Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:07 PM GMT

PDB ID	:	4H19
Title	:	Crystal structure of an enolase (mandelate racemase subgroup, target EFI-502087) from agrobacterium tumefaciens, with bound Mg and d-ribonohydroxamate, ordered loop
Authors	:	Vetting, M.W.; Bouvier, J.T.; Morisco, L.L.; Wasserman, S.R.; Sojitra, S.; Imker, H.J.; Gerlt, J.A.; Almo, S.C.; Enzyme Function Initiative (EFI)
Deposited on	:	2012-09-10
Resolution	:	1.80 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 (1)) were used in the production of this report:

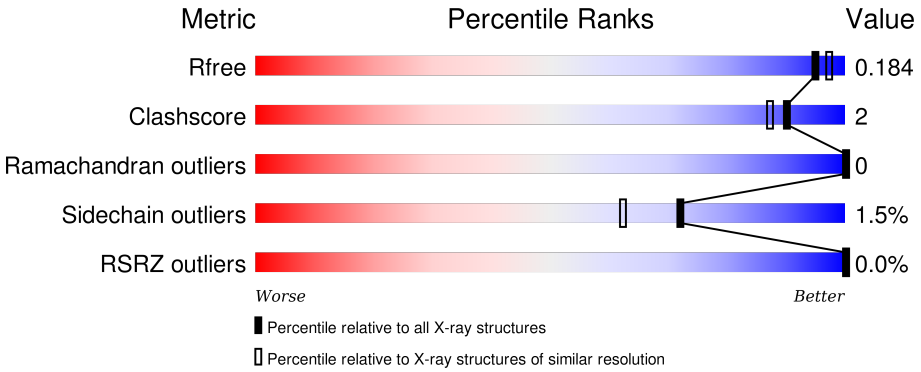
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 1.80 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}	91344	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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	372	93% 6% •
1	B	372	94% 6%
1	C	372	94% 6%
1	D	372	92% 7% •
1	E	372	93% 6% •

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Mol	Chain	Length	Quality of chain
1	F	372	92% 8%
1	G	372	92% 8%
1	H	372	93% 7%
1	I	372	91% 9%
1	J	372	94% 6%
1	K	372	91% 9%
1	L	372	94% 6%
1	M	372	93% 6%
1	N	372	95% 5%
1	O	372	92% 7%
1	P	372	93% 7%

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CL	A	403	-	-	-	X
3	CL	A	404	-	-	X	X
3	CL	B	403	-	-	X	X
3	CL	B	404	-	-	-	X
3	CL	C	403	-	-	-	X
3	CL	D	403	-	-	X	-
3	CL	D	404	-	-	X	X
3	CL	D	405	-	-	X	X
3	CL	E	402	-	-	X	X
3	CL	E	403	-	-	-	X
3	CL	F	402	-	-	-	X
3	CL	F	403	-	-	-	X
3	CL	G	403	-	-	-	X
3	CL	G	404	-	-	X	-
3	CL	H	403	-	-	-	X
3	CL	H	404	-	-	-	X
3	CL	I	402	-	-	-	X
3	CL	I	403	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CL	J	403	-	-	-	X
3	CL	K	403	-	-	-	X
3	CL	K	404	-	-	X	X
3	CL	L	402	-	-	X	-
3	CL	L	403	-	-	-	X
3	CL	M	403	-	-	-	X
3	CL	N	403	-	-	-	X
3	CL	O	403	-	-	X	X
3	CL	O	404	-	-	-	X
3	CL	P	402	-	-	-	X
3	CL	P	403	-	-	-	X
5	GOL	A	406	-	-	-	X
5	GOL	A	407	-	-	-	X
5	GOL	A	408	-	-	-	X
5	GOL	B	406	-	-	-	X
5	GOL	B	408	-	-	-	X
5	GOL	C	407	-	-	-	X
5	GOL	D	409	-	-	-	X
5	GOL	E	405	-	-	-	X
5	GOL	E	406	-	-	-	X
5	GOL	F	406	-	-	-	X
5	GOL	F	407	-	-	-	X
5	GOL	G	407	-	-	-	X
5	GOL	I	405	-	-	-	X
5	GOL	J	405	-	-	-	X
5	GOL	J	406	-	-	-	X
5	GOL	K	408	-	-	-	X
5	GOL	L	405	-	-	-	X
5	GOL	M	406	-	-	-	X
5	GOL	N	406	-	-	-	X
5	GOL	N	407	-	-	-	X
5	GOL	P	405	-	-	-	X
5	GOL	P	407	-	-	-	X
5	GOL	P	408	-	-	-	X
6	0YR	C	408	-	-	-	X
6	0YR	E	408	-	-	-	X
6	0YR	F	408	-	-	-	X
6	0YR	G	409	-	-	-	X
6	0YR	H	409	-	-	-	X
6	0YR	K	409	-	-	-	X
6	0YR	L	407	-	-	-	X
6	0YR	N	409	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	0YR	O	408	-	-	-	X
6	0YR	P	409	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 53008 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	372	Total	C	N	O	S	0	2	0
			2922	1868	505	543	6			
1	B	372	Total	C	N	O	S	0	1	0
			2913	1863	503	541	6			
1	C	372	Total	C	N	O	S	0	1	0
			2913	1863	503	541	6			
1	D	372	Total	C	N	O	S	0	2	0
			2924	1869	507	542	6			
1	E	372	Total	C	N	O	S	0	3	0
			2925	1869	505	545	6			
1	F	372	Total	C	N	O	S	0	2	0
			2919	1866	504	543	6			
1	G	372	Total	C	N	O	S	0	2	0
			2919	1866	504	543	6			
1	H	372	Total	C	N	O	S	0	0	0
			2907	1860	502	539	6			
1	I	372	Total	C	N	O	S	0	1	0
			2913	1863	503	541	6			
1	K	372	Total	C	N	O	S	0	2	0
			2919	1866	504	543	6			
1	L	372	Total	C	N	O	S	0	0	0
			2907	1860	502	539	6			
1	M	372	Total	C	N	O	S	0	1	0
			2913	1863	503	541	6			
1	N	372	Total	C	N	O	S	0	2	0
			2919	1866	504	543	6			
1	P	372	Total	C	N	O	S	0	2	0
			2922	1869	505	542	6			
1	J	372	Total	C	N	O	S	0	3	0
			2928	1871	505	546	6			
1	O	372	Total	C	N	O	S	0	2	0
			2919	1866	504	543	6			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Ca 1 1	0	0
2	J	1	Total Ca 1 1	0	0
2	D	1	Total Ca 1 1	0	0
2	K	1	Total Ca 1 1	0	0
2	H	1	Total Ca 1 1	0	0
2	B	1	Total Ca 1 1	0	0
2	A	1	Total Ca 1 1	0	0
2	N	1	Total Ca 1 1	0	0
2	O	1	Total Ca 1 1	0	0
2	M	1	Total Ca 1 1	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	P	3	Total Cl 3 3	0	0
3	G	3	Total Cl 3 3	0	0
3	J	2	Total Cl 2 2	0	0
3	D	5	Total Cl 5 5	0	0
3	K	3	Total Cl 3 3	0	0
3	E	3	Total Cl 3 3	0	0
3	H	3	Total Cl 3 3	0	0
3	B	3	Total Cl 3 3	0	0
3	I	3	Total Cl 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	3	Total Cl 3 3	0	0
3	A	3	Total Cl 3 3	0	0
3	N	3	Total Cl 3 3	0	0
3	O	3	Total Cl 3 3	0	0
3	L	3	Total Cl 3 3	0	0
3	F	3	Total Cl 3 3	0	0
3	M	3	Total Cl 3 3	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	P	1	Total Mg 1 1	0	0
4	G	1	Total Mg 1 1	0	0
4	J	1	Total Mg 1 1	0	0
4	D	1	Total Mg 1 1	0	0
4	K	1	Total Mg 1 1	0	0
4	E	1	Total Mg 1 1	0	0
4	H	1	Total Mg 1 1	0	0
4	B	1	Total Mg 1 1	0	0
4	I	1	Total Mg 1 1	0	0
4	C	1	Total Mg 1 1	0	0
4	A	1	Total Mg 1 1	0	0
4	N	1	Total Mg 1 1	0	0

