



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:55 AM UTC

PDB ID : 3WSV / pdb_00003wsv
Title : Crystal structure of minor L-lactate dehydrogenase from *Enterococcus mundtii* in the ligands-unbound form
Authors : Matoba, Y.; Sugiyama, M.
Deposited on : 2014-03-27
Resolution : 2.38 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

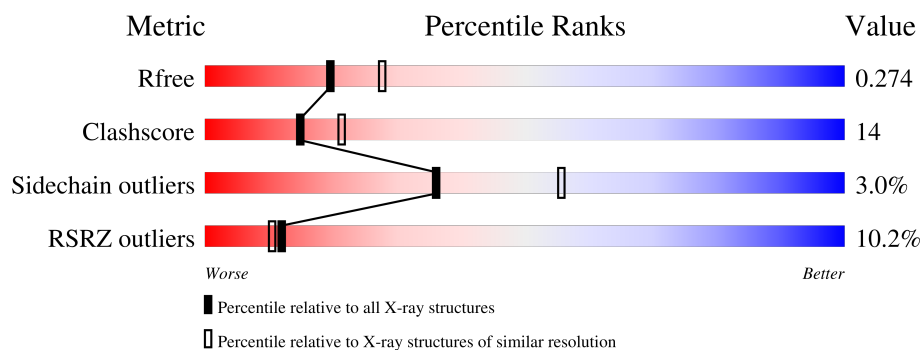
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.38 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	7164 (2.40-2.36)
Clashscore	190562	7722 (2.40-2.36)
Sidechain outliers	187428	7627 (2.40-2.36)
RSRZ outliers	180081	7170 (2.40-2.36)

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	322	16% 64% 31% ..
1	B	322	6% 72% 24% ..
1	C	322	11% 67% 26% ..
1	D	322	7% 76% 21% ..

2 Entry composition [i](#)

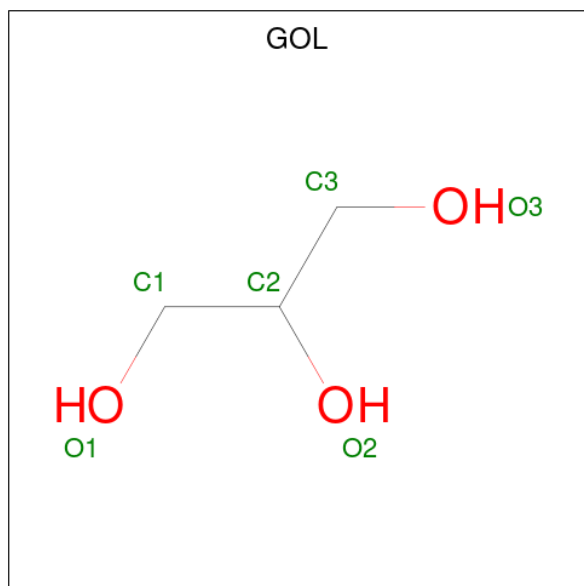
There are 3 unique types of molecules in this entry. The entry contains 10138 atoms, of which 0 are hydrogens and 0 are deuteriums.

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-lactate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	312	Total	C	N	O	S	0	0	0
			2400	1513	407	472	8			
1	B	317	Total	C	N	O	S	0	0	0
			2441	1538	415	481	7			
1	C	312	Total	C	N	O	S	0	0	0
			2400	1513	407	472	8			
1	D	317	Total	C	N	O	S	0	0	0
			2441	1538	415	481	7			

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



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

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

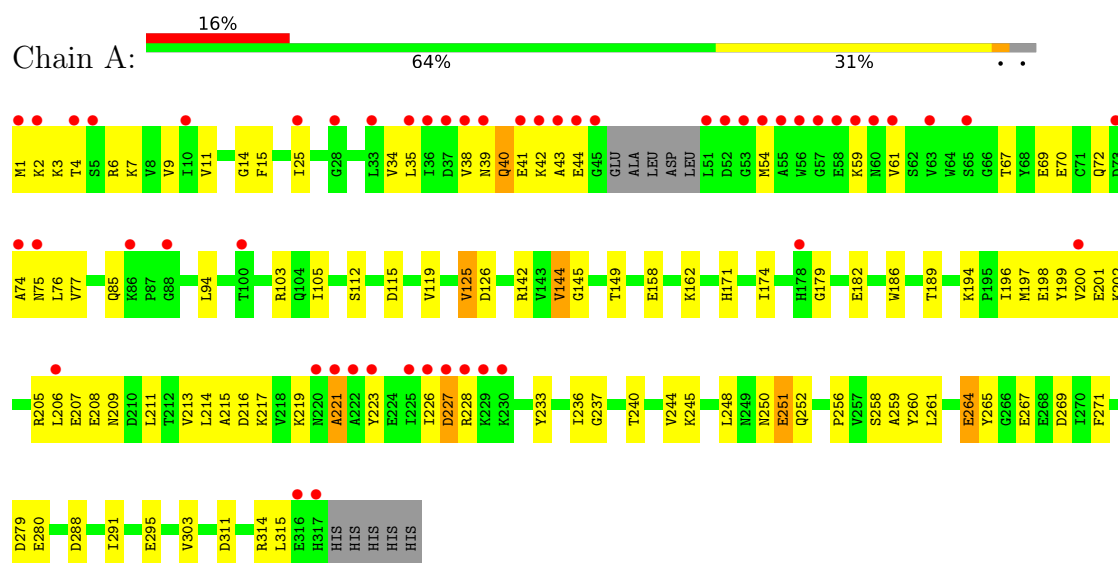
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	86	Total	O	0	0
			86	86		
3	B	121	Total	O	0	0
			121	121		
3	C	79	Total	O	0	0
			79	79		
3	D	122	Total	O	0	0
			122	122		

