



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 27, 2026 – 04:47 PM EDT

PDB ID : 3CYJ / pdb_00003cyj
Title : Crystal structure of a mandelate racemase/muconate lactonizing enzyme-like protein from *Rubrobacter xylanophilus*
Authors : Bonanno, J.B.; Freeman, J.; Bain, K.T.; Zhang, F.; Bravo, J.; Smith, D.; Wasserman, S.; Sauder, J.M.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2008-04-25
Resolution : 2.30 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

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>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

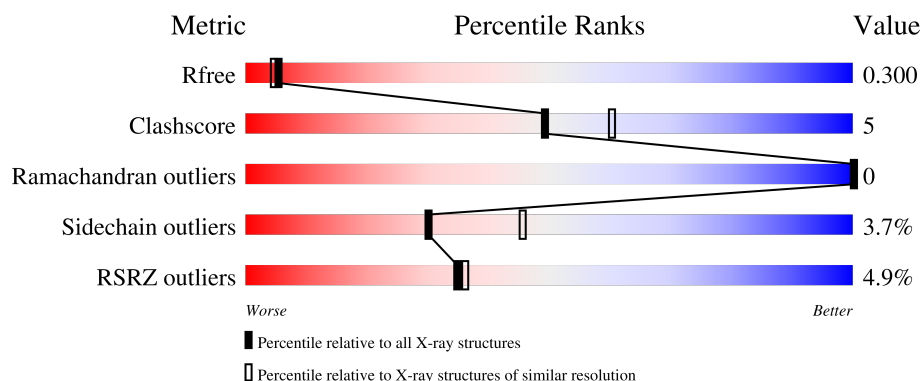
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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 $\leq 5\%$. 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	372	5% 83% 11% ..
1	B	372	2% 81% 15% ..
1	C	372	10% 85% 10% ..
1	D	372	2% 83% 12% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11364 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 Mandelate racemase/muconate lactonizing enzyme-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	359	Total	C	N	O	S	0	2	0
			2704	1703	487	503	11			
1	B	359	Total	C	N	O	S	0	3	0
			2725	1711	498	505	11			
1	C	359	Total	C	N	O	S	0	2	0
			2704	1703	487	503	11			
1	D	359	Total	C	N	O	S	0	1	0
			2705	1698	491	505	11			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	expression tag	UNP Q1ASJ4
A	0	SER	-	expression tag	UNP Q1ASJ4
A	1	LEU	-	expression tag	UNP Q1ASJ4
A	363	GLU	-	expression tag	UNP Q1ASJ4
A	364	GLY	-	expression tag	UNP Q1ASJ4
A	365	HIS	-	expression tag	UNP Q1ASJ4
A	366	HIS	-	expression tag	UNP Q1ASJ4
A	367	HIS	-	expression tag	UNP Q1ASJ4
A	368	HIS	-	expression tag	UNP Q1ASJ4
A	369	HIS	-	expression tag	UNP Q1ASJ4
A	370	HIS	-	expression tag	UNP Q1ASJ4
B	-1	MET	-	expression tag	UNP Q1ASJ4
B	0	SER	-	expression tag	UNP Q1ASJ4
B	1	LEU	-	expression tag	UNP Q1ASJ4
B	363	GLU	-	expression tag	UNP Q1ASJ4
B	364	GLY	-	expression tag	UNP Q1ASJ4
B	365	HIS	-	expression tag	UNP Q1ASJ4
B	366	HIS	-	expression tag	UNP Q1ASJ4
B	367	HIS	-	expression tag	UNP Q1ASJ4
B	368	HIS	-	expression tag	UNP Q1ASJ4
B	369	HIS	-	expression tag	UNP Q1ASJ4