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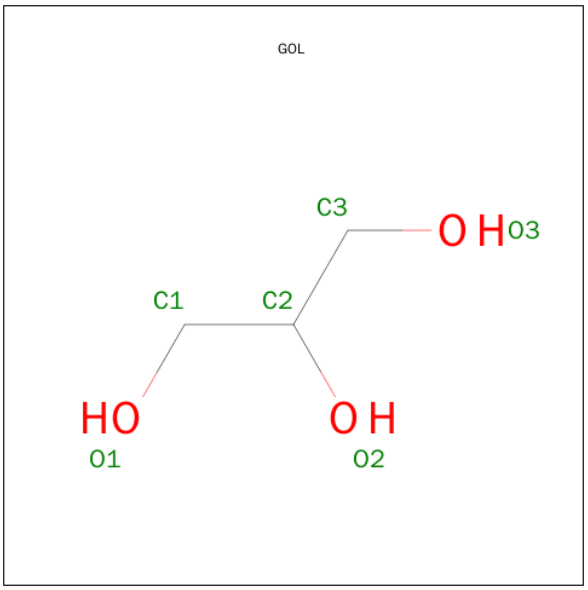
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	O	1	Total Mg 1 1	0	0
4	L	1	Total Mg 1 1	0	0
4	F	1	Total Mg 1 1	0	0
4	M	1	Total Mg 1 1	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		
5	E	1	Total	C	O	0	0
			6	3	3		
5	E	1	Total	C	O	0	0
			6	3	3		
5	E	1	Total	C	O	0	0
			6	3	3		
5	F	1	Total	C	O	0	0
			6	3	3		
5	F	1	Total	C	O	0	0
			6	3	3		
5	F	1	Total	C	O	0	0
			6	3	3		
5	G	1	Total	C	O	0	0
			6	3	3		
5	G	1	Total	C	O	0	0
			6	3	3		
5	G	1	Total	C	O	0	0
			6	3	3		
5	H	1	Total	C	O	0	0
			6	3	3		
5	H	1	Total	C	O	0	0
			6	3	3		
5	H	1	Total	C	O	0	0
			6	3	3		
5	I	1	Total	C	O	0	0
			6	3	3		
5	K	1	Total	C	O	0	0
			6	3	3		
5	K	1	Total	C	O	0	0
			6	3	3		

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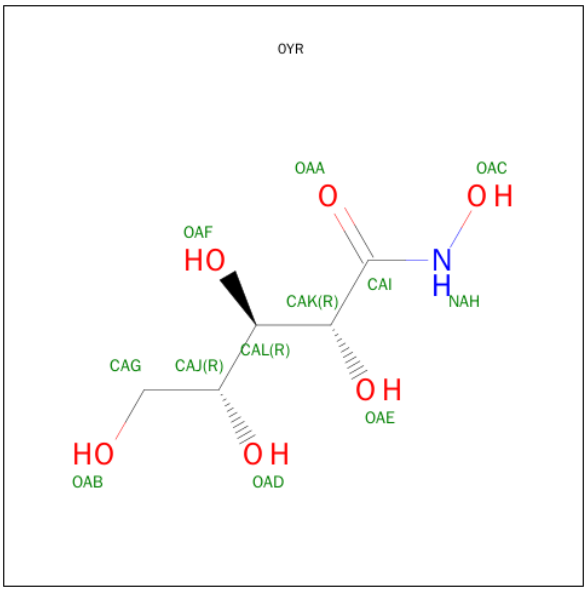
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	K	1	Total	C	O	0	0
			6	3	3		
5	L	1	Total	C	O	0	0
			6	3	3		
5	L	1	Total	C	O	0	0
			6	3	3		
5	M	1	Total	C	O	0	0
			6	3	3		
5	N	1	Total	C	O	0	0
			6	3	3		
5	N	1	Total	C	O	0	0
			6	3	3		
5	N	1	Total	C	O	0	0
			6	3	3		
5	P	1	Total	C	O	0	0
			6	3	3		
5	P	1	Total	C	O	0	0
			6	3	3		
5	P	1	Total	C	O	0	0
			6	3	3		
5	P	1	Total	C	O	0	0
			6	3	3		
5	J	1	Total	C	O	0	0
			6	3	3		
5	J	1	Total	C	O	0	0
			6	3	3		
5	J	1	Total	C	O	0	0
			6	3	3		
5	O	1	Total	C	O	0	0
			6	3	3		
5	O	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is (2R,3R,4R)-N,2,3,4,5-PENTAKIS(OXIDANYL)PENTANAMIDE (three-letter code: 0YR) (formula: $C_5H_{11}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C N O 12 5 1 6	0	0
6	B	1	Total C N O 12 5 1 6	0	0
6	C	1	Total C N O 12 5 1 6	0	0
6	D	1	Total C N O 12 5 1 6	0	0
6	E	1	Total C N O 12 5 1 6	0	0
6	F	1	Total C N O 12 5 1 6	0	0
6	G	1	Total C N O 12 5 1 6	0	0
6	H	1	Total C N O 12 5 1 6	0	0
6	I	1	Total C N O 12 5 1 6	0	0
6	K	1	Total C N O 12 5 1 6	0	0
6	L	1	Total C N O 12 5 1 6	0	0
6	M	1	Total C N O 12 5 1 6	0	0
6	N	1	Total C N O 12 5 1 6	0	0
6	P	1	Total C N O 12 5 1 6	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	J	1	Total C N O 12 5 1 6	0	0
6	O	1	Total C N O 12 5 1 6	0	0

- Molecule 7 is water.

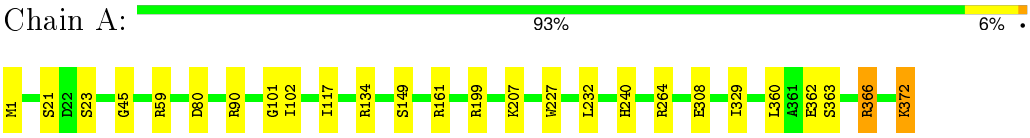
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	354	Total O 354 354	0	0
7	B	383	Total O 383 383	0	0
7	C	345	Total O 345 345	0	0
7	D	430	Total O 430 430	0	0
7	E	370	Total O 370 370	0	0
7	F	353	Total O 353 353	0	0
7	G	375	Total O 375 375	0	0
7	H	378	Total O 378 378	0	0
7	I	352	Total O 352 352	0	0
7	K	370	Total O 370 370	0	0
7	L	333	Total O 334 334	0	1
7	M	354	Total O 354 354	0	0
7	N	393	Total O 394 394	0	1
7	P	329	Total O 329 329	0	0
7	J	321	Total O 321 321	0	0
7	O	353	Total O 353 353	0	0

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 errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

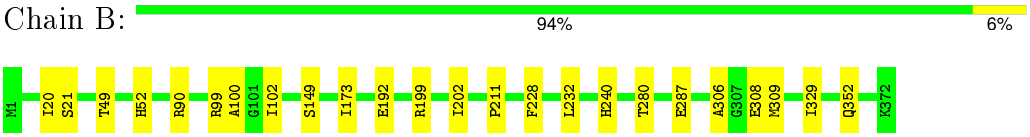
- Molecule 1: Mandelate racemase

Chain A:



