



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:02 AM UTC

PDB ID : 2PP0 / pdb_00002pp0
Title : Crystal structure of L-talarate/galactarate dehydratase from Salmonella typhimurium LT2
Authors : Fedorov, A.A.; Fedorov, E.V.; Yew, W.S.; Gerlt, J.A.; Almo, S.C.
Deposited on : 2007-04-27
Resolution : 2.20 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

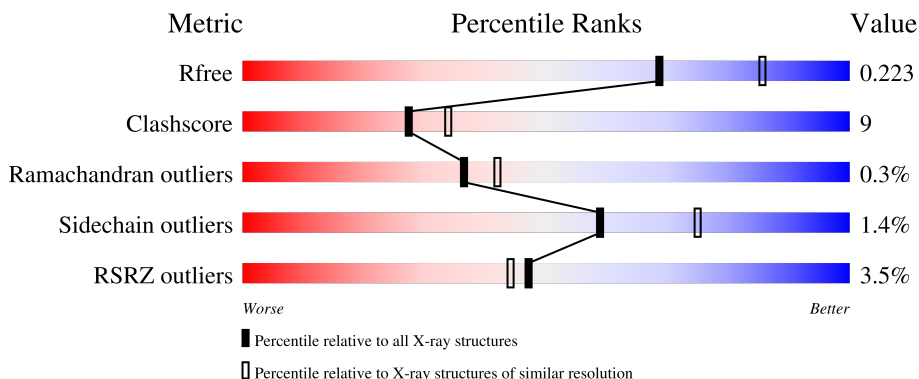
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


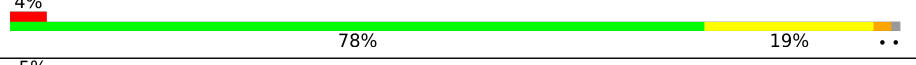

The reported resolution of this entry is 2.20 Å.

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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	398	 3% 80% 18% ..
1	B	398	 4% 78% 19% ..
1	C	398	 5% 79% 19% ..

2 Entry composition [i](#)

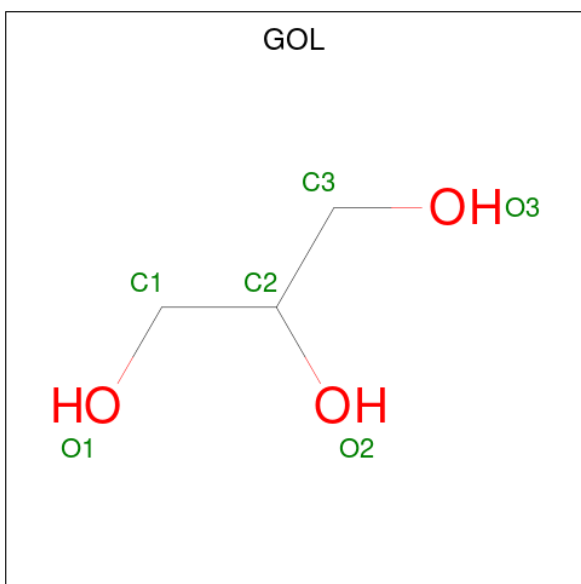
There are 3 unique types of molecules in this entry. The entry contains 9690 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 L-talarate/Galactarate Dehydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	395	Total 3081	C 1951	N 548	O 570	S 12	0	0	0
1	B	395	Total 3081	C 1951	N 548	O 570	S 12	0	0	0
1	C	395	Total 3081	C 1951	N 548	O 570	S 12	0	0	0