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	370	HIS	-	expression tag	UNP Q1ASJ4
C	-1	MET	-	expression tag	UNP Q1ASJ4
C	0	SER	-	expression tag	UNP Q1ASJ4
C	1	LEU	-	expression tag	UNP Q1ASJ4
C	363	GLU	-	expression tag	UNP Q1ASJ4
C	364	GLY	-	expression tag	UNP Q1ASJ4
C	365	HIS	-	expression tag	UNP Q1ASJ4
C	366	HIS	-	expression tag	UNP Q1ASJ4
C	367	HIS	-	expression tag	UNP Q1ASJ4
C	368	HIS	-	expression tag	UNP Q1ASJ4
C	369	HIS	-	expression tag	UNP Q1ASJ4
C	370	HIS	-	expression tag	UNP Q1ASJ4
D	-1	MET	-	expression tag	UNP Q1ASJ4
D	0	SER	-	expression tag	UNP Q1ASJ4
D	1	LEU	-	expression tag	UNP Q1ASJ4
D	363	GLU	-	expression tag	UNP Q1ASJ4
D	364	GLY	-	expression tag	UNP Q1ASJ4
D	365	HIS	-	expression tag	UNP Q1ASJ4
D	366	HIS	-	expression tag	UNP Q1ASJ4
D	367	HIS	-	expression tag	UNP Q1ASJ4
D	368	HIS	-	expression tag	UNP Q1ASJ4
D	369	HIS	-	expression tag	UNP Q1ASJ4
D	370	HIS	-	expression tag	UNP Q1ASJ4

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Na 1 1	0	0
2	C	1	Total Na 1 1	0	0

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

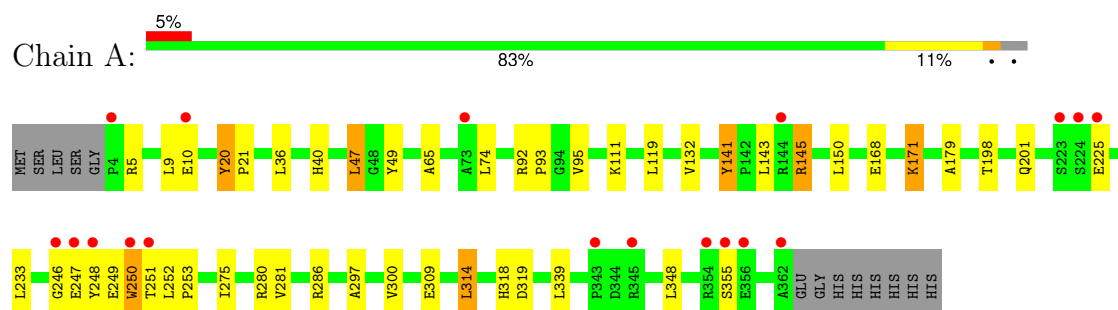
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	113	Total	O	0	0
			113	113		
4	B	137	Total	O	0	0
			137	137		
4	C	112	Total	O	0	0
			112	112		
4	D	150	Total	O	0	0
			150	150		

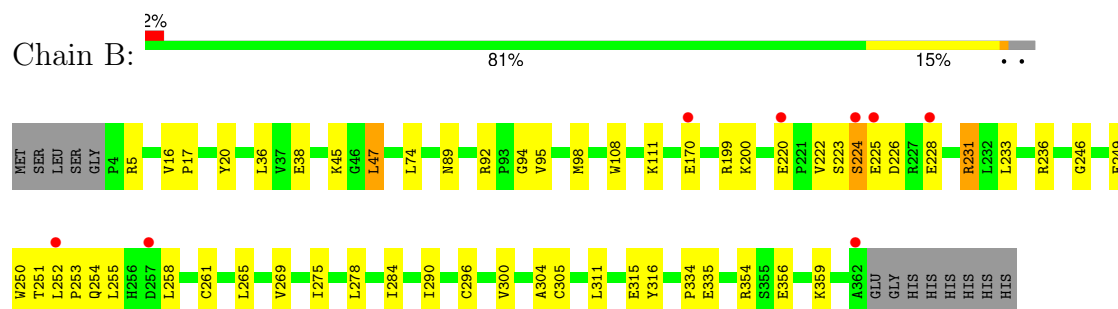
3 Residue-property plots [i](#)

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.

