Full wwPDB X-ray Structure Validation Report (i)

Feb 14, 2017 – 10:10 pm GMT

PDB ID	:	3WSV
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

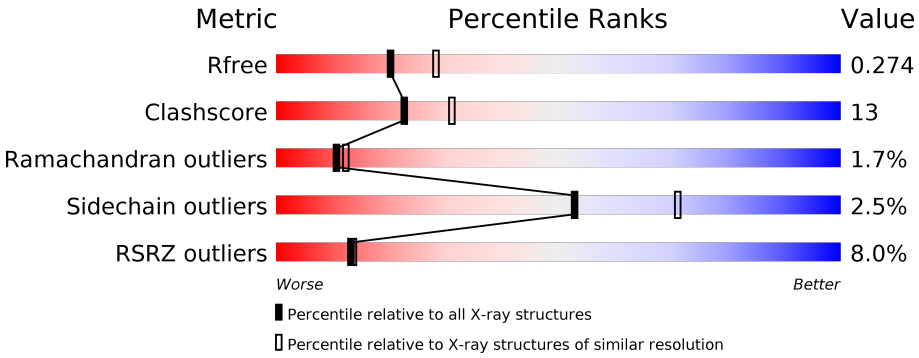
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 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}	100719	4388 (2.40-2.36)
Clashscore	112137	4984 (2.40-2.36)
Ramachandran outliers	110173	4907 (2.40-2.36)
Sidechain outliers	110143	4909 (2.40-2.36)
RSRZ outliers	101464	4423 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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	11% 65% 31%
1	B	322	5% 74% 23%
1	C	322	10% 67% 27%
1	D	322	6% 78% 20%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	B	401	-	-	-	X
2	GOL	B	402	-	-	-	X
2	GOL	C	501	-	-	-	X

2 Entry composition (i)

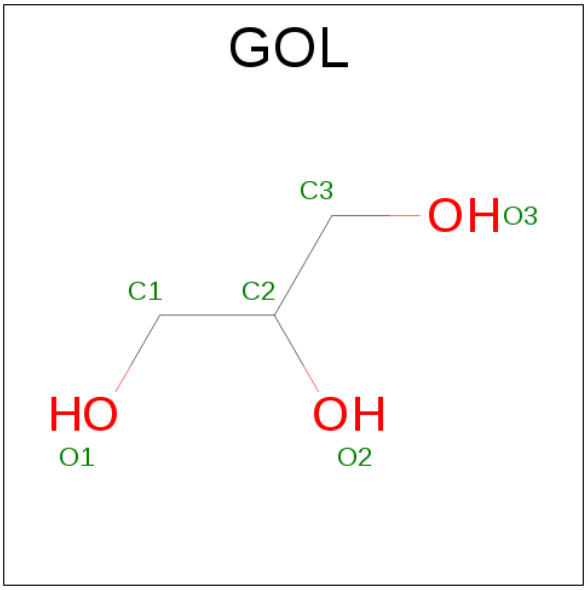
There are 3 unique types of molecules in this entry. The entry contains 10138 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (three-letter code: GOL) (formula: $C_3H_8O_3$).



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.