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

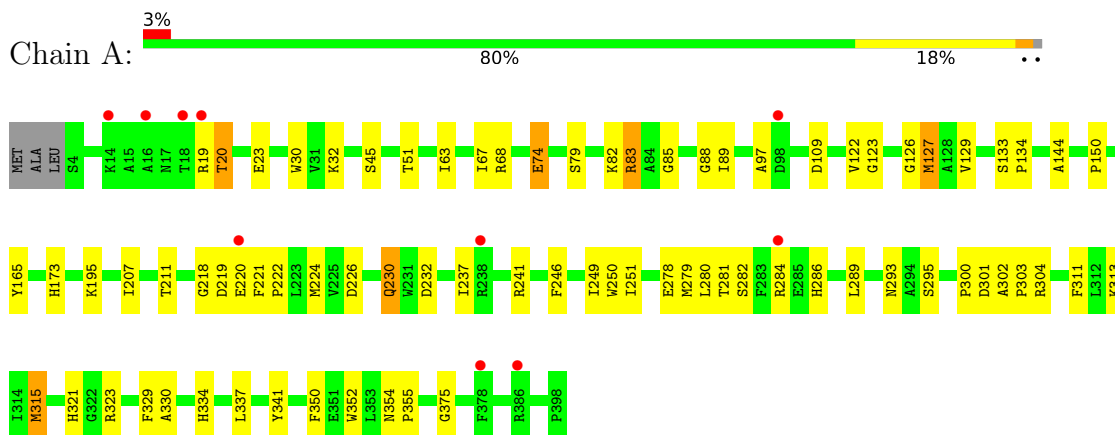
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	207	Total 207	O 207	0	0
3	B	102	Total 102	O 102	0	0
3	C	120	Total 120	O 120	0	0

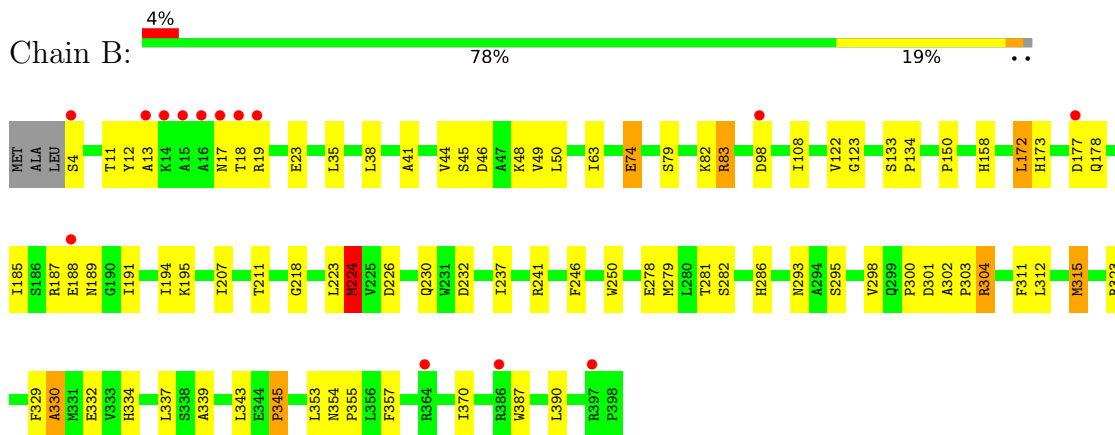
3 Residue-property plots [i](#)

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.

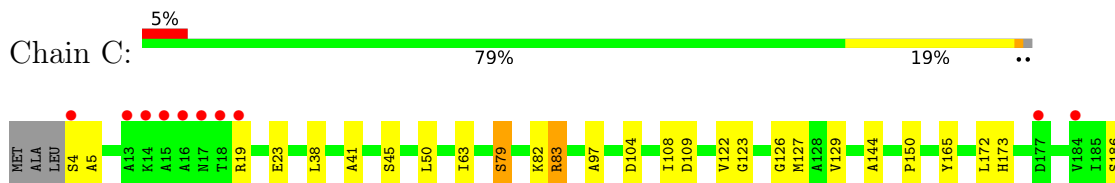
- Molecule 1: L-talarate/Galactarate Dehydratase