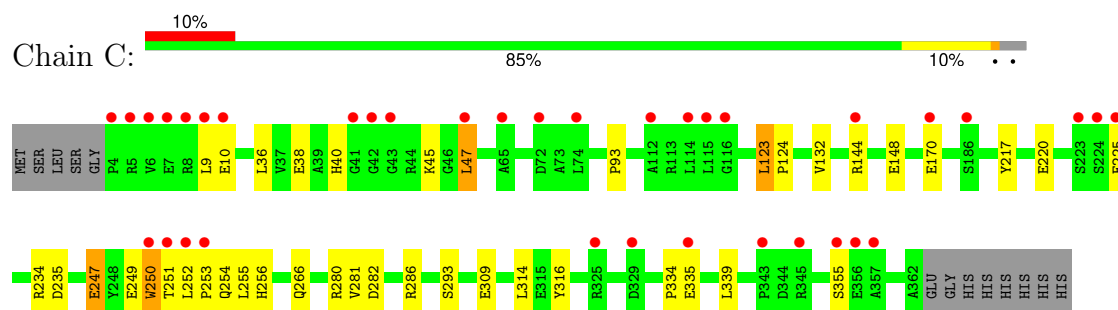
- Molecule 1: Mandelate racemase/muconate lactonizing enzyme-like protein



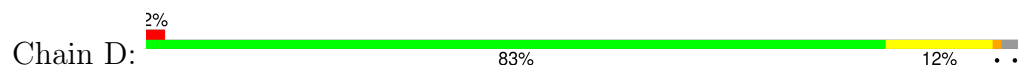
- Molecule 1: Mandelate racemase/muconate lactonizing enzyme-like protein

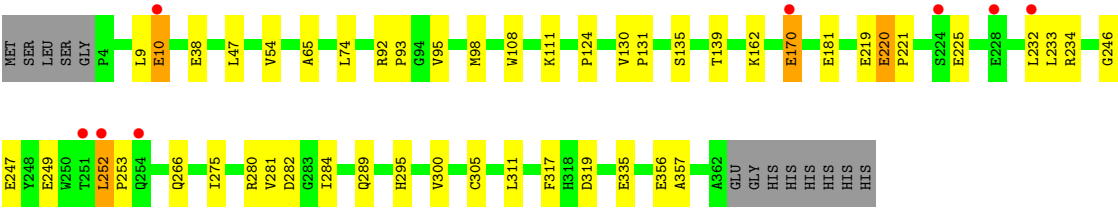


- Molecule 1: Mandelate racemase/muconate lactonizing enzyme-like protein



- Molecule 1: Mandelate racemase/muconate lactonizing enzyme-like protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	193.10Å 193.10Å 113.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 20.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.2 (20.00-2.30) 97.9 (20.00-2.30)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	0.16	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.55 (at 2.29Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.243 , 0.292 0.252 , 0.300	Depositor DCC
R_{free} test set	4688 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	28.2	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 44.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.57$, $\langle L^2 \rangle = 0.42$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11364	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 69.77 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.4988e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical 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: NA, 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	A	1.08	1/2773 (0.0%)	1.11	4/3769 (0.1%)
1	B	1.16	1/2795 (0.0%)	1.09	6/3793 (0.2%)
1	C	1.05	0/2773	1.06	4/3769 (0.1%)
1	D	1.17	0/2769	1.09	6/3761 (0.2%)
All	All	1.12	2/11110 (0.0%)	1.09	20/15092 (0.1%)

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	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	297	ALA	CA-CB	7.42	1.57	1.52
1	B	290	ILE	C-O	-5.54	1.18	1.24

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	247	GLU	N-CA-C	7.63	121.69	112.38
1	B	225	GLU	N-CA-C	-7.41	103.34	112.38
1	C	247	GLU	N-CA-C	6.58	120.17	111.75
1	B	20	TYR	CA-C-N	-6.23	113.34	119.76
1	B	20	TYR	C-N-CA	-6.23	113.34	119.76
1	B	199	ARG	N-CA-C	5.88	117.37	111.07
1	A	141	TYR	CA-C-N	-5.76	114.33	120.03

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	141	TYR	C-N-CA	-5.76	114.33	120.03
1	B	354	ARG	N-CA-C	5.67	117.14	111.07
1	D	124	PRO	CA-C-N	-5.44	115.10	122.77
1	D	124	PRO	C-N-CA	-5.44	115.10	122.77
1	D	300	VAL	CB-CA-C	-5.40	104.94	112.02
1	C	123	LEU	CA-C-N	-5.33	114.23	119.93
1	C	123	LEU	C-N-CA	-5.33	114.23	119.93
1	B	251	THR	N-CA-C	5.27	117.87	109.81
1	C	234	ARG	N-CA-C	-5.18	105.55	111.14
1	D	220	GLU	CA-C-N	-5.11	113.66	119.28
1	D	220	GLU	C-N-CA	-5.11	113.66	119.28
1	A	20	TYR	N-CA-C	-5.10	103.63	108.22
1	D	54	VAL	CB-CA-C	-5.04	104.69	112.05