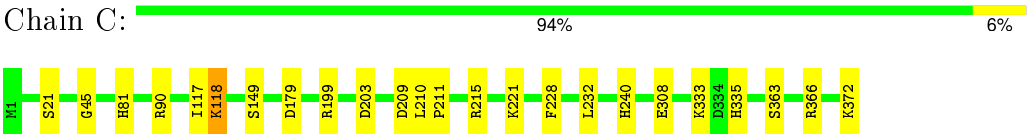
- Molecule 1: Mandelate racemase

Chain B:



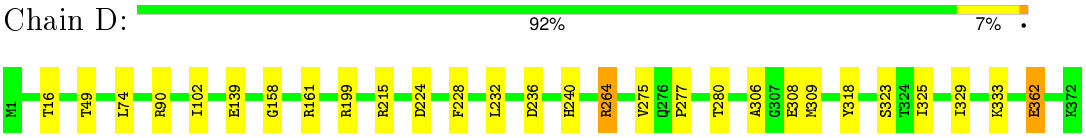
- Molecule 1: Mandelate racemase

Chain C:



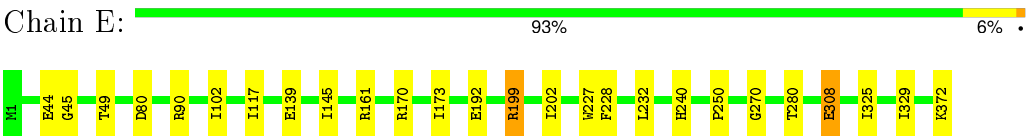
- Molecule 1: Mandelate racemase

Chain D:



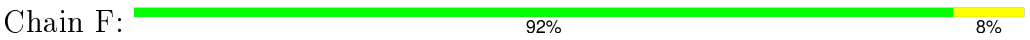
- Molecule 1: Mandelate racemase

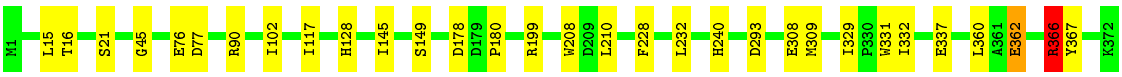
Chain E:



- Molecule 1: Mandelate racemase

Chain F:



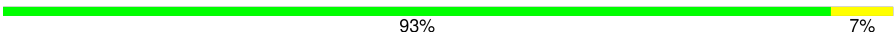


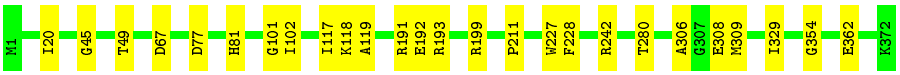
• Molecule 1: Mandelate racemase

Chain G:

• Molecule 1: Mandelate racemase

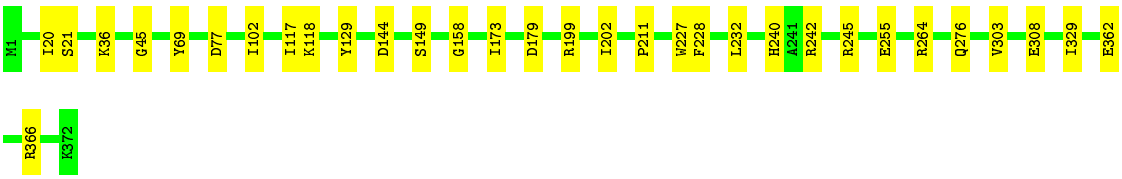
Chain H:





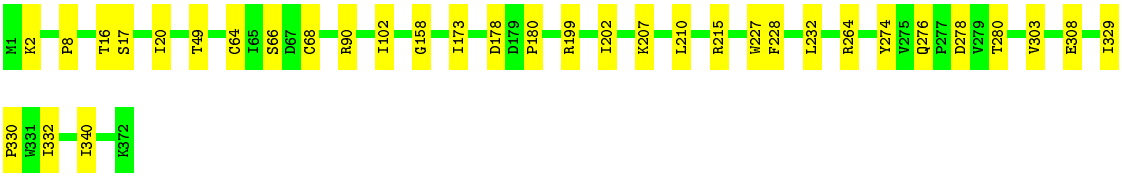
• Molecule 1: Mandelate racemase

Chain I:



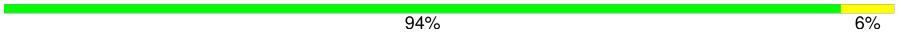
• Molecule 1: Mandelate racemase

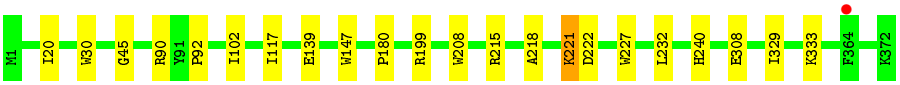
Chain K:



• Molecule 1: Mandelate racemase

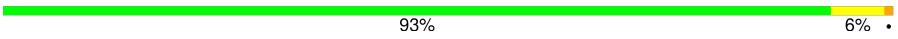
Chain L:





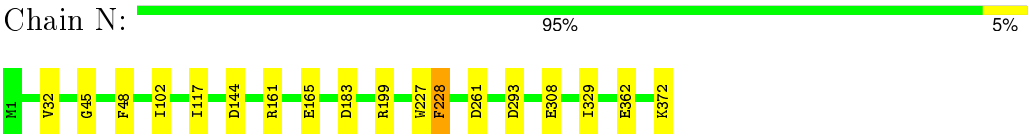
• Molecule 1: Mandelate racemase

Chain M:



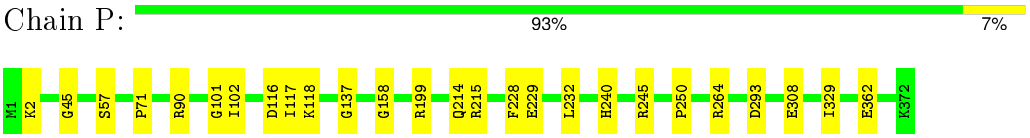
• Molecule 1: Mandelate racemase

Chain N:



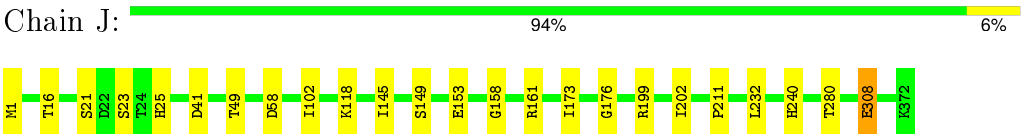
- Molecule 1: Mandelate racemase

Chain P:



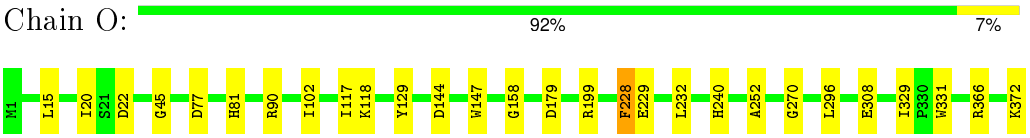
- Molecule 1: Mandelate racemase

Chain J:



- Molecule 1: Mandelate racemase

Chain O:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	178.36Å 395.69Å 177.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	197.84 – 1.80 197.84 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (197.84-1.80) 99.9 (197.84-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) >$ [1]	2.51 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.137 , 0.175 0.151 , 0.184	Depositor DCC
R_{free} test set	28792 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	15.3	Xtriage
Anisotropy	0.435	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 47.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	4 of 573402 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	53008	wwPDB-VP
Average B, all atoms (Å^2)	17.0	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 58.56 % 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 2.0094e-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, 0.375 respectively for untwinned datasets, and 0.333, 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, MG, CA, 0YR, CL