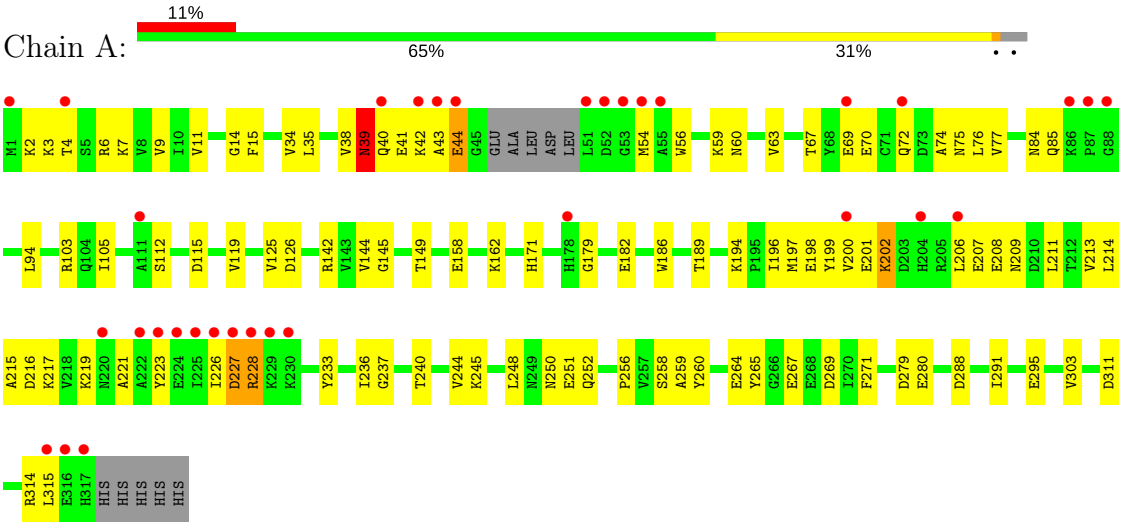
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	86	Total	O	0	0
			86	86		
3	B	121	Total	O	0	0
			121	121		
3	C	79	Total	O	0	0
			79	79		
3	D	122	Total	O	0	0
			122	122		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

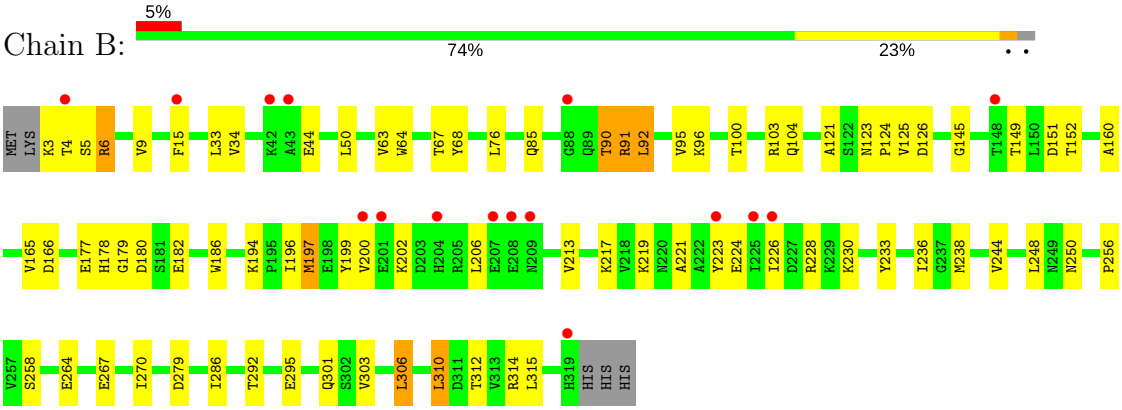
• Molecule 1: L-lactate dehydrogenase

Chain A:



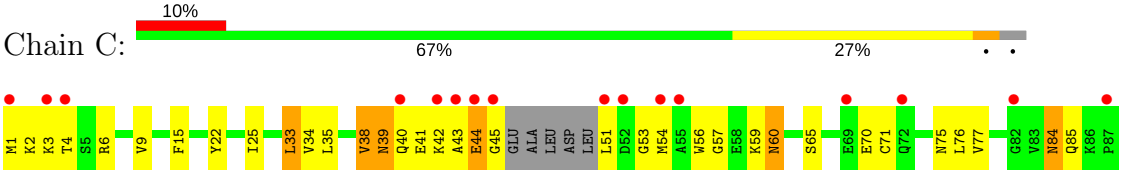
• Molecule 1: L-lactate dehydrogenase

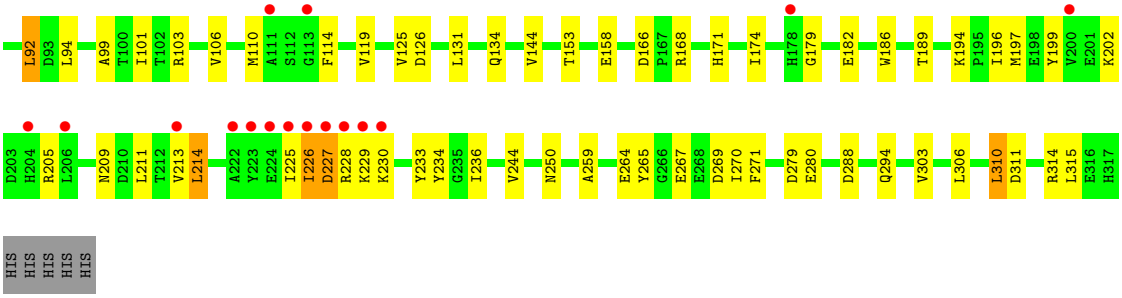
Chain B:



• Molecule 1: L-lactate dehydrogenase

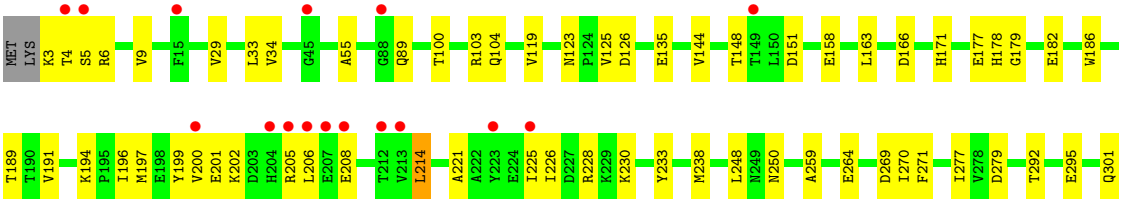
Chain C:





• Molecule 1: L-lactate dehydrogenase

Chain D:



4 Data and refinement statistics (i)

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 35.94 – 2.38	Depositor EDS
% Data completeness (in resolution range)	96.4 (29.96-2.38) 99.5 (35.94-2.38)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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	3629 reflections (5.05%)	DCC
Wilson B-factor (Å^2)	45.7	Xtriage
Anisotropy	0.639	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 44.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.57$, $< L^2 > = 0.42$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o,F_c correlation	0.95	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 $< |L| >$, $< L^2 >$ 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	0.34	0/2436	0.58	0/3304
1	B	0.35	0/2480	0.59	0/3368
1	C	0.34	0/2436	0.56	1/3304 (0.0%)
1	D	0.34	0/2480	0.58	0/3368
All	All	0.34	0/9832	0.58	1/13344 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	174	ILE	N-CA-C	-5.13	97.16	111.00

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	83	0
1	B	2441	0	2442	55	0
1	C	2400	0	2415	76	0
1	D	2441	0	2442	54	0
2	A	12	0	16	2	0
2	B	12	0	16	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	253	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 13.