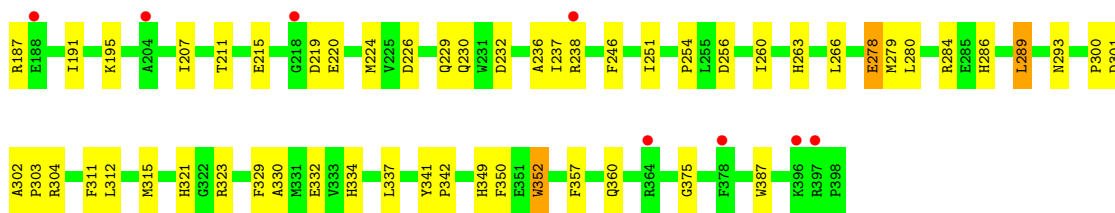


- Molecule 1: L-talarate/Galactarate Dehydratase



- Molecule 1: L-talarate/Galactarate Dehydratase





4 Data and refinement statistics

Property	Value	Source
Space group	P 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	173.89Å 173.89Å 123.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.87 – 2.20 24.87 – 2.20	Depositor EDS
% Data completeness (in resolution range)	90.3 (24.87-2.20) 90.2 (24.87-2.20)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.65 (at 2.00Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.207 , 0.223 0.207 , 0.223	Depositor DCC
R_{free} test set	6336 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	28.7	Xtrriage
Anisotropy	0.303	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 30.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9690	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.45% of the height of the origin peak. No significant pseudotranslation is detected.*

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: 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	0.46	1/3149 (0.0%)	0.94	15/4266 (0.4%)
1	B	0.42	2/3149 (0.1%)	0.92	11/4266 (0.3%)
1	C	0.40	1/3149 (0.0%)	0.93	15/4266 (0.4%)
All	All	0.43	4/9447 (0.0%)	0.93	41/12798 (0.3%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	127	MET	SD-CE	-10.27	1.53	1.79
1	B	315	MET	SD-CE	-7.63	1.60	1.79
1	B	224	MET	SD-CE	-7.30	1.61	1.79
1	C	127	MET	SD-CE	-5.10	1.66	1.79

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	230	GLN	N-CA-C	8.21	123.35	113.16
1	A	218	GLY	N-CA-C	-7.42	103.98	112.29
1	A	219	ASP	N-CA-C	7.36	119.30	111.28
1	B	150	PRO	N-CA-C	-7.33	100.41	111.41
1	B	230	GLN	N-CA-C	7.26	121.98	113.20
1	C	122	VAL	N-CA-C	7.23	118.34	111.91
1	C	220	GLU	N-CA-C	7.22	122.35	112.90
1	B	122	VAL	N-CA-C	7.06	118.19	111.91
1	C	230	GLN	N-CA-C	6.93	121.34	113.02
1	C	150	PRO	N-CA-C	-6.79	100.58	111.38
1	A	150	PRO	N-CA-C	-6.77	100.62	111.38
1	C	219	ASP	N-CA-C	6.45	119.13	111.33
1	B	123	GLY	N-CA-C	6.32	123.57	112.83
1	B	108	ILE	N-CA-C	6.27	116.44	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	352	TRP	N-CA-C	6.25	118.61	111.11
1	A	220	GLU	N-CA-C	6.24	120.09	112.23
1	C	123	GLY	N-CA-C	6.23	123.41	112.83
1	A	123	GLY	N-CA-C	6.01	123.05	112.83
1	C	97	ALA	N-CA-C	5.94	118.52	111.33
1	C	232	ASP	N-CA-C	-5.92	102.00	110.59
1	A	122	VAL	N-CA-C	5.84	117.10	111.91
1	B	232	ASP	N-CA-C	-5.79	101.90	110.46
1	C	352	TRP	N-CA-C	5.71	117.97	111.11
1	C	104	ASP	N-CA-C	-5.65	101.06	109.42
1	B	304	ARG	N-CA-C	5.65	118.37	111.82
1	C	350	PHE	N-CA-C	-5.61	100.54	109.23
1	C	251	ILE	N-CA-C	-5.51	99.70	107.75
1	A	232	ASP	N-CA-C	-5.50	101.83	110.36
1	C	349	HIS	N-CA-C	5.48	117.90	109.07
1	B	158	HIS	N-CA-C	-5.46	106.62	113.72
1	A	295	SER	N-CA-C	5.45	117.35	109.07
1	C	108	ILE	N-CA-C	5.40	116.03	110.36
1	A	350	PHE	N-CA-C	-5.39	99.89	109.06
1	C	79	SER	N-CA-C	-5.35	101.58	109.18
1	B	295	SER	N-CA-C	5.34	117.19	109.07
1	A	251	ILE	N-CA-C	-5.33	99.97	107.75
1	A	20	THR	N-CA-C	5.21	118.49	110.42
1	B	172	LEU	N-CA-C	5.20	119.25	113.01
1	A	249	ILE	N-CA-C	-5.19	105.47	110.72
1	A	97	ALA	N-CA-C	5.18	117.60	111.33
1	B	218	GLY	N-CA-C	-5.02	106.26	112.33