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	0.99	0/3003	1.01	10/4102 (0.2%)
1	B	1.00	1/2994 (0.0%)	0.95	2/4089 (0.0%)
1	C	1.01	0/2994	0.97	4/4089 (0.1%)
1	D	1.03	1/3005 (0.0%)	0.99	8/4104 (0.2%)
1	E	0.99	2/3006 (0.1%)	0.94	6/4105 (0.1%)
1	F	1.02	1/3000 (0.0%)	0.97	5/4097 (0.1%)
1	G	0.97	3/3000 (0.1%)	0.96	4/4097 (0.1%)
1	H	1.00	1/2988 (0.0%)	0.98	7/4081 (0.2%)
1	I	0.99	3/2994 (0.1%)	0.95	6/4089 (0.1%)
1	J	1.02	1/3009 (0.0%)	0.95	2/4109 (0.0%)
1	K	1.05	1/3000 (0.0%)	0.97	6/4097 (0.1%)
1	L	1.00	2/2988 (0.1%)	0.94	3/4081 (0.1%)
1	M	1.01	0/2994	0.96	7/4089 (0.2%)
1	N	0.97	0/3000	0.93	4/4097 (0.1%)
1	O	1.00	1/3000 (0.0%)	0.96	8/4097 (0.2%)
1	P	0.99	3/3003 (0.1%)	0.95	7/4100 (0.2%)
All	All	1.00	20/47978 (0.0%)	0.96	89/65523 (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	C	0	1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	362	GLU	CG-CD	6.06	1.61	1.51
1	H	362	GLU	CG-CD	5.94	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	362	GLU	CG-CD	5.92	1.60	1.51
1	O	270	GLY	C-O	5.89	1.33	1.23
1	P	57	SER	CB-OG	-5.87	1.34	1.42
1	G	362	GLU	CG-CD	5.83	1.60	1.51
1	K	274	TYR	CE1-CZ	-5.78	1.31	1.38
1	J	308	GLU	CD-OE2	5.75	1.31	1.25
1	E	308	GLU	CD-OE1	5.69	1.31	1.25
1	G	230	GLU	CD-OE1	5.68	1.31	1.25
1	F	76	GLU	CD-OE2	-5.57	1.19	1.25
1	I	362	GLU	CG-CD	5.56	1.60	1.51
1	I	69	TYR	CE1-CZ	-5.53	1.31	1.38
1	P	229	GLU	CD-OE2	5.52	1.31	1.25
1	B	287	GLU	CD-OE2	5.22	1.31	1.25
1	L	139	GLU	CD-OE2	-5.15	1.20	1.25
1	I	255	GLU	CD-OE2	5.15	1.31	1.25
1	E	44	GLU	CD-OE2	-5.09	1.20	1.25
1	L	30	TRP	CB-CG	-5.05	1.41	1.50
1	G	288	TYR	CZ-OH	-5.04	1.29	1.37

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	90	ARG	NE-CZ-NH1	10.35	125.48	120.30
1	O	77	ASP	CB-CG-OD1	9.45	126.81	118.30
1	P	90	ARG	NE-CZ-NH1	9.07	124.84	120.30
1	A	134	ARG	NE-CZ-NH1	-8.79	115.90	120.30
1	M	199	ARG	NE-CZ-NH2	8.66	124.63	120.30
1	D	264	ARG	NE-CZ-NH1	8.65	124.63	120.30
1	L	90	ARG	NE-CZ-NH1	8.47	124.53	120.30
1	F	366	ARG	NE-CZ-NH2	8.20	124.40	120.30
1	H	242	ARG	NE-CZ-NH1	-8.14	116.23	120.30
1	D	264	ARG	NE-CZ-NH2	-7.83	116.39	120.30
1	O	77	ASP	CB-CG-OD2	-7.79	111.29	118.30
1	K	278	ASP	CB-CG-OD2	-7.72	111.35	118.30
1	H	193	ARG	NE-CZ-NH1	7.27	123.94	120.30
1	L	215	ARG	NE-CZ-NH1	7.24	123.92	120.30
1	A	264	ARG	NE-CZ-NH2	-7.18	116.71	120.30
1	E	90	ARG	NE-CZ-NH1	7.13	123.87	120.30
1	G	90	ARG	NE-CZ-NH1	7.01	123.80	120.30
1	C	179	ASP	CB-CG-OD1	7.00	124.60	118.30
1	K	278	ASP	CB-CG-OD1	6.86	124.47	118.30
1	A	90	ARG	NE-CZ-NH1	6.54	123.57	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	99	ARG	NE-CZ-NH2	6.48	123.54	120.30
1	G	90	ARG	NE-CZ-NH2	-6.44	117.08	120.30
1	P	264	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	J	161	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	H	67	ASP	CB-CG-OD2	-6.24	112.69	118.30
1	A	80	ASP	CB-CG-OD1	6.24	123.91	118.30
1	P	116	ASP	CB-CG-OD1	6.21	123.89	118.30
1	K	90	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	O	90	ARG	NE-CZ-NH2	-6.17	117.21	120.30
1	K	215	ARG	NE-CZ-NH2	-6.17	117.22	120.30
1	I	245	ARG	NE-CZ-NH2	6.16	123.38	120.30
1	O	179	ASP	CB-CG-OD1	6.11	123.80	118.30
1	P	116	ASP	CB-CG-OD2	-5.94	112.96	118.30
1	P	245	ARG	NE-CZ-NH2	5.90	123.25	120.30
1	E	199	ARG	NE-CZ-NH2	5.88	123.24	120.30
1	I	179	ASP	CB-CG-OD1	5.88	123.59	118.30
1	C	209	ASP	CB-CG-OD2	-5.86	113.03	118.30
1	B	90	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	O	90	ARG	NE-CZ-NH1	5.85	123.22	120.30
1	F	178	ASP	CB-CG-OD1	5.82	123.54	118.30
1	D	215	ARG	NE-CZ-NH2	-5.79	117.40	120.30
1	J	58	ASP	CB-CG-OD1	5.77	123.50	118.30
1	C	90	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	E	90	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	K	178	ASP	CB-CG-OD1	5.75	123.48	118.30
1	M	179	ASP	CB-CG-OD1	5.73	123.46	118.30
1	D	215	ARG	NE-CZ-NH1	5.69	123.15	120.30
1	M	90	ARG	NE-CZ-NH1	5.69	123.14	120.30
1	O	228	PHE	CB-CG-CD2	-5.67	116.83	120.80
1	P	215	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	G	193	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	I	242	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	H	77	ASP	CB-CG-OD2	-5.61	113.25	118.30
1	L	90	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	M	224	ASP	CB-CG-OD1	5.59	123.33	118.30
1	A	161	ARG	NE-CZ-NH2	-5.53	117.54	120.30
1	A	372	LYS	CD-CE-NZ	5.50	124.35	111.70
1	D	236	ASP	CB-CG-OD2	-5.50	113.35	118.30
1	P	228	PHE	CB-CG-CD1	5.49	124.64	120.80
1	N	261	ASP	CB-CG-OD1	-5.44	113.40	118.30
1	O	144	ASP	CB-CG-OD1	5.44	123.20	118.30
1	D	224	ASP	CB-CG-OD1	5.44	123.19	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	161	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	E	170	ARG	NE-CZ-NH2	5.36	122.98	120.30
1	E	80	ASP	CB-CG-OD1	5.32	123.08	118.30
1	F	77	ASP	CB-CG-OD1	5.31	123.08	118.30
1	M	90	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	K	264	ARG	NE-CZ-NH1	5.29	122.95	120.30
1	H	191	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	H	77	ASP	CB-CG-OD1	5.24	123.02	118.30
1	D	74	LEU	CB-CG-CD1	-5.24	102.10	111.00
1	M	228	PHE	CB-CG-CD2	-5.22	117.15	120.80
1	I	144	ASP	CB-CG-OD1	5.20	122.98	118.30
1	N	228	PHE	CB-CG-CD1	5.20	124.44	120.80
1	G	99	ARG	NE-CZ-NH2	5.18	122.89	120.30
1	A	59	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	N	183	ASP	CB-CG-OD2	5.15	122.94	118.30
1	I	77	ASP	CB-CG-OD2	-5.13	113.68	118.30
1	A	90	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	A	59	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	H	242	ARG	NE-CZ-NH2	5.11	122.85	120.30
1	M	228	PHE	CB-CG-CD1	5.08	124.36	120.80
1	O	22	ASP	CB-CG-OD1	5.06	122.86	118.30
1	F	293	ASP	CB-CG-OD1	5.05	122.84	118.30
1	D	90	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	C	203	ASP	CB-CG-OD1	5.03	122.83	118.30
1	N	144	ASP	CB-CG-OD1	5.03	122.83	118.30
1	A	366	ARG	CG-CD-NE	5.01	122.33	111.80
1	I	144	ASP	CB-CG-OD2	-5.01	113.79	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	215	ARG	Sidechain