All (253) 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:C:158:GLU:HB3	1:C:214:LEU:HD11	1.57	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
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: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:B:200:VAL:HG22	1:B:206:LEU:HD12	1.73	0.69
1:D:89:GLN:H	1:D:89:GLN:CD	1.96	0.69
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:85:GLN:HE21	1:B:123:ASN:HB3	1.62	0.64
1:B:103:ARG:HD2	1:B:315:LEU:HD11	1.81	0.63
1:B:85:GLN:NE2	1:B:123:ASN:HB3	2.13	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
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: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: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:B:197:MET:HA	1:B:197:MET:CE	2.34	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:A:39:ASN:CG	1:A:40:GLN:H	2.08	0.57
1:C:186:TRP:HE3	1:C:196:ILE:HG21	1.70	0.56
1:C:119:VAL:HA	1:C:144:VAL:O	2.05	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:67:THR:HG22	1:B:68:TYR:N	2.22	0.55
1:B:3:LYS:HB2	3:B:610:HOH:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:CD1	1:A:223:TYR:O	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: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:O	1:C:270:ILE:HD12	2.10	0.52
1:D:264:GLU:H	1:D:264:GLU:CD	2.13	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: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
2:A:402:GOL:H31	1:D:277:ILE:HD11	1.92	0.51
1:A:67:THR:OG1	1:A:69:GLU:HG2	2.10	0.51
1:B:152:THR:HG22	2:B:401:GOL:H31	1.91	0.51
1:A:221:ALA:C	1:A:223:TYR:H	2.14	0.51
1:A:264:GLU:HA	1:A:288:ASP:OD2	2.11	0.51
1:A:35:LEU:HD11	1:A:54:MET:HE1	1.93	0.51
1:B:267:GLU:HG3	1:B:303:VAL:HG21	1.93	0.51
1:A:115:ASP:O	1:C:1:MET:HA	2.11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:D:270:ILE:HD12	1:D:270:ILE:O	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:A:7:LYS:HZ1	1:A:70:GLU:HG3	1.78	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:264:GLU:HA	1:C:288:ASP:OD2	2.14	0.48
1:C:84:ASN:CB	1:C:228:ARG:HH21	2.25	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:O	1:B:206:LEU:HD12	2.14	0.48
1:C:228:ARG:HH11	1:C:228:ARG:HG3	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:A:54:MET:HE2	1:A:63:VAL:HG11	1.96	0.47
1:D:171:HIS:O	1:D:189:THR:HA	2.15	0.47
1:C:197:MET:HE2	1:C:211:LEU:HD11	1.95	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:O	1:D:225:ILE:HG23	2.14	0.47
1:D:310:LEU:HD22	1:D:314:ARG:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:LEU:HD23	1:A:76:LEU:C	2.35	0.47
1:B:264:GLU:CD	1:B:264:GLU:H	2.17	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:186:TRP:HB3	1:C:197:MET:HE3	1.98	0.46
1:C:71:CYS:O	1:C:114:PHE:HD1	1.99	0.46
1:C:59:LYS:O	1:C:60:ASN:C	2.54	0.46
1:A:233:TYR:O	1:A:236:ILE:HG22	2.17	0.45
1:D:205:ARG:C	1:D:206:LEU:HD12	2.37	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: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:38:VAL:HG23	1:C:39:ASN:N	2.24	0.44
1:C:76:LEU:HD23	1:C:76:LEU:C	2.38	0.44
1:C:9:VAL:HB	1:C:77:VAL:HG22	2.00	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:HD3	1:C:3:LYS:HA	1.76	0.44
1:A:35:LEU:HD11	1:A:54:MET:CE	2.47	0.44
1:B:76:LEU:HD13	1:B:244:VAL:HG13	1.99	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:125:VAL:HG13	1:C:126:ASP:N	2.33	0.43
1:C:25:ILE:CD1	1:C:54:MET:HG3	2.48	0.43
1:A:119:VAL:HA	1:A:144:VAL:O	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:125:VAL:HG13	1:D:126:ASP:N	2.34	0.43
1:A:15:PHE:N	1:A:43:ALA:HB3	2.34	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
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:D:89:GLN:N	1:D:89:GLN:CD	2.67	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:200:VAL:HG12	1:A:206:LEU:HB3	2.01	0.42
1:A:103:ARG:NE	1:A:315:LEU:HD11	2.35	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:162:LYS:HD2	1:A:162:LYS:HA	1.87	0.42
1:A:226:ILE:HG22	1:A:227:ASP:N	2.33	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: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: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:N	1:C:294:GLN:OE1	2.47	0.41
1:A:207:GLU:HG2	1:A:209:ASN:H	1.85	0.41
1:C:194:LYS:HD3	1:C:199:TYR:CE1	2.54	0.41
1:C:51:LEU:HD21	1:C:65:SER:CB	2.51	0.41
1:A:186:TRP:CE3	1:A:196:ILE:HG21	2.55	0.41
1:C:234:TYR:HE2	1:D:233:TYR:HH	1.66	0.41
1:A:142:ARG:HD3	1:C:1:MET:SD	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:209:ASN:O	1:C:213:VAL:HG23	2.20	0.41
1:C:92:LEU:HD12	1:C:92:LEU:HA	1.91	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
1:A:315:LEU:N	1:A:315:LEU:CD1	2.84	0.41
1:A:39:ASN:ND2	1:A:40:GLN:H	2.19	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:145:GLY:HA3	1:B:258:SER:HB2	2.03	0.40
1:B:92:LEU:HD21	1:B:312:THR:OG1	2.21	0.40
1:B:149:THR:HA	1:B:256:PRO:HG2	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:D:163:LEU:HD12	1:D:191:VAL:HG21	2.03	0.40
1:D:208:GLU:OE1	1:D:208:GLU:HA	2.21	0.40
1:C:22:TYR:CZ	1:D:230:LYS:HE2	2.57	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)