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	3081	0	3064	54	0
1	B	3081	0	3064	64	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3081	0	3064	56	0
2	A	6	0	8	0	0
2	B	6	0	8	0	0
2	C	6	0	8	0	0
3	A	207	0	0	5	0
3	B	102	0	0	5	0
3	C	120	0	0	3	0
All	All	9690	0	9216	168	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 (168) 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:302:ALA:H	1:A:334:HIS:HE1	1.20	0.85
1:B:302:ALA:H	1:B:334:HIS:HE1	1.24	0.82
1:C:302:ALA:H	1:C:334:HIS:HE1	1.28	0.80
1:A:207:ILE:O	1:A:211:THR:HG23	1.81	0.79
1:C:45:SER:H	1:C:173:HIS:HD2	1.35	0.75
1:B:207:ILE:O	1:B:211:THR:HG23	1.87	0.74
1:B:17:ASN:HD22	1:B:18:THR:N	1.87	0.73
1:A:19:ARG:HG3	1:A:19:ARG:HH11	1.53	0.71
1:A:302:ALA:H	1:A:334:HIS:CE1	2.07	0.70
1:A:195:LYS:HD3	1:A:226:ASP:HB2	1.74	0.70
1:C:165:TYR:HE1	1:C:195:LYS:HE3	1.57	0.69
1:B:17:ASN:HD22	1:B:18:THR:H	1.38	0.69
1:A:302:ALA:HB3	1:A:303:PRO:HD3	1.74	0.68
1:C:45:SER:H	1:C:173:HIS:CD2	2.12	0.67
1:B:302:ALA:H	1:B:334:HIS:CE1	2.09	0.67
1:C:165:TYR:CE1	1:C:195:LYS:HE3	2.30	0.67
1:A:85:GLY:O	1:A:127:MET:CE	2.43	0.66
1:C:302:ALA:H	1:C:334:HIS:CE1	2.13	0.65
1:B:223:LEU:CA	1:B:224:MET:HE2	2.27	0.64
1:B:45:SER:H	1:B:173:HIS:HD2	1.45	0.64
1:C:236:ALA:HB1	1:C:266:LEU:HD21	1.80	0.64
1:A:211:THR:HG22	1:A:246:PHE:CZ	2.32	0.63
1:A:211:THR:HG22	1:A:246:PHE:HZ	1.63	0.63
1:C:329:PHE:O	1:C:334:HIS:HD2	1.81	0.63
1:B:194:ILE:O	1:B:224:MET:HE3	1.99	0.62
1:A:329:PHE:O	1:A:334:HIS:HD2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:GLY:O	1:A:127:MET:HE3	2.00	0.62
1:B:38:LEU:HD11	1:C:5:ALA:HB2	1.83	0.61
1:B:74:GLU:HG2	3:B:698:HOH:O	2.01	0.61
1:C:207:ILE:O	1:C:211:THR:HG23	2.00	0.61
1:B:301:ASP:OD1	1:B:303:PRO:HD2	2.01	0.60
1:B:19:ARG:HA	1:B:23:GLU:OE1	2.02	0.60
1:B:223:LEU:HA	1:B:224:MET:HE2	1.84	0.60
1:B:312:LEU:HD23	1:B:315:MET:CE	2.32	0.60
1:C:19:ARG:HH11	1:C:19:ARG:HG3	1.67	0.59
1:B:194:ILE:C	1:B:224:MET:HE3	2.28	0.59
1:B:293:ASN:HD22	1:B:323:ARG:HH21	1.50	0.59