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	2922	0	2862	13	0
1	B	2913	0	2854	14	0
1	C	2913	0	2854	12	0
1	D	2924	0	2867	15	0
1	E	2925	0	2862	13	0
1	F	2919	0	2858	16	0
1	G	2919	0	2858	18	0
1	H	2907	0	2850	15	0
1	I	2913	0	2854	13	0
1	J	2928	0	2863	14	0
1	K	2919	0	2858	19	0
1	L	2907	0	2850	9	0
1	M	2913	0	2854	12	0
1	N	2919	0	2858	7	0
1	O	2919	0	2858	16	0
1	P	2922	0	2866	14	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	D	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	M	1	0	0	0	0
2	N	1	0	0	0	0
2	O	1	0	0	0	0
3	A	3	0	0	3	0
3	B	3	0	0	3	0
3	C	3	0	0	2	0
3	D	5	0	0	6	0
3	E	3	0	0	3	0
3	F	3	0	0	2	0
3	G	3	0	0	3	0
3	H	3	0	0	2	0
3	I	3	0	0	2	0
3	J	2	0	0	1	0
3	K	3	0	0	4	0
3	L	3	0	0	3	0
3	M	3	0	0	1	0
3	N	3	0	0	2	0
3	O	3	0	0	3	0
3	P	3	0	0	2	0
4	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
4	K	1	0	0	0	0
4	L	1	0	0	0	0
4	M	1	0	0	0	0
4	N	1	0	0	0	0
4	O	1	0	0	0	0
4	P	1	0	0	0	0
5	A	24	0	31	0	0
5	B	18	0	24	0	0
5	C	18	0	24	0	0
5	D	18	0	24	1	0
5	E	18	0	24	3	0
5	F	18	0	24	0	0
5	G	18	0	24	1	0
5	H	18	0	24	0	0
5	I	6	0	8	0	0
5	J	18	0	24	0	0
5	K	18	0	24	1	0
5	L	12	0	16	0	0
5	M	6	0	8	1	0
5	N	18	0	23	0	0
5	O	12	0	16	0	0
5	P	24	0	32	2	0
6	A	12	0	10	0	0
6	B	12	0	10	0	0
6	C	12	0	10	0	0
6	D	12	0	10	0	0
6	E	12	0	10	0	0
6	F	12	0	10	0	0
6	G	12	0	10	0	0
6	H	12	0	10	0	0
6	I	12	0	10	0	0
6	J	12	0	10	0	0
6	K	12	0	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	L	12	0	10	0	0
6	M	12	0	10	0	0
6	N	12	0	10	0	0
6	O	12	0	10	0	0
6	P	12	0	10	0	0
7	A	354	0	0	5	1
7	B	383	0	0	4	0
7	C	345	0	0	6	0
7	D	430	0	0	5	0
7	E	370	0	0	3	0
7	F	353	0	0	1	3
7	G	375	0	0	5	0
7	H	378	0	0	6	0
7	I	352	0	0	3	1
7	J	321	0	0	4	0
7	K	370	0	0	6	3
7	L	334	0	0	0	0
7	M	354	0	0	0	0
7	N	394	0	0	1	0
7	O	353	0	0	6	0
7	P	329	0	0	5	0
All	All	53008	0	46236	216	5

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 2.

