ILE:HD13	1:X:441:ALA:CB	2.45	0.46
1:X:281:GLN:OE1	1:X:400:SER:HB2	2.15	0.46
1:O:51:ASN:HD21	1:O:96:GLN:NE2	2.13	0.46
1:X:498:LYS:HA	1:X:498:LYS:HD3	1.67	0.46
1:X:283:SER:HB3	1:X:289:THR:OG1	2.16	0.46
1:O:249:ALA:O	1:O:443:GLY:HA3	2.16	0.46
1:O:386:ALA:HA	1:O:423:GLN:HE22	1.79	0.46
1:X:284:ASP:HB3	1:X:286:ASP:N	2.24	0.46
1:O:438:GLU:HG3	1:O:438:GLU:O	2.16	0.46
1:X:124:MET:HE1	1:X:207:LEU:HD22	1.98	0.46
1:O:394:ASP:O	1:O:398:LYS:HG3	2.17	0.45
1:O:408:LYS:HZ3	1:O:432:GLN:HE21	1.64	0.45
1:X:457:ASP:O	1:X:460:GLU:HB2	2.16	0.45
1:X:81:THR:OG1	1:X:246:ASP:HA	2.17	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:X:30:GLY:HA3	1:X:68:SER:HB3	1.99	0.45
1:X:243:MET:HB2	1:X:243:MET:SD	2.55	0.45
1:O:20:ILE:HG23	1:O:28:LYS:HG3	1.98	0.45
1:X:461:LEU:HB2	1:X:463:SER:N	2.30	0.45
1:X:386:ALA:HA	1:X:423:GLN:NE2	2.32	0.45
1:O:6:TYR:CE2	1:O:70:ILE:HD12	2.52	0.45
1:O:124:MET:CE	1:O:128:LYS:CD	2.95	0.45
1:X:22:PHE:HA	1:X:27:LYS:O	2.17	0.45
1:X:124:MET:HE1	1:X:207:LEU:CD2	2.47	0.44
1:O:370:ARG:HD2	1:X:316:TRP:HB2	1.99	0.44
1:X:263:LYS:HA	1:X:408:LYS:O	2.18	0.44
1:O:154:GLU:CD	1:O:154:GLU:N	2.71	0.44
1:O:425:ASP:O	1:O:480:ARG:HD3	2.17	0.44
1:X:285:ASN:HA	1:X:285:ASN:HD22	1.40	0.43
1:O:283:SER:HB2	1:O:284:ASP:O	2.18	0.43
1:O:400:SER:HB3	1:O:402:ILE:HB	2.00	0.43
1:X:461:LEU:CA	1:X:463:SER:H	2.31	0.43
1:O:459:ASP:O	1:O:461:LEU:HG	2.18	0.43
1:O:231:TYR:O	1:O:234:TYR:HB2	2.19	0.43
1:X:8:MET:HB3	1:X:78:ILE:HD13	2.00	0.43
1:X:283:SER:O	1:X:284:ASP:O	2.37	0.43
1:X:181:VAL:CG2	1:X:219:LYS:HG3	2.48	0.43
1:O:330:SER:HA	1:O:378:VAL:HG11	2.01	0.42
1:O:400:SER:C	1:O:402:ILE:N	2.72	0.42
1:O:225:TYR:CE1	1:O:243:MET:HG3	2.54	0.42
1:X:426:ILE:HD12	1:X:427:LEU:N	2.35	0.42
1:O:54:TRP:CD1	1:O:173:LYS:HE2	2.54	0.42
1:X:329:GLN:OE1	1:X:332:GLU:OE1	2.38	0.42
1:O:172:TRP:CE2	1:O:177:GLY:HA2	2.54	0.42
1:O:498:LYS:HA	1:O:498:LYS:HD3	1.71	0.42
1:O:499:PHE:CZ	1:X:482:ASN:O	2.74	0.41
1:O:438:GLU:CG	1:O:441:ALA:HB3	2.47	0.41
1:O:327:SER:N	1:O:328:PRO:CD	2.83	0.41
1:X:318:ARG:O	1:X:322:ARG:HA	2.21	0.41
1:O:124:MET:HE3	1:O:128:LYS:CD	2.51	0.41
1:X:282:LEU:O	1:X:399:ASP:OD2	2.38	0.41
1:O:255:MET:HA	1:O:257:PHE:CZ	2.56	0.41
1:X:265:THR:HG23	1:X:410:ASP:OD2	2.21	0.41
1:X:370:ARG:NE	3:X:633:HOH:O	2.54	0.41
1:O:163:PHE:O	1:O:180:HIS:CE1	2.74	0.41
1:O:124:MET:CE	1:O:204:ILE:CG1	2.97	0.40
1:O:133:ILE:HA	1:O:191:MET:HE2	2.02	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:X:78:ILE:HG23	1:X:78:ILE:HD12	1.88	0.40
1:O:324:ILE:HG22	1:O:333:LEU:CD1	2.52	0.40
1:X:6:TYR:CE2	1:X:70:ILE:HD12	2.56	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	O	493/505 (98%)	466 (94%)	21 (4%)	6 (1%)	19	9
1	X	493/505 (98%)	466 (94%)	17 (3%)	10 (2%)	11	3
All	All	986/1010 (98%)	932 (94%)	38 (4%)	16 (2%)	14	5