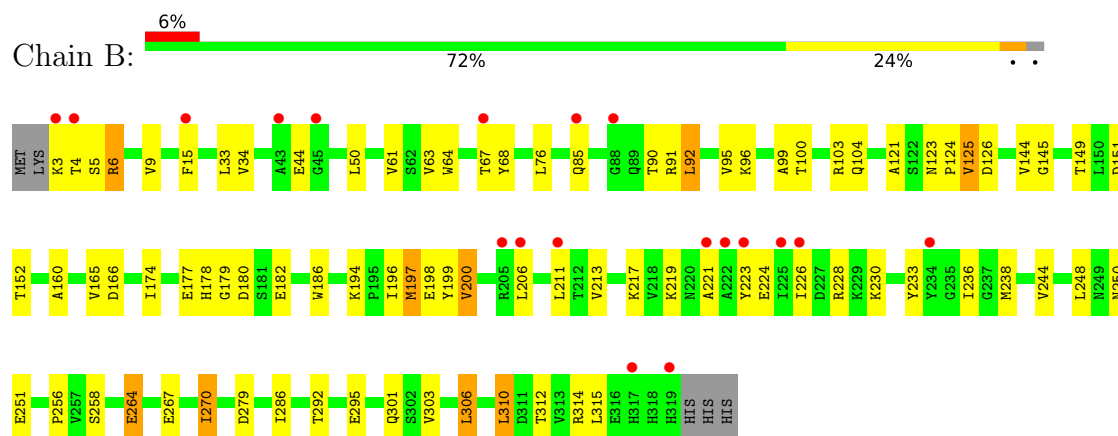
3 Residue-property plots [i](#)

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-lactate dehydrogenase

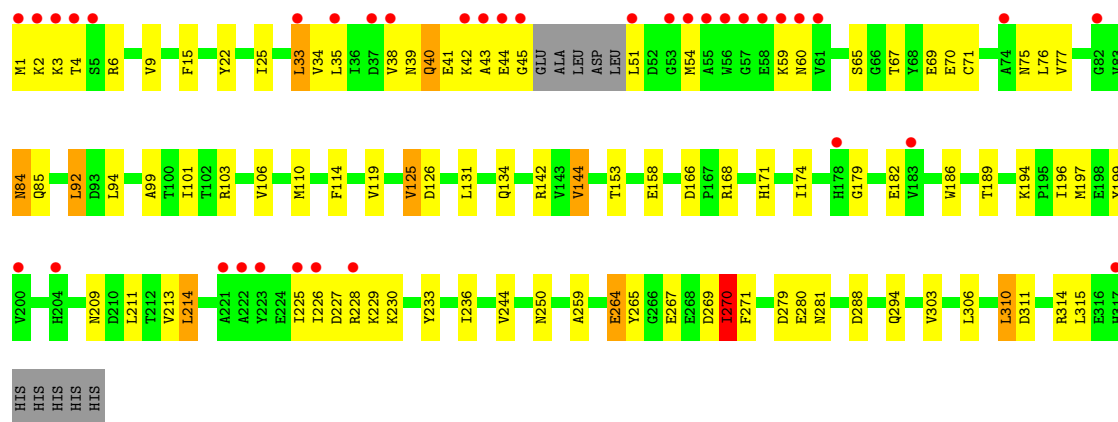


• Molecule 1: L-lactate dehydrogenase

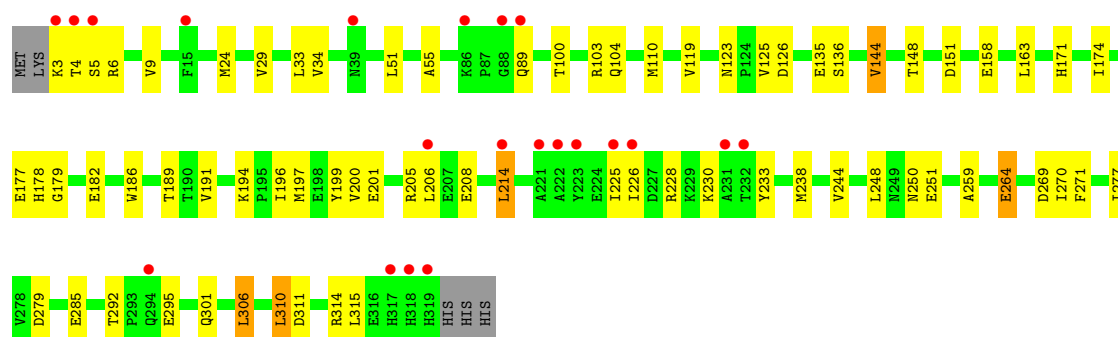
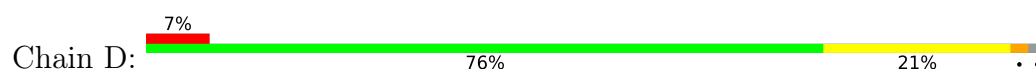


• Molecule 1: L-lactate dehydrogenase





● Molecule 1: L-lactate dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	104.43Å 127.82Å 133.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.96 – 2.38 29.96 – 2.38	Depositor EDS
% Data completeness (in resolution range)	96.4 (29.96-2.38) 99.4 (29.96-2.38)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.84 (at 2.39Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.232 , 0.271 0.237 , 0.274	Depositor DCC
R_{free} test set	3632 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	45.7	Xtriage
Anisotropy	0.639	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.57$, $\langle L^2 \rangle = 0.42$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10138	wwPDB-VP
Average B, all atoms (Å ²)	57.0	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 54.76 % 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 3.4886e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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

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	A	0.42	0/2436	0.89	7/3304 (0.2%)
1	B	0.44	0/2480	0.89	6/3368 (0.2%)
1	C	0.42	0/2436	0.87	5/3304 (0.2%)
1	D	0.43	0/2480	0.85	3/3368 (0.1%)
All	All	0.43	0/9832	0.87	21/13344 (0.2%)