All (216) 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:H:81:HIS:CD2	7:H:612:HOH:O	2.09	1.03
1:D:161:ARG:NH1	7:D:828:HOH:O	1.98	0.95
1:B:52:HIS:HD2	7:B:881:HOH:O	1.56	0.89
1:C:118:LYS:HE3	7:C:842:HOH:O	1.73	0.89
1:O:81:HIS:ND1	7:O:691:HOH:O	2.09	0.86
1:I:118:LYS:HE2	7:I:560:HOH:O	1.80	0.81
1:B:352:GLN:HG2	7:B:747:HOH:O	1.83	0.79
1:E:139:GLU:HB2	5:E:406:GOL:H11	1.73	0.70
1:C:335:HIS:HD2	7:C:681:HOH:O	1.74	0.69
1:K:16:THR:OG1	7:K:744:HOH:O	2.13	0.66
3:E:402:CL:CL	1:H:102:ILE:HG12	2.38	0.61
1:C:366:ARG:HD2	7:C:685:HOH:O	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:921:HOH:O	1:F:128:HIS:HD2	1.83	0.60
1:H:81:HIS:NE2	7:H:612:HOH:O	2.22	0.60
3:A:403:CL:CL	1:D:102:ILE:HG12	2.38	0.59
1:P:137:GLY:O	5:P:407:GOL:H32	2.01	0.59
3:F:402:CL:CL	1:K:102:ILE:HG12	2.40	0.58
1:G:372:LYS:CE	7:G:748:HOH:O	2.51	0.58
1:G:372:LYS:HE2	7:G:748:HOH:O	2.04	0.58
1:K:16:THR:CB	7:K:744:HOH:O	2.51	0.58
1:M:1:MET:HG2	1:M:121:LYS:HE3	1.86	0.58
1:E:102:ILE:HG12	3:H:403:CL:CL	2.41	0.57
1:A:362:GLU:O	1:A:366:ARG:HG3	2.05	0.57
1:P:71:PRO:HB2	5:P:408:GOL:H11	1.85	0.57
1:I:21:SER:HB2	1:I:149:SER:HB3	1.87	0.57
1:I:102:ILE:HG12	3:L:403:CL:CL	2.42	0.57
1:D:362:GLU:HG2	7:D:606:HOH:O	2.04	0.56
3:C:403:CL:CL	1:M:102:ILE:HG12	2.43	0.56
1:I:20:ILE:HD12	1:I:20:ILE:C	2.27	0.55
1:L:218:ALA:O	1:L:221:LYS:HD3	2.07	0.55
1:C:363:SER:HB3	7:C:681:HOH:O	2.06	0.55
1:B:192:GLU:HG3	7:B:802:HOH:O	2.07	0.55
3:B:403:CL:CL	1:G:102:ILE:HG12	2.44	0.54
1:L:45:GLY:HA3	1:L:117:ILE:HG13	1.90	0.53
1:L:221:LYS:HG2	1:L:222:ASP:N	2.23	0.53
1:P:250:PRO:HB3	1:J:211:PRO:HB3	1.90	0.53
1:A:366:ARG:NE	7:A:693:HOH:O	2.41	0.52
1:O:45:GLY:HA3	1:O:117:ILE:HG13	1.91	0.52
1:B:102:ILE:HG12	3:G:403:CL:CL	2.46	0.52
1:F:45:GLY:HA3	1:F:117:ILE:HG13	1.91	0.52
1:O:118:LYS:HE3	1:O:129:TYR:OH	2.09	0.52
1:J:21:SER:HB2	1:J:149:SER:HB3	1.91	0.52
1:O:329:ILE:O	3:O:404:CL:CL	2.64	0.52
1:L:20:ILE:HD13	1:L:147:TRP:CE3	2.45	0.52
1:F:366:ARG:HH21	1:F:366:ARG:HG2	1.73	0.52
1:C:221:LYS:HA	7:C:782:HOH:O	2.10	0.51
1:C:21:SER:HB2	1:C:149:SER:HB3	1.92	0.51
1:I:329:ILE:O	3:I:403:CL:CL	2.66	0.51
1:A:102:ILE:HG12	3:D:405:CL:CL	2.48	0.51
1:O:81:HIS:CE1	7:O:691:HOH:O	2.58	0.51
1:G:242:ARG:NH1	7:G:568:HOH:O	2.40	0.51
3:N:403:CL:CL	1:J:102:ILE:HG12	2.48	0.51
1:E:372:LYS:HE3	7:E:659:HOH:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:158:GLY:HA3	7:O:522:HOH:O	2.11	0.50
1:F:102:ILE:HG12	3:K:403:CL:CL	2.48	0.50
1:D:362:GLU:HG3	7:D:930:HOH:O	2.11	0.50
3:P:402:CL:CL	1:O:102:ILE:HG12	2.48	0.50
1:G:139:GLU:HG3	5:G:407:GOL:H32	1.92	0.50
1:C:372:LYS:HA	7:C:721:HOH:O	2.12	0.50
1:K:2:LYS:CE	7:K:804:HOH:O	2.59	0.50
1:J:1:MET:HG3	1:J:41:ASP:OD2	2.11	0.50
1:O:20:ILE:C	1:O:20:ILE:HD12	2.32	0.50
1:A:372:LYS:HE3	7:A:853:HOH:O	2.12	0.49
1:C:45:GLY:HA3	1:C:117:ILE:HG13	1.93	0.49
5:E:407:GOL:H11	1:G:299:ARG:NH1	2.28	0.49
1:O:232:LEU:HB2	1:O:240:HIS:CE1	2.48	0.49
1:A:21:SER:HB2	1:A:149:SER:HB3	1.95	0.49
1:E:270:GLY:HA2	7:E:834:HOH:O	2.13	0.49
1:H:45:GLY:HA3	1:H:117:ILE:HG13	1.95	0.48
1:F:145:ILE:C	1:F:145:ILE:HD12	2.33	0.48
1:F:232:LEU:HB2	1:F:240:HIS:CE1	2.48	0.48
1:J:49:THR:HA	1:J:280:THR:HB	1.95	0.48
1:O:20:ILE:HD13	1:O:147:TRP:CE3	2.48	0.48
1:K:329:ILE:O	3:K:404:CL:CL	2.68	0.48
1:K:2:LYS:HE3	7:K:804:HOH:O	2.13	0.48
1:L:180:PRO:HB3	1:L:208:TRP:CH2	2.49	0.48
3:I:402:CL:CL	1:L:102:ILE:HG12	2.50	0.48
1:P:102:ILE:HG12	3:O:403:CL:CL	2.51	0.48
1:A:360:LEU:O	1:A:363:SER:HB2	2.14	0.47
1:N:45:GLY:HA3	1:N:117:ILE:HG13	1.95	0.47
1:K:16:THR:CA	7:K:744:HOH:O	2.61	0.47
1:D:232:LEU:HB2	1:D:240:HIS:CE1	2.50	0.47
1:J:145:ILE:C	1:J:145:ILE:HD12	2.35	0.47
1:G:232:LEU:HB2	1:G:240:HIS:CE1	2.50	0.47
1:P:118[A]:LYS:CE	7:P:629:HOH:O	2.62	0.47
1:B:352:GLN:CG	7:B:747:HOH:O	2.53	0.47
1:I:158:GLY:HA3	7:I:579:HOH:O	2.13	0.47
1:F:329:ILE:O	3:F:403:CL:CL	2.70	0.47
1:D:139:GLU:HG3	5:D:409:GOL:H32	1.97	0.47
1:N:102:ILE:HG12	3:J:403:CL:CL	2.51	0.47
1:P:329:ILE:O	3:P:403:CL:CL	2.69	0.47
1:K:180:PRO:HB2	5:K:406:GOL:H31	1.97	0.47
1:N:372:LYS:HE3	7:N:605:HOH:O	2.14	0.47
1:J:158:GLY:HA3	7:J:605:HOH:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:16:THR:HG21	7:J:781:HOH:O	2.15	0.47
1:P:214:GLN:NE2	7:P:760:HOH:O	2.47	0.47
1:A:329:ILE:O	3:A:404:CL:CL	2.70	0.47
1:I:173:ILE:O	1:I:202:ILE:HA	2.14	0.47
1:M:232:LEU:HB2	1:M:240:HIS:CE1	2.50	0.47
1:B:211:PRO:HB3	1:E:250:PRO:HB3	1.97	0.46
1:H:329:ILE:O	3:H:404:CL:CL	2.69	0.46
1:P:45:GLY:HA3	1:P:117:ILE:HG13	1.97	0.46
1:A:372:LYS:CE	7:A:853:HOH:O	2.63	0.46
1:A:232:LEU:HB2	1:A:240:HIS:CE1	2.50	0.46
3:A:404:CL:CL	7:A:505:HOH:O	2.58	0.46
1:E:192:GLU:HG3	7:E:654:HOH:O	2.15	0.46
1:B:100:ALA:O	3:B:403:CL:CL	2.71	0.46
1:E:329:ILE:O	3:E:403:CL:CL	2.71	0.46
1:F:309:MET:HG3	1:F:332:ILE:HG12	1.97	0.45
1:A:23:SER:O	1:A:207:LYS:HE2	2.17	0.45
1:K:340:ILE:O	1:K:340:ILE:HG13	2.17	0.45
1:C:81:HIS:ND1	1:C:118:LYS:NZ	2.62	0.45
1:K:330:PRO:C	3:K:404:CL:CL	2.92	0.45
1:I:45:GLY:HA3	1:I:117:ILE:HG13	1.99	0.45
1:C:232:LEU:HB2	1:C:240:HIS:CE1	2.52	0.45
1:M:21:SER:HB2	1:M:149:SER:HB3	1.99	0.45
1:N:32:VAL:HG13	1:N:48:PHE:CD1	2.52	0.45
1:I:276:GLN:HG2	1:I:303:VAL:HG23	1.99	0.45
1:I:232:LEU:HB2	1:I:240:HIS:CE1	2.52	0.45
1:F:180:PRO:HB3	1:F:208:TRP:CH2	2.52	0.44
1:D:329:ILE:O	3:D:403:CL:CL	2.72	0.44
1:K:49:THR:HA	1:K:280:THR:HB	1.99	0.44
1:C:333:LYS:N	3:C:402:CL:CL	2.86	0.44
1:A:45:GLY:HA3	1:A:117:ILE:HG13	2.00	0.44
1:J:23:SER:HB3	1:J:176:GLY:HA3	1.98	0.44
1:J:173:ILE:O	1:J:202:ILE:HA	2.17	0.44
1:B:49:THR:HA	1:B:280:THR:HB	2.00	0.44
1:D:323:SER:HB3	3:D:404:CL:CL	2.54	0.44
1:J:153:GLU:HG3	7:J:748:HOH:O	2.17	0.44
1:L:329:ILE:O	3:L:402:CL:CL	2.72	0.44
1:O:229:GLU:HA	1:O:252:ALA:O	2.17	0.44
1:P:118[A]:LYS:NZ	7:P:629:HOH:O	2.38	0.44
1:B:21:SER:HB2	1:B:149:SER:HB3	2.00	0.44
1:J:16:THR:CG2	7:J:781:HOH:O	2.65	0.44
1:G:250:PRO:HB3	1:H:211:PRO:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:192:GLU:HG3	7:H:873:HOH:O	2.17	0.44
1:P:232:LEU:HB2	1:P:240:HIS:CE1	2.53	0.43
1:J:232:LEU:HB2	1:J:240:HIS:CE1	2.53	0.43
1:G:276:GLN:HG2	1:G:303:VAL:HG23	2.00	0.43
1:D:306:ALA:HB1	1:D:309:MET:HA	2.00	0.43
1:O:372:LYS:CE	7:O:684:HOH:O	2.66	0.43
1:H:49:THR:HA	1:H:280:THR:HB	2.01	0.43
1:K:20:ILE:C	1:K:20:ILE:HD12	2.38	0.43
1:G:20:ILE:HD12	1:G:20:ILE:C	2.39	0.43
1:P:2:LYS:HE2	7:P:723:HOH:O	2.18	0.43
1:O:118:LYS:HD3	7:O:691:HOH:O	2.18	0.43
1:E:232:LEU:HB2	1:E:240:HIS:CE1	2.53	0.43
1:K:332:ILE:N	3:K:404:CL:CL	2.82	0.43
1:F:337:GLU:HG2	1:F:360:LEU:HD23	2.00	0.43
1:E:49:THR:HA	1:E:280:THR:HB	2.01	0.43
1:K:210:LEU:HA	1:K:232:LEU:HD21	2.01	0.43
1:K:276:GLN:HG2	1:K:303:VAL:HG23	2.01	0.43
1:L:232:LEU:HB2	1:L:240:HIS:CE1	2.54	0.43
1:J:21:SER:HA	1:J:25:HIS:O	2.18	0.42
1:D:325:ILE:O	3:D:404:CL:CL	2.74	0.42
1:H:306:ALA:HB1	1:H:309:MET:HA	2.01	0.42
1:K:158:GLY:HA3	7:K:542:HOH:O	2.18	0.42
1:B:306:ALA:HB1	1:B:309:MET:HA	2.01	0.42
1:N:329:ILE:O	3:N:404:CL:CL	2.74	0.42
1:G:55:LEU:HD21	1:G:59:ARG:NH2	2.35	0.42
1:E:45:GLY:HA3	1:E:117:ILE:HG13	2.00	0.42
1:G:16:THR:HB	7:G:624:HOH:O	2.19	0.42
1:G:242:ARG:NH2	7:G:699:HOH:O	2.46	0.42
1:M:1:MET:HG3	1:M:41:ASP:OD2	2.20	0.42
1:B:232:LEU:HB2	1:B:240:HIS:CE1	2.54	0.42
1:L:333:LYS:N	3:L:402:CL:CL	2.90	0.42
1:G:45:GLY:HA3	1:G:117:ILE:HG13	2.02	0.42
1:I:36:LYS:NZ	7:I:820:HOH:O	2.53	0.42
3:E:402:CL:CL	1:H:101:GLY:HA3	2.57	0.42
1:F:366:ARG:HG2	1:F:366:ARG:NH2	2.34	0.42
1:D:333:LYS:N	3:D:403:CL:CL	2.90	0.42
1:D:16:THR:HG22	1:D:16:THR:O	2.20	0.42
1:N:293:ASP:OD2	1:P:293:ASP:OD2	2.38	0.42
1:F:366:ARG:HD3	1:F:367:TYR:CZ	2.55	0.41
1:O:372:LYS:HE3	7:O:684:HOH:O	2.19	0.41
1:H:20:ILE:C	1:H:20:ILE:HD12	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:158:GLY:HA3	7:P:618:HOH:O	2.19	0.41
1:B:20:ILE:C	1:B:20:ILE:HD12	2.40	0.41
1:F:15:LEU:HD22	1:F:331:TRP:CD2	2.56	0.41
1:O:15:LEU:HD22	1:O:331:TRP:CD2	2.55	0.41
1:M:329:ILE:O	3:M:403:CL:CL	2.75	0.41
1:D:158:GLY:HA3	7:D:562:HOH:O	2.21	0.41
1:K:8:PRO:HG3	1:K:66:SER:HB3	2.02	0.41
1:E:173:ILE:O	1:E:202:ILE:HA	2.21	0.41
1:M:64:CYS:O	1:M:68:CYS:HB2	2.20	0.41
1:H:118:LYS:CE	7:H:721:HOH:O	2.68	0.41
1:D:49:THR:HA	1:D:280:THR:HB	2.02	0.41
1:B:329:ILE:O	3:B:404:CL:CL	2.75	0.41
1:F:210:LEU:HA	1:F:232:LEU:HD21	2.02	0.41
1:H:119:ALA:HB3	1:H:354:GLY:HA2	2.03	0.41
1:D:275:VAL:HG12	1:D:277:PRO:HD3	2.03	0.41
1:M:276:GLN:HG2	1:M:303:VAL:HG23	2.01	0.41
1:F:362:GLU:OE1	7:F:513:HOH:O	2.22	0.41
1:I:118:LYS:HE3	1:I:129:TYR:OH	2.21	0.41
1:M:21:SER:HA	1:M:25:HIS:O	2.21	0.41
1:M:180:PRO:HB2	5:M:406:GOL:H31	2.02	0.41
1:G:145:ILE:C	1:G:145:ILE:HD12	2.41	0.41
1:K:173:ILE:O	1:K:202:ILE:HA	2.19	0.41
1:K:64:CYS:O	1:K:68:CYS:HB2	2.21	0.41
1:A:1:MET:CE	7:A:779:HOH:O	2.69	0.41
1:I:211:PRO:HB3	1:M:250:PRO:HB3	2.03	0.41
1:A:101:GLY:HA3	3:D:405:CL:CL	2.58	0.41
1:G:332:ILE:N	3:G:404:CL:CL	2.81	0.41
1:H:118:LYS:CE	7:H:537:HOH:O	2.69	0.40
1:B:173:ILE:O	1:B:202:ILE:HA	2.21	0.40
1:F:21:SER:HB2	1:F:149:SER:HB3	2.02	0.40
1:M:20:ILE:HD12	1:M:20:ILE:C	2.42	0.40
1:O:296:LEU:HD23	1:O:296:LEU:C	2.41	0.40
1:E:145:ILE:C	1:E:145:ILE:HD12	2.42	0.40
1:C:210:LEU:N	1:C:211:PRO:HD2	2.37	0.40
1:H:118:LYS:HE3	7:H:537:HOH:O	2.20	0.40
1:G:21:SER:HB2	1:G:149:SER:HB3	2.03	0.40
1:E:325:ILE:HG22	5:E:406:GOL:H12	2.04	0.40
1:P:101:GLY:HA3	3:O:403:CL:CL	2.59	0.40
1:G:333:LYS:N	3:G:404:CL:CL	2.92	0.40
1:N:161:ARG:HG3	1:N:165:GLU:CD	2.42	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:852:HOH:O	7:K:868:HOH:O[3_553]	1.34	0.86
7:F:853:HOH:O	7:K:870:HOH:O[3_553]	1.61	0.59
7:K:825:HOH:O	7:K:825:HOH:O[3_553]	1.76	0.44
7:A:818:HOH:O	7:A:818:HOH:O[3_553]	2.02	0.18
7:F:841:HOH:O	7:I:838:HOH:O[3_554]	2.06	0.14