1:C:302:ALA:HB3	1:C:303:PRO:HD3	1.83	0.59
1:C:195:LYS:HD3	1:C:226:ASP:HB2	1.85	0.59
1:A:45:SER:H	1:A:173:HIS:CD2	2.21	0.58
1:B:329:PHE:O	1:B:334:HIS:HD2	1.85	0.58
1:B:63:ILE:HD12	1:B:63:ILE:N	2.18	0.58
1:B:82:LYS:O	1:B:83:ARG:HB2	2.03	0.58
1:A:45:SER:H	1:A:173:HIS:HD2	1.50	0.58
1:C:301:ASP:OD1	1:C:303:PRO:HD2	2.04	0.57
1:B:223:LEU:C	1:B:224:MET:HE2	2.29	0.57
1:A:293:ASN:HD22	1:A:323:ARG:HH21	1.52	0.57
1:A:165:TYR:CE1	1:A:195:LYS:HE3	2.40	0.56
1:C:260:ILE:HG12	1:C:289:LEU:HD22	1.85	0.56
1:C:293:ASN:HD22	1:C:323:ARG:HH21	1.54	0.56
1:B:45:SER:HB2	1:B:49:VAL:HB	1.87	0.56
1:C:82:LYS:O	1:C:83:ARG:HB2	2.05	0.56
1:A:63:ILE:HD12	1:A:63:ILE:N	2.22	0.55
1:A:301:ASP:OD1	1:A:303:PRO:HD2	2.06	0.55
1:C:311:PHE:CD2	1:C:337:LEU:HD13	2.42	0.55
1:B:17:ASN:ND2	1:B:19:ARG:H	2.03	0.55
1:A:19:ARG:HG3	1:A:19:ARG:NH1	2.22	0.54
1:C:38:LEU:HD12	1:C:387:TRP:CZ3	2.42	0.54
1:A:82:LYS:O	1:A:83:ARG:HB2	2.07	0.54
1:C:312:LEU:HD23	1:C:315:MET:HE2	1.90	0.54
1:B:13:ALA:HB1	1:C:360:GLN:HG3	1.89	0.54
1:B:224:MET:HE2	1:B:224:MET:N	2.22	0.54
1:B:17:ASN:ND2	1:B:18:THR:N	2.57	0.52
1:A:300:PRO:HB2	1:A:311:PHE:CE1	2.44	0.52
1:B:50:LEU:HD22	1:B:172:LEU:HD13	1.91	0.52
1:B:187:ARG:HA	1:B:191:ILE:HG22	1.91	0.52
1:B:237:ILE:O	1:B:241:ARG:HG2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:19:ARG:HG3	1:C:19:ARG:NH1	2.23	0.52
1:A:280:LEU:HD11	1:A:289:LEU:HD22	1.92	0.52
1:A:315:MET:HG2	1:A:341:TYR:CD1	2.45	0.51
1:B:302:ALA:HB3	1:B:303:PRO:HD3	1.91	0.51
1:C:79:SER:HA	1:C:303:PRO:HB3	1.93	0.51
1:C:126:GLY:O	1:C:129:VAL:HG22	2.11	0.51
1:A:20:THR:OG1	1:A:23:GLU:HG2	2.10	0.51
1:C:211:THR:HG22	1:C:246:PHE:CZ	2.46	0.51
1:C:341:TYR:CD1	1:C:342:PRO:HD2	2.46	0.50
1:A:51:THR:HG21	1:A:230:GLN:HE21	1.76	0.50
1:A:126:GLY:O	1:A:129:VAL:HG22	2.10	0.50
1:A:329:PHE:CG	1:A:330:ALA:N	2.78	0.50
1:B:298:VAL:HG12	1:B:300:PRO:HD3	1.94	0.50
1:A:74:GLU:HG2	3:A:654:HOH:O	2.13	0.49
1:C:300:PRO:HB2	1:C:311:PHE:CE1	2.48	0.49