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	221	ALA	N-CA-C	-8.90	102.55	113.50
1	C	125	VAL	N-CA-C	8.68	118.75	110.42
1	C	174	ILE	N-CA-C	-7.87	97.16	108.17
1	B	125	VAL	N-CA-C	7.54	118.27	110.36
1	A	125	VAL	N-CA-C	7.36	118.09	110.36
1	A	174	ILE	N-CA-C	-7.04	98.31	108.17
1	C	40	GLN	N-CA-C	-6.66	105.04	112.57
1	B	251	GLU	N-CA-C	6.63	118.59	111.36
1	B	174	ILE	N-CA-C	-6.55	98.99	108.36
1	D	144	VAL	N-CA-C	6.42	117.11	107.75
1	D	174	ILE	N-CA-C	-6.40	99.21	108.36
1	B	200	VAL	CB-CA-C	-6.08	106.54	111.71
1	B	144	VAL	N-CA-C	5.98	116.47	107.80
1	A	40	GLN	N-CA-C	-5.80	106.06	113.02
1	C	144	VAL	N-CA-C	5.55	115.86	107.75
1	A	144	VAL	N-CA-C	5.38	115.60	107.75
1	D	251	GLU	N-CA-C	5.31	117.98	111.82
1	A	251	GLU	N-CA-C	5.23	117.72	111.71
1	C	270	ILE	CB-CA-C	-5.22	106.83	111.74
1	B	99	ALA	N-CA-C	-5.20	105.69	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	205	ARG	N-CA-C	-5.15	106.95	113.18

There are no chirality outliers.

There are no planarity outliers.