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	372/372 (100%)	362 (97%)	10 (3%)	0	100	100
1	B	371/372 (100%)	361 (97%)	10 (3%)	0	100	100
1	C	371/372 (100%)	361 (97%)	10 (3%)	0	100	100
1	D	372/372 (100%)	361 (97%)	11 (3%)	0	100	100
1	E	373/372 (100%)	366 (98%)	7 (2%)	0	100	100
1	F	372/372 (100%)	361 (97%)	11 (3%)	0	100	100
1	G	372/372 (100%)	358 (96%)	14 (4%)	0	100	100
1	H	370/372 (100%)	361 (98%)	9 (2%)	0	100	100
1	I	371/372 (100%)	363 (98%)	8 (2%)	0	100	100
1	J	373/372 (100%)	363 (97%)	10 (3%)	0	100	100
1	K	372/372 (100%)	359 (96%)	13 (4%)	0	100	100
1	L	370/372 (100%)	359 (97%)	11 (3%)	0	100	100
1	M	371/372 (100%)	362 (98%)	9 (2%)	0	100	100
1	N	372/372 (100%)	360 (97%)	12 (3%)	0	100	100
1	O	372/372 (100%)	361 (97%)	11 (3%)	0	100	100
1	P	372/372 (100%)	363 (98%)	9 (2%)	0	100	100
All	All	5946/5952 (100%)	5781 (97%)	165 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	306/304 (101%)	303 (99%)	3 (1%)	82	77
1	B	305/304 (100%)	302 (99%)	3 (1%)	82	77
1	C	305/304 (100%)	301 (99%)	4 (1%)	76	68
1	D	306/304 (101%)	301 (98%)	5 (2%)	70	59
1	E	307/304 (101%)	303 (99%)	4 (1%)	76	68
1	F	306/304 (101%)	300 (98%)	6 (2%)	63	49
1	G	306/304 (101%)	301 (98%)	5 (2%)	70	59
1	H	304/304 (100%)	300 (99%)	4 (1%)	76	68
1	I	305/304 (100%)	299 (98%)	6 (2%)	63	49
1	J	307/304 (101%)	304 (99%)	3 (1%)	82	77
1	K	306/304 (101%)	300 (98%)	6 (2%)	63	49
1	L	304/304 (100%)	299 (98%)	5 (2%)	70	59
1	M	305/304 (100%)	299 (98%)	6 (2%)	63	49
1	N	306/304 (101%)	301 (98%)	5 (2%)	70	59
1	O	306/304 (101%)	302 (99%)	4 (1%)	76	68
1	P	306/304 (101%)	304 (99%)	2 (1%)	88	86
All	All	4890/4864 (100%)	4819 (98%)	71 (2%)	72	62