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	O	283	SER
1	O	461	LEU
1	X	283	SER
1	X	284	ASP
1	X	461	LEU
1	X	469	GLN
1	O	340	ASP
1	O	468	GLY
1	X	285	ASN
1	X	401	GLY
1	X	462	LYS
1	X	470	MET
1	X	282	LEU
1	O	466	GLU
1	X	433	ARG
1	O	284	ASP

### 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	O	401/408 (98%)	381 (95%)	20 (5%)	34	26
1	X	401/408 (98%)	380 (95%)	21 (5%)	32	25
All	All	802/816 (98%)	761 (95%)	41 (5%)	33	25

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	12	GLN
1	O	29	ILE
1	O	124	MET
1	O	143	ARG
1	O	149	ILE
1	O	165	THR
1	O	189	ARG
1	O	229	ARG
1	O	263	LYS
1	O	284	ASP
1	O	415	LYS
1	O	426	ILE
1	O	429	ILE
1	O	439	THR
1	O	456	LYS
1	O	461	LEU
1	O	464	MET
1	O	467	GLU
1	O	469	GLN
1	O	488	LYS
1	X	12	GLN
1	X	61	ILE
1	X	92	LYS
1	X	150	GLU
1	X	189	ARG
1	X	243	MET
1	X	263	LYS
1	X	282	LEU
1	X	284	ASP

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Mol	Chain	Res	Type
1	X	285	ASN
1	X	328	PRO
1	X	329	GLN
1	X	332	GLU
1	X	370	ARG
1	X	403	ASP
1	X	415	LYS
1	X	438	GLU
1	X	460	GLU
1	X	461	LEU
1	X	467	GLU
1	X	469	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	O	12	GLN
1	O	96	GLN
1	O	196	HIS
1	O	221	ASN
1	O	281	GLN
1	O	383	GLN
1	O	423	GLN
1	O	432	GLN
1	X	12	GLN
1	X	115	GLN
1	X	180	HIS
1	X	186	ASN
1	X	221	ASN
1	X	285	ASN
1	X	329	GLN
1	X	383	GLN
1	X	423	GLN
1	X	432	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

2 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	GOL	O	507	-	5,5,5	0.87	0	5,5,5	1.46	1 (20%)
2	GOL	X	507	-	5,5,5	0.87	0	5,5,5	1.45	1 (20%)

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	O	507	-	-	0/4/4/4	0/0/0/0
2	GOL	X	507	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	507	GOL	C3-C2-C1	-2.61	99.75	111.26
2	X	507	GOL	C3-C2-C1	-2.61	99.76	111.26

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

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 ⓘ

### 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	495/505 (98%)	0.02	17 (3%) 43 43	14, 24, 46, 79	0
1	X	495/505 (98%)	0.03	16 (3%) 45 45	15, 23, 46, 71	0
All	All	990/1010 (98%)	0.03	33 (3%) 44 44	14, 23, 46, 79	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	461	LEU	7.5
1	O	462	LYS	5.5
1	X	461	LEU	5.1
1	O	466	GLU	4.8
1	X	467	GLU	4.6
1	O	467	GLU	4.4
1	X	466	GLU	4.3
1	O	402	ILE	4.2
1	X	234	TYR	4.2
1	O	400	SER	3.7
1	X	285	ASN	3.6
1	X	401	GLY	3.6
1	X	435	ALA	3.6
1	X	469	GLN	3.6
1	O	285	ASN	3.5
1	O	499	PHE	3.4
1	X	402	ILE	3.1
1	X	462	LYS	3.1
1	X	284	ASP	3.0
1	O	465	ALA	3.0
1	O	459	ASP	2.9
1	X	281	GLN	2.9
1	O	234	TYR	2.9
1	X	399	ASP	2.6

*Continued on next page...*

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Mol	Chain	Res	Type	RSRZ
1	O	457	ASP	2.5
1	O	458	LEU	2.5
1	X	329	GLN	2.3
1	O	283	SER	2.3
1	O	29	ILE	2.3
1	O	435	ALA	2.2
1	X	403	ASP	2.2
1	X	463	SER	2.2
1	O	336	LYS	2.1

## 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 ⓘ

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	GOL	O	507	6/6	0.26	5.64	15,16,18,18	0
2	GOL	X	507	6/6	0.22	2.45	15,16,18,18	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.