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	2400	0	2415	86	0
1	B	2441	0	2442	61	0
1	C	2400	0	2415	82	0
1	D	2441	0	2442	57	0
2	A	12	0	16	3	0
2	B	12	0	16	1	0
2	C	18	0	24	0	0
2	D	6	0	8	0	0
3	A	86	0	0	1	0
3	B	121	0	0	3	0
3	C	79	0	0	1	0
3	D	122	0	0	3	0
All	All	10138	0	9778	270	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 (270) 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:250:ASN:HB2	1:A:280:GLU:HG3	1.57	0.87
1:B:226:ILE:HD11	1:B:230:LYS:HD2	1.55	0.86
1:B:197:MET:HE3	1:B:197:MET:HA	1.57	0.85
1:C:158:GLU:HB3	1:C:214:LEU:HD11	1.57	0.85
1:A:35:LEU:HD11	1:A:54:MET:HE2	1.56	0.85
1:A:2:LYS:HG3	1:C:75:ASN:ND2	1.96	0.81
1:C:38:VAL:HG23	1:C:39:ASN:H	1.47	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MET:HE3	1:C:142:ARG:HD3	1.63	0.80
1:C:186:TRP:HB3	1:C:197:MET:HE3	1.63	0.79
1:B:197:MET:HE1	1:B:211:LEU:HD11	1.65	0.79
1:A:6:ARG:HG2	1:C:4:THR:HB	1.65	0.78
1:A:38:VAL:O	1:A:39:ASN:HB2	1.84	0.77
1:A:217:LYS:O	1:A:221:ALA:HB2	1.83	0.77
1:B:92:LEU:HD22	1:B:96:LYS:HE3	1.68	0.75
1:A:85:GLN:HB2	1:A:94:LEU:HD22	1.67	0.75
1:A:200:VAL:HG23	1:A:201:GLU:HG3	1.69	0.74
1:D:103:ARG:HD2	1:D:315:LEU:HD21	1.69	0.74
1:C:197:MET:HE1	1:C:211:LEU:CD1	2.17	0.74
1:D:89:GLN:CD	1:D:89:GLN:H	1.96	0.73
1:A:39:ASN:HB3	1:A:41:GLU:HG2	1.70	0.72
1:D:177:GLU:OE1	1:D:306:LEU:HG	1.90	0.72
1:B:90:THR:O	1:B:91:ARG:HB2	1.91	0.70
1:C:166:ASP:OD2	1:C:168:ARG:HB2	1.92	0.69
1:A:186:TRP:HB3	1:A:197:MET:HE3	1.75	0.69
1:B:200:VAL:HG22	1:B:206:LEU:HD12	1.73	0.69
1:C:197:MET:HE1	1:C:211:LEU:HD11	1.74	0.68
1:C:85:GLN:HB2	1:C:94:LEU:HD22	1.74	0.68
1:D:5:SER:HB2	3:D:592:HOH:O	1.94	0.67
1:D:226:ILE:HD11	1:D:230:LYS:HD2	1.77	0.67
1:C:310:LEU:HD22	1:C:314:ARG:HB3	1.76	0.67
1:C:34:VAL:HG11	1:C:70:GLU:HG3	1.78	0.66
1:C:158:GLU:HB3	1:C:214:LEU:CD1	2.25	0.66
1:C:51:LEU:HD21	1:C:65:SER:OG	1.96	0.66
1:A:250:ASN:OD1	1:A:279:ASP:HB2	1.95	0.65
1:A:76:LEU:HD13	1:A:244:VAL:HG13	1.79	0.65
1:D:205:ARG:O	1:D:206:LEU:HD12	1.96	0.65
1:A:4:THR:HB	1:C:6:ARG:HG2	1.79	0.65
1:C:42:LYS:HG3	1:C:43:ALA:H	1.61	0.64
1:B:221:ALA:HA	1:B:224:GLU:HG2	1.79	0.64
1:A:1:MET:HE1	1:C:281:ASN:HA	1.78	0.64
1:B:85:GLN:HE21	1:B:123:ASN:HB3	1.62	0.64
1:B:85:GLN:NE2	1:B:123:ASN:HB3	2.13	0.63
1:B:103:ARG:HD2	1:B:315:LEU:HD11	1.81	0.63
1:B:180:ASP:HA	1:B:219:LYS:HD2	1.80	0.63
1:D:151:ASP:OD1	1:D:178:HIS:HB2	1.98	0.63
1:C:250:ASN:OD1	1:C:280:GLU:HG2	1.99	0.62
1:A:3:LYS:HE3	3:C:667:HOH:O	1.99	0.62
1:B:15:PHE:CZ	1:B:44:GLU:HG2	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:134:GLN:HB3	1:C:315:LEU:HD12	1.80	0.62
1:B:200:VAL:HG22	1:B:206:LEU:CD1	2.30	0.61
1:C:103:ARG:NH2	1:C:131:LEU:HD22	2.16	0.61
1:A:39:ASN:CG	1:A:40:GLN:H	2.08	0.61
1:B:5:SER:HB2	3:B:610:HOH:O	2.01	0.60
1:D:301:GLN:HG2	3:D:608:HOH:O	2.02	0.60
1:B:233:TYR:O	1:B:238:MET:HG3	2.01	0.60
1:D:103:ARG:HH11	1:D:103:ARG:HG2	1.67	0.60
1:B:151:ASP:OD1	1:B:178:HIS:HB2	2.02	0.59
1:C:1:MET:HE3	1:C:3:LYS:NZ	2.18	0.59
1:D:186:TRP:HE3	1:D:196:ILE:HG21	1.67	0.58
1:A:250:ASN:CB	1:A:280:GLU:HG3	2.31	0.58
1:A:228:ARG:HG3	1:A:228:ARG:HH11	1.67	0.58
1:D:3:LYS:HG2	1:D:4:THR:H	1.68	0.58
1:D:29:VAL:HG12	1:D:248:LEU:HD12	1.86	0.58
1:D:100:THR:O	1:D:104:GLN:HG3	2.04	0.58
1:A:75:ASN:ND2	1:C:2:LYS:HB3	2.19	0.57
1:C:84:ASN:HB3	1:C:228:ARG:HH21	1.68	0.57
1:D:250:ASN:OD1	1:D:279:ASP:HB2	2.03	0.57
1:A:72:GLN:HG2	1:A:112:SER:O	2.05	0.57
1:D:264:GLU:H	1:D:264:GLU:CD	2.13	0.57
1:C:119:VAL:HA	1:C:144:VAL:O	2.05	0.56
1:C:186:TRP:HE3	1:C:196:ILE:HG21	1.70	0.56
1:A:221:ALA:C	1:A:223:TYR:H	2.14	0.56
1:D:179:GLY:O	1:D:182:GLU:HG2	2.06	0.55
1:A:267:GLU:HG3	1:A:303:VAL:HG21	1.88	0.55
1:A:215:ALA:O	1:A:219:LYS:HB2	2.05	0.55
1:A:223:TYR:HD1	1:A:223:TYR:O	1.89	0.55
1:C:269:ASP:O	1:C:270:ILE:HG23	2.07	0.55
1:B:3:LYS:HB2	3:B:610:HOH:O	2.07	0.54
1:A:125:VAL:HG13	1:A:126:ASP:N	2.23	0.54
1:B:177:GLU:OE1	1:B:306:LEU:HG	2.08	0.54
1:A:228:ARG:HG2	1:A:233:TYR:OH	2.08	0.54
1:B:4:THR:HG21	1:D:248:LEU:HA	1.89	0.54
1:A:194:LYS:HD3	1:A:199:TYR:CE1	2.42	0.54
1:B:292:THR:OG1	1:B:295:GLU:HG3	2.08	0.54