1:C:63:ILE:HD12	1:C:63:ILE:N	2.27	0.48
1:A:68:ARG:HG2	1:A:74:GLU:HB2	1.94	0.48
1:A:144:ALA:HB3	1:A:375:GLY:HA2	1.95	0.48
1:B:300:PRO:HG2	1:B:311:PHE:CE1	2.49	0.48
1:C:50:LEU:HD22	1:C:172:LEU:HD13	1.96	0.48
1:A:79:SER:HA	1:A:303:PRO:HB3	1.96	0.47
1:B:45:SER:HB2	1:B:49:VAL:CB	2.45	0.47
1:C:19:ARG:HA	1:C:23:GLU:OE1	2.14	0.47
1:C:45:SER:HB2	1:C:173:HIS:HB3	1.95	0.47
1:A:280:LEU:HB2	1:A:286:HIS:CE1	2.50	0.47
1:B:194:ILE:O	1:B:224:MET:CE	2.60	0.47
1:B:12:TYR:CE2	1:C:186:SER:HA	2.50	0.46
1:B:45:SER:HA	3:B:657:HOH:O	2.15	0.46
1:C:321:HIS:HE1	3:C:659:HOH:O	1.99	0.46
1:A:89:ILE:N	1:A:127:MET:HE2	2.31	0.46
1:B:278:GLU:HG3	1:B:279:MET:N	2.30	0.46
1:A:284:ARG:HG3	3:A:805:HOH:O	2.14	0.46
1:B:301:ASP:HB3	1:B:304:ARG:HB2	1.98	0.46
1:C:280:LEU:HB2	1:C:286:HIS:CE1	2.51	0.46
1:B:286:HIS:HE1	3:B:615:HOH:O	1.98	0.46
1:B:329:PHE:CG	1:B:330:ALA:N	2.84	0.45
1:A:237:ILE:O	1:A:241:ARG:HG2	2.16	0.45
1:A:278:GLU:HG3	1:A:279:MET:N	2.29	0.45
1:B:354:ASN:N	1:B:355:PRO:HD2	2.31	0.45
1:A:286:HIS:HE1	3:A:604:HOH:O	2.00	0.45
1:B:4:SER:HB2	1:C:41:ALA:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:HIS:HE1	3:A:749:HOH:O	2.00	0.45
1:B:311:PHE:CD2	1:B:337:LEU:HD13	2.52	0.44
1:C:301:ASP:HB3	1:C:304:ARG:HB2	2.00	0.44
1:C:38:LEU:HD21	1:C:352:TRP:O	2.17	0.44
1:C:278:GLU:HG3	1:C:279:MET:N	2.33	0.44
1:B:211:THR:HG22	1:B:246:PHE:CZ	2.53	0.44
1:C:229:GLN:HB3	1:C:256:ASP:HA	2.00	0.44
1:A:301:ASP:HB3	1:A:304:ARG:HB2	2.00	0.44
1:A:311:PHE:CD2	1:A:337:LEU:HD13	2.53	0.43
1:B:133:SER:HB2	1:B:134:PRO:HD3	1.99	0.43
1:C:82:LYS:NZ	1:C:329:PHE:CE2	2.83	0.43
1:C:237:ILE:HG23	1:C:238:ARG:N	2.34	0.43
1:B:38:LEU:CD1	1:C:5:ALA:HB2	2.48	0.43
1:A:88:GLY:CA	1:A:127:MET:HE2	2.49	0.43
1:A:313:LYS:HD3	3:A:784:HOH:O	2.17	0.43
1:B:250:TRP:C	1:B:250:TRP:CD1	2.96	0.43
1:C:144:ALA:HB3	1:C:375:GLY:HA2	2.00	0.43
1:C:211:THR:HG22	1:C:246:PHE:HZ	1.82	0.43
1:C:293:ASN:ND2	1:C:323:ARG:HH21	2.16	0.43
1:A:315:MET:HG2	1:A:341:TYR:HD1	1.81	0.43