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	224	SER	Peptide

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	2704	0	2648	35	0
1	B	2725	0	2690	31	0
1	C	2704	0	2648	29	0
1	D	2705	0	2653	26	1
2	A	1	0	0	0	0
2	C	1	0	0	0	0
3	A	6	0	8	0	0
3	C	6	0	8	0	0
4	A	113	0	0	1	1
4	B	137	0	0	2	0
4	C	112	0	0	0	0
4	D	150	0	0	1	0
All	All	11364	0	10655	115	1

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 5.

All (115) 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:47:LEU:C	1:A:47:LEU:HD23	1.81	1.06
1:C:93:PRO:HB3	1:C:250[B]:TRP:CD2	2.02	0.94
1:D:282:ASP:HB2	4:D:497:HOH:O	1.78	0.84
1:C:40:HIS:CE1	1:C:45:LYS:HD3	2.14	0.82
1:D:252:LEU:HD23	1:D:284:ILE:HD11	1.60	0.82
1:A:47:LEU:HD23	1:A:47:LEU:O	1.78	0.82
1:A:47:LEU:C	1:A:47:LEU:CD2	2.56	0.77
1:C:36:LEU:HD11	1:C:47:LEU:HG	1.68	0.76
1:A:93:PRO:HB3	1:A:250[B]:TRP:CG	2.21	0.75
1:A:93:PRO:HB3	1:A:250[B]:TRP:CD2	2.22	0.74
1:C:93:PRO:HB3	1:C:250[B]:TRP:CG	2.22	0.74
1:A:280:ARG:NH1	1:C:309:GLU:OE1	2.25	0.69
1:B:170:GLU:H	1:B:170:GLU:CD	2.01	0.68
1:D:252:LEU:CD2	1:D:284:ILE:HD11	2.23	0.68
1:A:309:GLU:OE1	1:C:280:ARG:NH1	2.26	0.65
1:C:144:ARG:O	1:C:148:GLU:HG3	1.96	0.65
1:A:251:THR:HB	1:A:253:PRO:HD2	1.79	0.64
1:A:248:TYR:O	1:A:250[A]:TRP:NE1	2.31	0.63
1:B:94:GLY:C	1:B:98:MET:HE3	2.24	0.62
1:C:220:GLU:OE2	1:C:247:GLU:HG2	2.01	0.61
1:B:47:LEU:C	1:B:47:LEU:HD23	2.27	0.60
1:A:10:GLU:OE2	1:A:40:HIS:HE1	1.86	0.58
1:B:269:VAL:HG11	1:B:300:VAL:HG13	1.86	0.57
1:C:132:VAL:HG11	1:C:339:LEU:HG	1.85	0.57
1:B:38:GLU:OE1	1:B:45:LYS:HE3	2.04	0.57
1:D:170:GLU:H	1:D:170:GLU:CD	2.12	0.56
1:C:250[B]:TRP:CD1	1:C:251:THR:HG23	2.40	0.56
1:B:228:GLU:OE2	1:B:231[A]:ARG:NH2	2.37	0.55
1:A:286:ARG:NH2	4:A:394:HOH:O	2.36	0.55
1:B:236[A]:ARG:HH11	1:B:236[A]:ARG:HG3	1.73	0.53
1:D:305:CYS:HB3	1:D:311:LEU:HD22	1.90	0.53
1:B:89:ASN:OD1	4:B:474:HOH:O	2.19	0.53
1:B:356:GLU:O	1:B:359:LYS:HB3	2.09	0.53
1:C:170:GLU:O	1:C:170:GLU:HG2	2.09	0.53
1:C:253:PRO:HA	1:C:256:HIS:HB3	1.91	0.53
1:D:74:LEU:O	1:D:111:LYS:HE3	2.09	0.53
1:C:251:THR:O	1:C:254:GLN:HB2	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:246:GLY:HA3	1:D:266:GLN:O	2.09	0.52
1:C:249:GLU:HG3	1:C:254:GLN:HB3	1.91	0.52
1:A:252:LEU:N	1:A:253:PRO:CD	2.73	0.52
1:C:93:PRO:HB3	1:C:250[B]:TRP:CE2	2.43	0.52
1:B:305:CYS:HB3	1:B:311:LEU:HD22	1.91	0.52
1:A:47:LEU:O	1:A:47:LEU:CD2	2.52	0.52
1:B:255:LEU:HD22	1:B:265:LEU:HD21	1.91	0.52
1:A:119:LEU:HD21	1:A:275:ILE:CD1	2.40	0.51
1:A:251:THR:CB	1:A:253:PRO:HD2	2.40	0.51
1:A:119:LEU:HD21	1:A:275:ILE:HD13	1.93	0.51
1:C:217:TYR:OH	1:C:266:GLN:NE2	2.44	0.51
1:B:222:VAL:O	4:B:472:HOH:O	2.19	0.51
1:D:9:LEU:HD12	1:D:65:ALA:HA	1.93	0.50
1:D:219:GLU:HG2	1:D:220:GLU:HG3	1.93	0.50