1:B:100:THR:O	1:B:104:GLN:HG3	2.08	0.54
1:C:226:ILE:HG22	1:C:227:ASP:N	2.22	0.54
1:C:267:GLU:HG3	1:C:303:VAL:HG21	1.88	0.54
1:A:14:GLY:HA3	1:A:43:ALA:HB3	1.89	0.53
1:A:25:ILE:HD11	1:A:54:MET:HE3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:ARG:HG3	1:B:248:LEU:HD13	1.89	0.53
1:D:123:ASN:HA	1:D:125:VAL:N	2.24	0.53
1:A:223:TYR:O	1:A:223:TYR:CD1	2.62	0.53
1:C:250:ASN:OD1	1:C:279:ASP:HB2	2.08	0.53
1:A:228:ARG:HG3	1:A:228:ARG:NH1	2.23	0.53
1:A:260:TYR:CZ	1:A:269:ASP:HA	2.44	0.53
1:B:67:THR:HG22	1:B:68:TYR:N	2.22	0.53
1:C:42:LYS:NZ	1:C:45:GLY:HA2	2.23	0.52
1:A:207:GLU:HG2	1:A:208:GLU:N	2.23	0.52
1:C:76:LEU:HD13	1:C:244:VAL:HG13	1.91	0.52
1:C:311:ASP:HA	1:C:314:ARG:HD2	1.90	0.52
1:A:198:GLU:HG2	1:A:202:LYS:HE2	1.92	0.52
1:C:270:ILE:HD12	1:C:270:ILE:O	2.10	0.52
1:C:103:ARG:HH21	1:C:131:LEU:HD22	1.73	0.52
1:C:227:ASP:O	1:C:228:ARG:HB2	2.10	0.52
1:B:197:MET:HA	1:B:197:MET:CE	2.34	0.52
1:A:76:LEU:C	1:A:76:LEU:HD23	2.35	0.52
1:B:179:GLY:O	1:B:182:GLU:HG2	2.10	0.51
1:C:171:HIS:O	1:C:189:THR:HA	2.10	0.51
1:D:200:VAL:HG12	1:D:206:LEU:HB2	1.92	0.51
1:A:67:THR:OG1	1:A:69:GLU:HG2	2.10	0.51
2:A:402:GOL:H31	1:D:277:ILE:HD11	1.92	0.51
1:B:152:THR:HG22	2:B:401:GOL:H31	1.91	0.51
1:B:264:GLU:CD	1:B:264:GLU:H	2.17	0.51
1:A:264:GLU:HA	1:A:288:ASP:OD2	2.11	0.51
1:A:115:ASP:O	1:C:1:MET:HA	2.11	0.51
1:B:267:GLU:HG3	1:B:303:VAL:HG21	1.93	0.51
1:D:200:VAL:HG12	1:D:206:LEU:CB	2.41	0.51
1:B:9:VAL:HG22	1:B:34:VAL:HB	1.92	0.51
1:C:42:LYS:HG3	1:C:43:ALA:N	2.25	0.51
1:C:43:ALA:O	1:C:44:GLU:HB3	2.11	0.51
1:A:200:VAL:HG12	1:A:206:LEU:CB	2.41	0.50
1:A:311:ASP:OD1	1:A:314:ARG:NH1	2.44	0.50
1:B:85:GLN:NE2	1:B:223:TYR:HE1	2.09	0.50
1:B:250:ASN:OD1	1:B:279:ASP:HB2	2.11	0.50
1:C:59:LYS:O	1:C:60:ASN:C	2.54	0.50
1:D:103:ARG:NH1	1:D:135:GLU:OE1	2.45	0.50
1:D:103:ARG:CD	1:D:315:LEU:HD21	2.40	0.50
1:A:158:GLU:HB3	1:A:214:LEU:CD2	2.42	0.50
1:A:179:GLY:O	1:A:182:GLU:HG2	2.11	0.50
1:C:179:GLY:O	1:C:182:GLU:HG2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:205:ARG:C	1:D:206:LEU:HD12	2.37	0.50
1:D:270:ILE:O	1:D:270:ILE:HD12	2.12	0.49
1:A:34:VAL:HG21	1:A:70:GLU:HG2	1.93	0.49
1:B:125:VAL:HG13	1:B:126:ASP:N	2.27	0.49
1:B:310:LEU:HD22	1:B:314:ARG:HB3	1.93	0.49
1:A:209:ASN:O	1:A:213:VAL:HG23	2.13	0.49
1:C:42:LYS:CG	1:C:43:ALA:H	2.24	0.49
1:C:76:LEU:HD23	1:C:76:LEU:C	2.38	0.49
1:B:95:VAL:HG22	1:B:124:PRO:HG3	1.93	0.49
1:A:186:TRP:HE3	1:A:196:ILE:HG21	1.79	0.48
1:C:84:ASN:CB	1:C:228:ARG:HH21	2.25	0.48
1:C:264:GLU:HA	1:C:288:ASP:OD2	2.14	0.48
1:D:3:LYS:HG2	1:D:4:THR:N	2.28	0.48
1:D:200:VAL:HG23	1:D:201:GLU:HG3	1.93	0.48
1:A:7:LYS:HB3	1:A:74:ALA:HA	1.95	0.48
1:B:194:LYS:HD3	1:B:199:TYR:CE1	2.49	0.48
1:A:15:PHE:HB3	1:A:233:TYR:CE2	2.49	0.48
1:D:148:THR:HA	3:D:517:HOH:O	2.13	0.48
1:A:42:LYS:HG3	1:A:44:GLU:H	1.78	0.48
1:C:15:PHE:CD2	1:C:43:ALA:HB1	2.49	0.48
1:B:206:LEU:HD12	1:B:206:LEU:O	2.14	0.48
1:C:228:ARG:HG3	1:C:228:ARG:HH11	1.79	0.48
1:C:41:GLU:HB3	1:C:101:ILE:HD13	1.96	0.47
1:C:230:LYS:HA	1:D:228:ARG:HG3	1.95	0.47
1:A:76:LEU:HD23	1:A:77:VAL:N	2.30	0.47
1:A:248:LEU:HD22	1:C:4:THR:HG21	1.97	0.47
1:C:33:LEU:HD13	1:C:35:LEU:HD21	1.95	0.47
1:D:89:GLN:CD	1:D:89:GLN:N	2.67	0.47
1:D:171:HIS:O	1:D:189:THR:HA	2.15	0.47
1:C:233:TYR:O	1:C:236:ILE:HG22	2.15	0.47
1:D:194:LYS:HD3	1:D:199:TYR:CE1	2.50	0.47
1:D:225:ILE:HG23	1:D:225:ILE:O	2.14	0.47
1:D:310:LEU:HD22	1:D:314:ARG:HB3	1.97	0.47
1:A:245:LYS:HE2	3:A:565:HOH:O	2.14	0.46
1:A:315:LEU:N	1:A:315:LEU:HD12	2.30	0.46
1:A:34:VAL:HG11	1:A:70:GLU:HG2	1.98	0.46
1:D:197:MET:O	1:D:200:VAL:HG22	2.15	0.46
1:B:160:ALA:HB1	1:B:165:VAL:O	2.16	0.46
1:B:121:ALA:HB1	1:B:236:ILE:HD11	1.98	0.46
1:D:311:ASP:HA	1:D:314:ARG:HD2	1.98	0.46
1:C:71:CYS:O	1:C:114:PHE:HD1	1.99	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:TYR:O	1:A:236:ILE:HG22	2.17	0.45
1:B:213:VAL:O	1:B:217:LYS:HG3	2.17	0.45
1:D:233:TYR:O	1:D:238:MET:HG3	2.17	0.45
1:A:291:ILE:HB	1:A:295:GLU:OE1	2.16	0.45
1:C:153:THR:HG22	1:D:55:ALA:HB1	1.97	0.45
1:C:38:VAL:O	1:C:39:ASN:CG	2.60	0.45