1:A:354:ASN:HB2	1:A:355:PRO:HD3	1.99	0.43
1:B:35:LEU:HD23	1:B:390:LEU:HD12	2.01	0.43
1:B:46:ASP:CG	1:B:48:LYS:HZ2	2.26	0.43
1:A:85:GLY:O	1:A:89:ILE:HG13	2.19	0.43
1:C:211:THR:O	1:C:215:GLU:HB2	2.19	0.43
1:B:11:THR:HG23	3:B:632:HOH:O	2.19	0.43
1:C:286:HIS:HE1	3:C:608:HOH:O	2.00	0.43
1:A:281:THR:O	1:A:282:SER:HB3	2.19	0.42
1:B:38:LEU:HD12	1:B:387:TRP:CZ3	2.54	0.42
1:A:45:SER:HB2	1:A:173:HIS:HB3	2.02	0.42
1:A:133:SER:HB2	1:A:134:PRO:HD3	2.00	0.42
1:B:18:THR:HG22	1:B:18:THR:O	2.19	0.42
1:C:254:PRO:HD2	1:C:263:HIS:CE1	2.54	0.42
1:A:195:LYS:HD3	1:A:226:ASP:CB	2.47	0.42
1:B:195:LYS:HD2	1:B:226:ASP:HB2	2.01	0.42
1:B:339:ALA:HB2	1:B:370:ILE:HD11	2.01	0.42
1:B:343:LEU:O	1:B:345:PRO:HD3	2.20	0.42
1:A:221:PHE:HA	1:A:222:PRO:HD3	1.94	0.41
1:C:187:ARG:HA	1:C:191:ILE:HG22	2.03	0.41
1:B:185:ILE:O	1:B:189:ASN:ND2	2.51	0.41
1:A:88:GLY:HA3	1:A:127:MET:HE2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:LEU:HD22	1:B:353:LEU:HD23	2.03	0.41
1:B:44:VAL:HA	1:B:173:HIS:CD2	2.56	0.41
1:C:329:PHE:CG	1:C:330:ALA:N	2.84	0.41
1:B:41:ALA:HB2	1:C:4:SER:HB2	2.02	0.41
1:A:67:ILE:O	1:A:74:GLU:HA	2.20	0.41
1:B:281:THR:O	1:B:282:SER:HB3	2.21	0.41
1:C:254:PRO:HD2	1:C:263:HIS:HE1	1.85	0.41
1:A:88:GLY:HA3	1:A:127:MET:CE	2.51	0.41
1:B:286:HIS:HD2	3:B:658:HOH:O	2.02	0.41
1:C:332:GLU:H	1:C:332:GLU:CD	2.29	0.40
1:A:30:TRP:CZ2	1:A:32:LYS:HB2	2.56	0.40
1:B:312:LEU:HD23	1:B:315:MET:HE1	2.03	0.40
1:C:332:GLU:HG2	1:C:357:PHE:CE2	2.56	0.40
1:B:177:ASP:OD2	1:B:178:GLN:N	2.54	0.40
1:C:284:ARG:HG3	3:C:617:HOH:O	2.22	0.40
1:A:250:TRP:CD1	1:A:250:TRP:C	3.00	0.40
1:C:329:PHE:O	1:C:330:ALA:C	2.63	0.40
1:B:79:SER:HA	1:B:303:PRO:HB3	2.03	0.40
1:B:332:GLU:HG2	1:B:357:PHE:CE2	2.57	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	A	393/398 (99%)	383 (98%)	9 (2%)	1 (0%)	36	42
1	B	393/398 (99%)	381 (97%)	10 (2%)	2 (0%)	24	27
1	C	393/398 (99%)	382 (97%)	10 (2%)	1 (0%)	36	42
All	All	1179/1194 (99%)	1146 (97%)	29 (2%)	4 (0%)	36	42