1:A:168:GLU:OE1	1:A:171:LYS:HD3	2.11	0.50
1:D:252:LEU:HD11	1:D:280:ARG:CB	2.42	0.50
1:D:234:ARG:C	1:D:234:ARG:HD2	2.37	0.50
1:A:246:GLY:O	1:A:249:GLU:OE1	2.31	0.49
1:B:223:SER:O	1:B:224:SER:CB	2.57	0.49
1:A:92:ARG:N	1:A:93:PRO:CD	2.75	0.49
1:C:225:GLU:HG2	1:D:253:PRO:HG2	1.95	0.49
1:D:95:VAL:HA	1:D:98:MET:HE3	1.95	0.48
1:A:20:TYR:CG	1:A:21:PRO:HD2	2.50	0.47
1:A:36:LEU:HD11	1:A:47:LEU:HG	1.97	0.47
1:A:150:LEU:HD12	1:A:179:ALA:HB1	1.95	0.47
1:B:98:MET:HE2	1:B:250:TRP:CH2	2.50	0.47
1:A:74:LEU:O	1:A:111:LYS:HE3	2.15	0.46
1:B:36:LEU:HD11	1:B:47:LEU:HG	1.96	0.46
1:D:130:VAL:HA	1:D:131:PRO:HD3	1.82	0.46
1:C:38:GLU:OE1	1:C:45:LYS:HD2	2.17	0.45
1:D:10:GLU:HG3	1:D:38:GLU:HB2	1.97	0.45
1:A:95:VAL:HB	1:B:95:VAL:HB	1.98	0.45
1:B:108:TRP:CD1	1:B:275:ILE:HB	2.52	0.45
1:B:252:LEU:HB3	1:B:253:PRO:HD3	1.98	0.45
1:B:246:GLY:HA2	1:B:258:LEU:CD2	2.47	0.44
1:D:252:LEU:HD11	1:D:280:ARG:HB3	1.99	0.44
1:C:93:PRO:HB2	1:D:93:PRO:HG2	1.99	0.44
1:B:200:LYS:HA	1:B:200:LYS:HD3	1.85	0.44
1:B:231[A]:ARG:HG3	1:B:261:CYS:HA	2.00	0.44
1:D:221:PRO:HG2	1:D:233:LEU:HD12	1.99	0.44
1:B:224:SER:C	1:B:226:ASP:N	2.71	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:316:TYR:CZ	1:B:334:PRO:HG3	2.54	0.43
1:A:132:VAL:HG11	1:A:339:LEU:HG	1.99	0.43
1:D:92:ARG:N	1:D:93:PRO:CD	2.81	0.43
1:D:95:VAL:HA	1:D:98:MET:CE	2.48	0.43
1:B:236[A]:ARG:NH1	1:C:235:ASP:O	2.52	0.43
1:D:162:LYS:NZ	1:D:219:GLU:OE1	2.51	0.43
1:C:316:TYR:CZ	1:C:334:PRO:HG3	2.54	0.42
1:B:74:LEU:O	1:B:111:LYS:HE3	2.19	0.42
1:C:249:GLU:CG	1:C:254:GLN:HB3	2.50	0.42
1:C:252:LEU:HD21	1:C:280:ARG:HB3	2.02	0.42
1:D:108:TRP:CD1	1:D:275:ILE:HB	2.55	0.42
1:D:356:GLU:O	1:D:357:ALA:C	2.60	0.42
1:A:9:LEU:HD12	1:A:65:ALA:HA	2.02	0.42
1:A:141:TYR:CG	1:A:145:ARG:HG2	2.54	0.42
1:B:249:GLU:HG3	1:B:254:GLN:HB3	2.02	0.42
1:D:135:SER:HB3	1:D:317:PHE:HA	2.01	0.42
1:A:314:LEU:C	1:A:314:LEU:HD12	2.45	0.42
1:B:16:VAL:HA	1:B:17:PRO:HD3	1.92	0.42
1:B:278:LEU:HD23	1:B:304:ALA:HB1	2.02	0.42
1:A:10:GLU:CD	1:A:40:HIS:HE1	2.28	0.41
1:A:93:PRO:HB3	1:A:250[B]:TRP:CD1	2.53	0.41
1:C:123:LEU:O	1:C:124:PRO:C	2.62	0.41
1:A:171:LYS:HB2	1:A:171:LYS:HE3	1.70	0.41
1:C:286:ARG:HA	1:C:286:ARG:HD2	1.91	0.41
1:A:49:TYR:CZ	1:A:300:VAL:HG23	2.56	0.41
1:C:47:LEU:C	1:C:47:LEU:HD23	2.46	0.41
1:D:317:PHE:CE2	1:D:319:ASP:HB2	2.56	0.41
1:C:250[B]:TRP:NE1	1:C:251:THR:HG23	2.37	0.40
1:C:266:GLN:HA	1:C:293:SER:O	2.21	0.40
1:B:296:CYS:H	1:B:315:GLU:HB3	1.85	0.40
1:D:247:GLU:HB2	1:D:295:HIS:CD2	2.56	0.40
1:A:198:THR:OG1	1:A:201:GLN:HB2	2.21	0.40
1:A:318:HIS:O	1:A:319:ASP:C	2.64	0.40
1:B:38:GLU:CD	1:B:45:LYS:HE3	2.46	0.40
1:C:255:LEU:HD23	1:C:255:LEU:HA	1.94	0.40
1:A:119:LEU:HD23	1:A:348:LEU:HD21	2.02	0.40
1:B:224:SER:C	1:B:226:ASP:H	2.30	0.40