1:B:123:ASN:HA	1:B:125:VAL:N	2.32	0.44
1:B:63:VAL:O	1:B:64:TRP:HB3	2.16	0.44
1:C:158:GLU:CB	1:C:214:LEU:HD11	2.39	0.44
1:B:4:THR:HG21	1:D:248:LEU:HD23	1.98	0.44
1:C:9:VAL:HB	1:C:77:VAL:HG22	2.00	0.44
1:C:38:VAL:HG23	1:C:39:ASN:N	2.24	0.44
1:D:292:THR:OG1	1:D:295:GLU:HG3	2.18	0.44
1:B:270:ILE:HD12	1:B:270:ILE:O	2.17	0.44
1:C:39:ASN:HB3	1:C:40:GLN:H	1.51	0.44
1:A:251:GLU:O	1:A:252:GLN:HB2	2.18	0.44
1:B:186:TRP:HE3	1:B:196:ILE:HG21	1.82	0.44
1:C:3:LYS:HA	1:C:3:LYS:HD3	1.76	0.44
1:B:76:LEU:HD13	1:B:244:VAL:HG13	1.99	0.44
1:B:206:LEU:HD12	1:B:206:LEU:C	2.43	0.44
1:D:119:VAL:HA	1:D:144:VAL:O	2.17	0.44
1:C:76:LEU:HD23	1:C:77:VAL:N	2.32	0.43
1:A:149:THR:HA	1:A:256:PRO:HG2	1.99	0.43
1:C:25:ILE:CD1	1:C:54:MET:HG3	2.48	0.43
1:C:125:VAL:HG13	1:C:126:ASP:N	2.33	0.43
1:C:197:MET:HE1	1:C:211:LEU:HD13	1.99	0.43
1:A:119:VAL:HA	1:A:144:VAL:O	2.18	0.43
2:A:402:GOL:H32	1:D:285:GLU:CD	2.44	0.43
1:C:44:GLU:OE2	1:C:229:LYS:HE2	2.17	0.43
1:A:171:HIS:O	1:A:189:THR:HA	2.18	0.43
1:A:213:VAL:O	1:A:217:LYS:HG3	2.19	0.43
1:C:106:VAL:O	1:C:110:MET:HG2	2.18	0.43
1:A:11:VAL:HG11	1:A:105:ILE:CG2	2.49	0.43
1:B:198:GLU:C	1:B:200:VAL:N	2.76	0.43
1:D:125:VAL:HG13	1:D:126:ASP:N	2.34	0.43
1:A:196:ILE:HG23	1:A:197:MET:HE2	2.01	0.43
1:A:15:PHE:N	1:A:43:ALA:HB3	2.34	0.43
1:A:221:ALA:C	1:A:223:TYR:N	2.76	0.43
1:A:259:ALA:O	1:A:271:PHE:HA	2.19	0.43
1:B:301:GLN:HG2	3:B:574:HOH:O	2.18	0.43
1:B:67:THR:CG2	1:B:68:TYR:N	2.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:33:LEU:CD1	1:C:35:LEU:HD21	2.49	0.43
1:C:259:ALA:O	1:C:271:PHE:HA	2.19	0.42
1:D:3:LYS:CG	1:D:4:THR:H	2.32	0.42
1:C:264:GLU:O	1:C:265:TYR:HB2	2.20	0.42
1:A:145:GLY:HA3	1:A:258:SER:HB2	2.00	0.42
1:B:315:LEU:HD12	1:B:315:LEU:N	2.35	0.42
1:C:186:TRP:CE3	1:C:196:ILE:HG21	2.53	0.42
1:A:103:ARG:NE	1:A:315:LEU:HD11	2.35	0.42
1:A:200:VAL:HG12	1:A:206:LEU:HB3	2.01	0.42
1:C:99:ALA:HB1	1:C:131:LEU:CD1	2.49	0.42
1:D:196:ILE:O	1:D:199:TYR:HB2	2.19	0.42
2:A:402:GOL:H31	1:D:277:ILE:CD1	2.50	0.42
1:B:248:LEU:CD2	1:D:4:THR:HG21	2.50	0.42
1:A:240:THR:O	1:A:244:VAL:HG23	2.19	0.42
1:B:103:ARG:NH1	1:B:315:LEU:HG	2.35	0.42
1:D:269:ASP:O	1:D:270:ILE:HG23	2.20	0.42
1:A:4:THR:CG2	1:C:75:ASN:ND2	2.83	0.42
1:A:69:GLU:HG3	1:A:70:GLU:N	2.35	0.42
1:A:162:LYS:HA	1:A:162:LYS:HD2	1.87	0.42
1:A:226:ILE:HG22	1:A:227:ASP:N	2.33	0.42
1:C:42:LYS:CE	1:C:45:GLY:HA2	2.50	0.42
1:D:9:VAL:HG22	1:D:34:VAL:HB	2.00	0.42
1:A:216:ASP:HA	1:A:219:LYS:HB3	2.02	0.42
1:D:110:MET:HE2	1:D:136:SER:O	2.20	0.42
1:D:259:ALA:O	1:D:271:PHE:HA	2.19	0.42
1:C:54:MET:SD	1:C:54:MET:N	2.93	0.41
1:C:294:GLN:OE1	1:C:294:GLN:N	2.47	0.41
1:A:207:GLU:HG2	1:A:209:ASN:H	1.85	0.41
1:B:198:GLU:C	1:B:200:VAL:H	2.28	0.41
1:C:51:LEU:HD21	1:C:65:SER:CB	2.51	0.41
1:C:67:THR:C	1:C:69:GLU:H	2.26	0.41
1:C:194:LYS:HD3	1:C:199:TYR:CE1	2.54	0.41
1:A:186:TRP:CE3	1:A:196:ILE:HG21	2.55	0.41
1:D:24:MET:HE1	1:D:244:VAL:HG11	2.02	0.41
1:A:142:ARG:HD3	1:C:1:MET:SD	2.60	0.41
1:A:197:MET:O	1:A:200:VAL:HG22	2.21	0.41
1:B:264:GLU:HG3	1:B:286:ILE:HG21	2.01	0.41
1:C:92:LEU:HD12	1:C:92:LEU:HA	1.91	0.41
1:C:209:ASN:O	1:C:213:VAL:HG23	2.20	0.41
1:A:236:ILE:HG23	1:A:237:GLY:N	2.35	0.41
1:A:264:GLU:O	1:A:265:TYR:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:LEU:N	1:A:315:LEU:CD1	2.84	0.41
1:B:197:MET:HE1	1:B:211:LEU:CD1	2.44	0.41
1:D:158:GLU:HB2	1:D:214:LEU:HD11	2.03	0.41
1:A:9:VAL:HB	1:A:77:VAL:HG22	2.03	0.41
1:B:15:PHE:CD1	1:B:228:ARG:HD3	2.56	0.41
1:B:92:LEU:HD21	1:B:312:THR:OG1	2.21	0.40
1:B:145:GLY:HA3	1:B:258:SER:HB2	2.03	0.40
1:B:92:LEU:HD22	1:B:96:LYS:CE	2.46	0.40
1:B:92:LEU:O	1:B:96:LYS:HG3	2.22	0.40
1:B:149:THR:HA	1:B:256:PRO:HG2	2.03	0.40
1:D:270:ILE:HD12	1:D:270:ILE:C	2.46	0.40
1:A:39:ASN:ND2	1:A:40:GLN:H	2.19	0.40
1:D:163:LEU:HD12	1:D:191:VAL:HG21	2.03	0.40
1:C:22:TYR:CZ	1:D:230:LYS:HE2	2.57	0.40
1:D:208:GLU:OE1	1:D:208:GLU:HA	2.21	0.40
1:A:186:TRP:CZ3	1:A:211:LEU:HD12	2.57	0.40
1:A:194:LYS:HD3	1:A:199:TYR:CZ	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