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	83	ARG
1	B	83	ARG
1	C	83	ARG
1	B	330	ALA

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	318/320 (99%)	314 (99%)	4 (1%)	61	76
1	B	318/320 (99%)	313 (98%)	5 (2%)	55	71
1	C	318/320 (99%)	314 (99%)	4 (1%)	61	76
All	All	954/960 (99%)	941 (99%)	13 (1%)	59	75

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	GLU
1	A	109	ASP
1	A	224	MET
1	A	315	MET
1	B	74	GLU
1	B	98	ASP
1	B	188	GLU
1	B	224	MET
1	B	345	PRO
1	C	109	ASP
1	C	224	MET
1	C	278	GLU
1	C	289	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	106	ASN

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Mol	Chain	Res	Type
1	A	163	GLN
1	A	173	HIS
1	A	230	GLN
1	A	247	ASN
1	A	263	HIS
1	A	286	HIS
1	A	293	ASN
1	A	321	HIS
1	A	334	HIS
1	B	17	ASN
1	B	163	GLN
1	B	173	HIS
1	B	178	GLN
1	B	230	GLN
1	B	247	ASN
1	B	263	HIS
1	B	265	GLN
1	B	286	HIS
1	B	293	ASN
1	B	321	HIS
1	B	334	HIS
1	B	358	ASN
1	B	360	GLN
1	C	17	ASN
1	C	99	ASN
1	C	106	ASN
1	C	158	HIS
1	C	163	GLN
1	C	173	HIS
1	C	230	GLN
1	C	245	GLN
1	C	247	ASN
1	C	263	HIS
1	C	286	HIS
1	C	293	ASN
1	C	321	HIS
1	C	334	HIS
1	C	358	ASN

5.3.3 RNA ⓘ

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](#)

3 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	A	601	-	5,5,5	0.37	0	5,5,5	0.42	0
2	GOL	C	603	-	5,5,5	0.37	0	5,5,5	0.36	0
2	GOL	B	602	-	5,5,5	0.29	0	5,5,5	0.38	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	A	601	-	-	2/4/4/4	-
2	GOL	C	603	-	-	1/4/4/4	-
2	GOL	B	602	-	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	GOL	O1-C1-C2-C3
2	A	601	GOL	O1-C1-C2-O2
2	B	602	GOL	O2-C2-C3-O3
2	C	603	GOL	O1-C1-C2-O2

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	395/398 (99%)	-0.16	10 (2%) 58 55	22, 28, 42, 57	0
1	B	395/398 (99%)	0.23	14 (3%) 47 44	24, 34, 48, 59	0
1	C	395/398 (99%)	0.19	18 (4%) 37 34	23, 33, 47, 60	0
All	All	1185/1194 (99%)	0.08	42 (3%) 47 44	22, 31, 47, 60	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	16	ALA	10.2
1	B	17	ASN	9.1
1	C	17	ASN	7.8
1	C	15	ALA	7.5
1	B	15	ALA	7.1
1	C	16	ALA	6.4
1	C	13	ALA	5.4
1	C	14	LYS	4.6
1	B	18	THR	4.3
1	A	16	ALA	4.2
1	B	14	LYS	4.1
1	A	19	ARG	3.3
1	C	188	GLU	3.3
1	A	378	PHE	3.3
1	A	14	LYS	3.1
1	B	4	SER	3.1
1	C	19	ARG	3.1
1	C	4	SER	3.0
1	B	177	ASP	2.9
1	C	18	THR	2.9
1	B	98	ASP	2.9
1	B	386	ARG	2.8
1	A	98	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	238	ARG	2.8
1	B	397	ARG	2.7
1	A	18	THR	2.7
1	A	220	GLU	2.6
1	A	238	ARG	2.6
1	B	13	ALA	2.5
1	C	218	GLY	2.4
1	C	184	VAL	2.4
1	C	378	PHE	2.3
1	C	364	ARG	2.3
1	C	177	ASP	2.3
1	B	19	ARG	2.2
1	C	397	ARG	2.1
1	A	284	ARG	2.1
1	B	364	ARG	2.1
1	C	204	ALA	2.1
1	B	188	GLU	2.1
1	C	396	LYS	2.0
1	A	386	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(Å ²)	Q<0.9
2	GOL	B	602	6/6	0.89	0.13	41,42,44,45	0
2	GOL	C	603	6/6	0.92	0.12	42,43,45,45	0
2	GOL	A	601	6/6	0.93	0.13	35,40,42,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.