All (1) 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)
1:D:289:GLN:OE1	4:A:442:HOH:O[7_556]	2.16	0.04

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	A	359/372 (96%)	350 (98%)	9 (2%)	0	100	100
1	B	360/372 (97%)	353 (98%)	7 (2%)	0	100	100
1	C	359/372 (96%)	352 (98%)	7 (2%)	0	100	100
1	D	358/372 (96%)	351 (98%)	7 (2%)	0	100	100
All	All	1436/1488 (96%)	1406 (98%)	30 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	267/282 (95%)	255 (96%)	12 (4%)	24	37
1	B	271/282 (96%)	262 (97%)	9 (3%)	33	50
1	C	267/282 (95%)	257 (96%)	10 (4%)	30	45
1	D	268/282 (95%)	257 (96%)	11 (4%)	27	41
All	All	1073/1128 (95%)	1031 (96%)	42 (4%)	30	43

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ARG
1	A	47	LEU
1	A	143	LEU
1	A	145	ARG
1	A	171	LYS
1	A	225	GLU
1	A	233	LEU
1	A	250[A]	TRP
1	A	250[B]	TRP
1	A	281	VAL
1	A	314	LEU
1	A	355	SER
1	B	5	ARG
1	B	47	LEU
1	B	92	ARG
1	B	220	GLU
1	B	231[A]	ARG
1	B	231[B]	ARG
1	B	233	LEU
1	B	284	ILE
1	B	335	GLU
1	C	9	LEU
1	C	10	GLU
1	C	47	LEU
1	C	250[A]	TRP
1	C	250[B]	TRP
1	C	281	VAL
1	C	282	ASP
1	C	314	LEU
1	C	335	GLU
1	C	355	SER
1	D	10	GLU
1	D	47	LEU
1	D	139	THR
1	D	170	GLU
1	D	181	GLU
1	D	225	GLU
1	D	232	LEU
1	D	249	GLU
1	D	252	LEU
1	D	281	VAL
1	D	335	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	HIS
1	A	147	GLN
1	A	256	HIS
1	A	288	HIS
1	B	266	GLN
1	B	295	HIS
1	C	266	GLN
1	D	40	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are 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	GOL	C	372	-	5,5,5	0.28	0	5,5,5	0.71	0
3	GOL	A	372	-	5,5,5	0.44	0	5,5,5	1.19	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
3	GOL	C	372	-	-	0/4/4/4	-
3	GOL	A	372	-	-	3/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	372	GOL	O2-C2-C1	2.18	118.21	109.18