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	262/271 (97%)	257 (98%)	5 (2%)	50 69
1	B	266/271 (98%)	255 (96%)	11 (4%)	27 43
1	C	262/271 (97%)	253 (97%)	9 (3%)	32 51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	266/271 (98%)	259 (97%)	7 (3%)	40 60
All	All	1056/1084 (97%)	1024 (97%)	32 (3%)	36 56

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	LYS
1	A	61	VAL
1	A	227	ASP
1	A	261	LEU
1	A	264	GLU
1	B	6	ARG
1	B	33	LEU
1	B	50	LEU
1	B	61	VAL
1	B	92	LEU
1	B	166	ASP
1	B	197	MET
1	B	264	GLU
1	B	270	ILE
1	B	306	LEU
1	B	310	LEU
1	C	33	LEU
1	C	84	ASN
1	C	92	LEU
1	C	214	LEU
1	C	225	ILE
1	C	264	GLU
1	C	270	ILE
1	C	306	LEU
1	C	310	LEU
1	D	6	ARG
1	D	33	LEU
1	D	51	LEU
1	D	214	LEU
1	D	264	GLU
1	D	306	LEU
1	D	310	LEU

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

Mol	Chain	Res	Type
1	A	39	ASN
1	A	85	GLN
1	A	123	ASN
1	A	209	ASN
1	A	252	GLN
1	B	26	ASN
1	B	27	GLN
1	B	72	GLN
1	B	85	GLN
1	B	220	ASN
1	B	317	HIS
1	B	318	HIS
1	C	60	ASN
1	C	85	GLN
1	C	89	GLN
1	D	72	GLN
1	D	204	HIS
1	D	319	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](#)

8 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	D	401	-	5,5,5	0.40	0	5,5,5	0.32	0
2	GOL	C	503	-	5,5,5	0.45	0	5,5,5	0.28	0
2	GOL	A	402	-	5,5,5	0.37	0	5,5,5	0.24	0
2	GOL	B	402	-	5,5,5	0.42	0	5,5,5	0.27	0
2	GOL	B	401	-	5,5,5	0.45	0	5,5,5	0.24	0
2	GOL	A	401	-	5,5,5	0.33	0	5,5,5	0.29	0
2	GOL	C	502	-	5,5,5	0.34	0	5,5,5	0.29	0
2	GOL	C	501	-	5,5,5	0.38	0	5,5,5	0.25	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	D	401	-	-	4/4/4/4	-
2	GOL	C	503	-	-	2/4/4/4	-
2	GOL	A	402	-	-	0/4/4/4	-
2	GOL	B	402	-	-	2/4/4/4	-
2	GOL	B	401	-	-	2/4/4/4	-
2	GOL	A	401	-	-	4/4/4/4	-
2	GOL	C	502	-	-	4/4/4/4	-
2	GOL	C	501	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	GOL	O1-C1-C2-O2
2	A	401	GOL	O1-C1-C2-C3
2	A	401	GOL	C1-C2-C3-O3
2	B	402	GOL	C1-C2-C3-O3
2	B	402	GOL	O2-C2-C3-O3
2	C	501	GOL	O1-C1-C2-C3
2	D	401	GOL	C1-C2-C3-O3
2	A	401	GOL	O2-C2-C3-O3
2	B	401	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
2	C	502	GOL	O1-C1-C2-C3
2	C	502	GOL	C1-C2-C3-O3
2	C	503	GOL	O1-C1-C2-C3
2	D	401	GOL	O1-C1-C2-C3
2	C	501	GOL	O1-C1-C2-O2
2	D	401	GOL	O2-C2-C3-O3
2	B	401	GOL	O1-C1-C2-O2
2	C	502	GOL	O1-C1-C2-O2
2	C	502	GOL	O2-C2-C3-O3
2	C	503	GOL	O1-C1-C2-O2
2	D	401	GOL	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	402	GOL	3	0
2	B	401	GOL	1	0