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	308/322 (96%)	283 (92%)	19 (6%)	6 (2%)	9 10
1	B	315/322 (98%)	296 (94%)	16 (5%)	3 (1%)	18 24
1	C	308/322 (96%)	281 (91%)	17 (6%)	10 (3%)	5 3
1	D	315/322 (98%)	297 (94%)	16 (5%)	2 (1%)	28 39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1246/1288 (97%)	1157 (93%)	68 (6%)	21 (2%)	11 12

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	39	ASN
1	A	60	ASN
1	C	39	ASN
1	B	90	THR
1	B	202	LYS
1	C	60	ASN
1	C	226	ILE
1	D	202	LYS
1	A	44	GLU
1	A	56	TRP
1	C	56	TRP
1	C	202	LYS
1	C	227	ASP
1	D	221	ALA
1	B	91	ARG
1	C	53	GLY
1	C	57	GLY
1	A	202	LYS
1	A	228	ARG
1	C	44	GLU
1	C	38	VAL

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%)	258 (98%)	4 (2%)	70 84
1	B	266/271 (98%)	258 (97%)	8 (3%)	46 65
1	C	262/271 (97%)	254 (97%)	8 (3%)	45 64
1	D	266/271 (98%)	260 (98%)	6 (2%)	56 73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1056/1084 (97%)	1030 (98%)	26 (2%)	53 71

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

Mol	Chain	Res	Type
1	A	39	ASN
1	A	59	LYS
1	A	84	ASN
1	A	227	ASP
1	B	6	ARG
1	B	33	LEU
1	B	50	LEU
1	B	92	LEU
1	B	166	ASP
1	B	197	MET
1	B	306	LEU
1	B	310	LEU
1	C	33	LEU
1	C	84	ASN
1	C	92	LEU
1	C	205	ARG
1	C	214	LEU
1	C	225	ILE
1	C	306	LEU
1	C	310	LEU
1	D	6	ARG
1	D	33	LEU
1	D	166	ASP
1	D	214	LEU
1	D	306	LEU
1	D	310	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	ASN
1	A	252	GLN
1	B	27	GLN
1	B	72	GLN
1	B	85	GLN
1	B	220	ASN

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Mol	Chain	Res	Type
1	B	318	HIS
1	C	85	GLN
1	D	72	GLN