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	372	GOL	O1-C1-C2-C3
3	A	372	GOL	O1-C1-C2-O2
3	A	372	GOL	O2-C2-C3-O3

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	359/372 (96%)	0.63	18 (5%) 34 35	23, 45, 57, 70	2 (0%)
1	B	359/372 (96%)	0.26	8 (2%) 62 64	19, 39, 53, 65	3 (0%)
1	C	359/372 (96%)	0.78	36 (10%) 12 14	24, 45, 60, 71	2 (0%)
1	D	359/372 (96%)	0.27	8 (2%) 62 64	18, 39, 52, 61	1 (0%)
All	All	1436/1488 (96%)	0.48	70 (4%) 35 36	18, 42, 56, 71	8 (0%)

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	250[A]	TRP	7.1
1	C	250[A]	TRP	5.9
1	B	224	SER	4.8
1	C	42	GLY	4.1
1	C	251	THR	3.9
1	C	224	SER	3.5
1	D	224	SER	3.4
1	A	355	SER	3.3
1	C	357	ALA	3.2
1	A	4	PRO	3.2
1	C	355	SER	3.2
1	C	225	GLU	3.1
1	C	252	LEU	3.0
1	A	354	ARG	3.0
1	A	362	ALA	3.0
1	D	232	LEU	2.9
1	C	144	ARG	2.9
1	A	251	THR	2.9
1	C	114	LEU	2.8
1	C	170	GLU	2.8
1	C	41	GLY	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	343	PRO	2.8
1	C	356	GLU	2.7
1	A	345	ARG	2.7
1	C	47	LEU	2.6
1	C	72	ASP	2.6
1	C	329	ASP	2.6
1	B	252	LEU	2.5
1	C	74	LEU	2.5
1	D	252	LEU	2.5
1	C	43	GLY	2.5
1	B	220	GLU	2.5
1	C	5	ARG	2.4
1	C	7	GLU	2.4
1	A	223	SER	2.4
1	C	186	SER	2.4
1	D	10	GLU	2.4
1	C	65	ALA	2.4
1	D	251	THR	2.4
1	C	223	SER	2.4
1	A	225	GLU	2.3
1	C	10	GLU	2.3
1	C	4	PRO	2.3
1	B	228	GLU	2.3
1	B	170	GLU	2.3
1	C	6	VAL	2.3
1	C	115	LEU	2.2
1	A	246	GLY	2.2
1	B	362	ALA	2.2
1	D	228	GLU	2.2
1	B	257	ASP	2.2
1	B	225	GLU	2.2
1	C	343	PRO	2.2
1	C	116	GLY	2.2
1	C	112	ALA	2.2
1	A	224	SER	2.1
1	A	247	GLU	2.1
1	A	356	GLU	2.1
1	C	325	ARG	2.1
1	C	335	GLU	2.1
1	D	254	GLN	2.1
1	A	144	ARG	2.1
1	D	170	GLU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	9	LEU	2.1
1	A	10	GLU	2.0
1	A	73	ALA	2.0
1	C	253	PRO	2.0
1	A	248	TYR	2.0
1	C	8	ARG	2.0
1	C	345	ARG	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	A	372	6/6	0.83	0.17	50,54,58,60	0
3	GOL	C	372	6/6	0.84	0.17	53,57,60,66	0
2	NA	A	371	1/1	0.87	0.12	55,55,55,55	0
2	NA	C	371	1/1	0.89	0.14	58,58,58,58	0

6.5 Other polymers [i](#)

There are no such residues in this entry.