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	312/322 (96%)	0.80	52 (16%) 4 4	33, 53, 108, 121	0
1	B	317/322 (98%)	0.39	19 (5%) 27 26	32, 49, 82, 98	0
1	C	312/322 (96%)	0.70	36 (11%) 9 8	33, 53, 110, 132	0
1	D	317/322 (98%)	0.36	21 (6%) 24 23	32, 49, 86, 99	0
All	All	1258/1288 (97%)	0.56	128 (10%) 12 10	32, 51, 96, 132	0

All (128) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	43	ALA	8.6
1	C	55	ALA	8.1
1	A	51	LEU	6.9
1	A	225	ILE	6.4
1	C	225	ILE	6.3
1	C	51	LEU	6.0
1	C	4	THR	5.9
1	A	45	GLY	5.7
1	A	226	ILE	5.4
1	D	226	ILE	5.4
1	A	54	MET	5.3
1	A	43	ALA	5.0
1	C	45	GLY	4.9
1	A	55	ALA	4.7
1	A	222	ALA	4.6
1	C	38	VAL	4.5
1	D	318	HIS	4.3
1	B	222	ALA	4.3
1	C	226	ILE	4.3
1	B	226	ILE	4.2
1	C	222	ALA	4.1

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Mol	Chain	Res	Type	RSRZ
1	D	4	THR	4.1
1	B	223	TYR	4.1
1	A	178	HIS	4.0
1	B	225	ILE	4.0
1	A	227	ASP	3.9
1	C	59	LYS	3.8
1	A	4	THR	3.8
1	A	59	LYS	3.8
1	A	223	TYR	3.7
1	A	5	SER	3.7
1	A	229	LYS	3.7
1	D	319	HIS	3.6
1	C	54	MET	3.6
1	C	44	GLU	3.6
1	A	42	LYS	3.5
1	A	38	VAL	3.5
1	B	4	THR	3.5
1	D	225	ILE	3.5
1	D	221	ALA	3.4
1	A	56	TRP	3.3
1	A	228	ARG	3.2
1	D	317	HIS	3.2
1	D	206	LEU	3.2
1	B	88	GLY	3.1
1	B	319	HIS	3.1
1	C	223	TYR	3.1
1	C	56	TRP	3.1
1	C	2	LYS	3.1
1	C	5	SER	3.1
1	A	2	LYS	3.1
1	C	33	LEU	3.0
1	A	317	HIS	3.0
1	D	5	SER	2.9
1	A	86	LYS	2.9
1	D	86	LYS	2.9
1	D	214	LEU	2.9
1	A	1	MET	2.9
1	B	221	ALA	2.9
1	B	234	TYR	2.8
1	B	85	GLN	2.8
1	A	200	VAL	2.8
1	C	178	HIS	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	316	GLU	2.8
1	A	220	ASN	2.8
1	B	15	PHE	2.8
1	C	61	VAL	2.8
1	D	39	ASN	2.7
1	B	206	LEU	2.7
1	D	231	ALA	2.7
1	A	57	GLY	2.7
1	C	57	GLY	2.7
1	C	53	GLY	2.6
1	C	204	HIS	2.6
1	B	43	ALA	2.6
1	A	44	GLU	2.6
1	A	61	VAL	2.6
1	A	60	ASN	2.6
1	A	35	LEU	2.5
1	D	223	TYR	2.5
1	A	58	GLU	2.5
1	C	35	LEU	2.5
1	A	33	LEU	2.5
1	A	230	LYS	2.5
1	A	52	ASP	2.5
1	D	88	GLY	2.4
1	C	1	MET	2.4
1	C	200	VAL	2.4
1	A	221	ALA	2.4
1	C	228	ARG	2.4
1	C	317	HIS	2.4
1	A	37	ASP	2.3
1	C	60	ASN	2.3
1	C	42	LYS	2.3
1	B	67	THR	2.3
1	D	232	THR	2.3
1	A	63	VAL	2.3
1	D	89	GLN	2.3
1	C	3	LYS	2.3
1	C	37	ASP	2.3
1	A	39	ASN	2.3
1	A	53	GLY	2.3
1	D	222	ALA	2.3
1	A	75	ASN	2.2
1	C	221	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	294	GLN	2.2
1	D	3	LYS	2.2
1	A	25	ILE	2.2
1	A	100	THR	2.2
1	C	74	ALA	2.2
1	A	206	LEU	2.2
1	B	205	ARG	2.2
1	A	41	GLU	2.2
1	B	3	LYS	2.2
1	A	88	GLY	2.2
1	A	65	SER	2.2
1	A	10	ILE	2.1
1	A	73	ASP	2.1
1	D	15	PHE	2.1
1	C	58	GLU	2.1
1	A	74	ALA	2.1
1	A	28	GLY	2.1
1	B	211	LEU	2.1
1	C	183	VAL	2.1
1	B	317	HIS	2.0
1	B	45	GLY	2.0
1	C	82	GLY	2.0
1	A	36	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 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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GOL	C	501	6/6	0.71	0.19	90,92,92,92	0
2	GOL	C	502	6/6	0.71	0.14	95,98,98,99	0
2	GOL	A	401	6/6	0.72	0.11	91,93,93,94	0
2	GOL	C	503	6/6	0.74	0.16	80,81,82,82	0
2	GOL	B	402	6/6	0.76	0.21	86,87,88,88	0
2	GOL	B	401	6/6	0.86	0.17	57,62,63,64	0
2	GOL	D	401	6/6	0.90	0.13	56,60,62,62	0
2	GOL	A	402	6/6	0.91	0.11	74,77,77,77	0

6.5 Other polymers [i](#)

There are no such residues in this entry.