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 carbohydrates 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	A	401	-	5,5,5	0.27	0	5,5,5	0.24	0
2	GOL	A	402	-	5,5,5	0.32	0	5,5,5	0.20	0
2	GOL	B	401	-	5,5,5	0.39	0	5,5,5	0.19	0
2	GOL	B	402	-	5,5,5	0.36	0	5,5,5	0.22	0
2	GOL	C	501	-	5,5,5	0.32	0	5,5,5	0.20	0
2	GOL	C	502	-	5,5,5	0.29	0	5,5,5	0.24	0
2	GOL	C	503	-	5,5,5	0.39	0	5,5,5	0.25	0
2	GOL	D	401	-	5,5,5	0.34	0	5,5,5	0.27	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	401	-	-	0/4/4/4	0/0/0/0
2	GOL	A	402	-	-	0/4/4/4	0/0/0/0
2	GOL	B	401	-	-	0/4/4/4	0/0/0/0
2	GOL	B	402	-	-	0/4/4/4	0/0/0/0
2	GOL	C	501	-	-	0/4/4/4	0/0/0/0
2	GOL	C	502	-	-	0/4/4/4	0/0/0/0
2	GOL	C	503	-	-	0/4/4/4	0/0/0/0
2	GOL	D	401	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	402	GOL	2	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, 95^{th} 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%)	0.70	34 (10%) 6 7	33, 53, 108, 121	0
1	B	317/322 (98%)	0.33	16 (5%) 30 32	32, 49, 82, 98	0
1	C	312/322 (96%)	0.63	32 (10%) 7 8	33, 53, 110, 132	0
1	D	317/322 (98%)	0.29	19 (5%) 23 24	32, 49, 86, 99	0
All	All	1258/1288 (97%)	0.49	101 (8%) 13 14	32, 51, 96, 132	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	225	ILE	10.4
1	A	54	MET	7.2
1	C	43	ALA	7.0
1	C	45	GLY	6.7
1	A	225	ILE	6.7
1	A	227	ASP	6.7
1	A	55	ALA	6.2
1	C	223	TYR	6.1
1	C	44	GLU	6.0
1	A	317	HIS	5.9
1	D	318	HIS	5.8
1	B	225	ILE	5.8
1	C	222	ALA	5.7
1	A	223	TYR	5.5
1	C	4	THR	5.5
1	A	226	ILE	5.5
1	C	55	ALA	5.1
1	C	54	MET	4.9
1	A	4	THR	4.9
1	A	224	GLU	4.8
1	D	200	VAL	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	200	VAL	4.4
1	A	87	PRO	4.4
1	A	222	ALA	4.3
1	C	42	LYS	4.2
1	D	204	HIS	4.2
1	D	317	HIS	4.1
1	A	316	GLU	4.1
1	C	204	HIS	4.1
1	C	226	ILE	4.0
1	C	224	GLU	4.0
1	A	42	LYS	4.0
1	A	229	LYS	3.8
1	A	228	ARG	3.8
1	A	44	GLU	3.8
1	C	228	ARG	3.7
1	C	40	GLN	3.7
1	D	225	ILE	3.7
1	B	223	TYR	3.7
1	B	43	ALA	3.6
1	C	51	LEU	3.6
1	A	86	LYS	3.6
1	A	51	LEU	3.4
1	C	200	VAL	3.4
1	A	111	ALA	3.4
1	D	15	PHE	3.4
1	C	227	ASP	3.3
1	A	43	ALA	3.3
1	B	319	HIS	3.3
1	B	15	PHE	3.2
1	A	230	LYS	3.2
1	C	87	PRO	3.2
1	B	208	GLU	3.2
1	C	3	LYS	3.1
1	A	204	HIS	3.1
1	D	208	GLU	3.1
1	C	229	LYS	3.1
1	A	40	GLN	3.1
1	D	4	THR	3.0
1	A	52	ASP	3.0
1	B	204	HIS	2.9
1	D	223	TYR	2.9
1	A	69	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	206	LEU	2.9
1	C	230	LYS	2.8
1	B	4	THR	2.8
1	A	220	ASN	2.7
1	A	88	GLY	2.7
1	D	207	GLU	2.7
1	B	201	GLU	2.6
1	C	111	ALA	2.6
1	A	178	HIS	2.6
1	D	316	GLU	2.5
1	C	69	GLU	2.5
1	A	72	GLN	2.5
1	C	72	GLN	2.5
1	D	213	VAL	2.5
1	D	5	SER	2.4
1	C	52	ASP	2.4
1	C	1	MET	2.4
1	C	206	LEU	2.4
1	C	113	GLY	2.4
1	A	1	MET	2.4
1	A	53	GLY	2.4
1	C	178	HIS	2.3
1	B	207	GLU	2.3
1	B	42	LYS	2.3
1	C	82	GLY	2.3
1	D	88	GLY	2.2
1	B	226	ILE	2.2
1	D	149	THR	2.2
1	D	212	THR	2.2
1	B	200	VAL	2.2
1	A	315	LEU	2.2
1	B	209	ASN	2.2
1	C	213	VAL	2.2
1	B	148	THR	2.2
1	D	45	GLY	2.1
1	A	206	LEU	2.1
1	B	88	GLY	2.1
1	D	205	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 carbohydrates 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. 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^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
2	GOL	B	402	6/6	0.72	0.32	6.35	86,87,88,88	0
2	GOL	C	501	6/6	0.71	0.38	5.93	90,92,92,92	0
2	GOL	B	401	6/6	0.84	0.32	3.78	57,62,63,64	0
2	GOL	D	401	6/6	0.90	0.24	1.34	56,60,62,62	0
2	GOL	A	402	6/6	0.90	0.16	-0.48	74,77,77,77	0
2	GOL	A	401	6/6	0.78	0.31	-	91,93,93,94	0
2	GOL	C	502	6/6	0.60	0.24	-	95,98,98,99	0
2	GOL	C	503	6/6	0.64	0.48	-	80,81,82,82	0

6.5 Other polymers (i)

There are no such residues in this entry.