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	199	ARG
1	A	227	TRP
1	A	308	GLU
1	B	199	ARG
1	B	228	PHE
1	B	308	GLU

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Mol	Chain	Res	Type
1	C	118	LYS
1	C	199	ARG
1	C	228	PHE
1	C	308	GLU
1	D	199	ARG
1	D	228	PHE
1	D	264	ARG
1	D	308	GLU
1	D	318	TYR
1	E	199	ARG
1	E	227	TRP
1	E	228	PHE
1	E	308	GLU
1	F	16	THR
1	F	199	ARG
1	F	228	PHE
1	F	308	GLU
1	F	362	GLU
1	F	366	ARG
1	G	16	THR
1	G	199	ARG
1	G	227	TRP
1	G	228	PHE
1	G	308	GLU
1	H	199	ARG
1	H	227	TRP
1	H	228	PHE
1	H	308	GLU
1	I	199	ARG
1	I	227	TRP
1	I	228	PHE
1	I	264	ARG
1	I	308	GLU
1	I	366	ARG
1	K	17	SER
1	K	199	ARG
1	K	207	LYS
1	K	227	TRP
1	K	228	PHE
1	K	308	GLU
1	L	92	PRO
1	L	199	ARG

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Mol	Chain	Res	Type
1	L	221	LYS
1	L	227	TRP
1	L	308	GLU
1	M	199	ARG
1	M	227	TRP
1	M	228	PHE
1	M	264	ARG
1	M	308	GLU
1	M	362	GLU
1	N	199	ARG
1	N	227	TRP
1	N	228	PHE
1	N	308	GLU
1	N	362	GLU
1	P	199	ARG
1	P	308	GLU
1	J	118	LYS
1	J	199	ARG
1	J	308	GLU
1	O	199	ARG
1	O	228	PHE
1	O	308	GLU
1	O	366	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	52	HIS
1	B	214	GLN
1	C	214	GLN
1	C	335	HIS
1	D	214	GLN
1	E	214	GLN
1	F	128	HIS
1	F	214	GLN
1	H	214	GLN
1	K	214	GLN
1	M	214	GLN
1	P	214	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 135 ligands modelled in this entry, 75 are monoatomic - leaving 60 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	$\#\|Z\| > 2$
5	GOL	A	406	-	5,5,5	0.46	0	5,5,5	0.59	0
5	GOL	A	407	-	5,5,5	1.37	0	5,5,5	2.14	1 (20%)
5	GOL	A	408	-	5,5,5	0.20	0	5,5,5	1.08	0
5	GOL	A	409	-	5,5,5	0.63	0	5,5,5	0.74	0
6	0YR	A	410	4	10,11,11	1.71	2 (20%)	12,14,14	1.90	7 (58%)
5	GOL	B	406	-	5,5,5	0.54	0	5,5,5	0.58	0
5	GOL	B	407	-	5,5,5	0.49	0	5,5,5	0.92	0
5	GOL	B	408	-	5,5,5	0.17	0	5,5,5	0.83	0
6	0YR	B	409	4	10,11,11	2.02	4 (40%)	12,14,14	1.78	4 (33%)
5	GOL	C	405	-	5,5,5	0.54	0	5,5,5	0.64	0
5	GOL	C	406	-	5,5,5	0.88	0	5,5,5	1.66	2 (40%)
5	GOL	C	407	-	5,5,5	0.76	0	5,5,5	0.41	0
6	0YR	C	408	4	10,11,11	1.81	3 (30%)	12,14,14	1.37	2 (16%)
5	GOL	D	408	-	5,5,5	0.61	0	5,5,5	0.42	0
5	GOL	D	409	-	5,5,5	0.65	0	5,5,5	1.67	2 (40%)
5	GOL	D	410	-	5,5,5	0.59	0	5,5,5	1.15	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	0YR	D	411	4	10,11,11	2.01	2 (20%)	12,14,14	1.76	3 (25%)
5	GOL	E	405	-	5,5,5	0.83	0	5,5,5	0.66	0
5	GOL	E	406	-	5,5,5	0.69	0	5,5,5	0.58	0
5	GOL	E	407	-	5,5,5	0.71	0	5,5,5	1.50	1 (20%)
6	0YR	E	408	4	10,11,11	1.69	2 (20%)	12,14,14	1.79	4 (33%)
5	GOL	F	405	-	5,5,5	0.30	0	5,5,5	0.63	0
5	GOL	F	406	-	5,5,5	0.64	0	5,5,5	0.61	0
5	GOL	F	407	-	5,5,5	0.56	0	5,5,5	1.26	0
6	0YR	F	408	4	10,11,11	1.83	2 (20%)	12,14,14	2.23	6 (50%)
5	GOL	G	406	-	5,5,5	0.67	0	5,5,5	0.53	0
5	GOL	G	407	-	5,5,5	0.95	0	5,5,5	2.04	3 (60%)
5	GOL	G	408	-	5,5,5	0.57	0	5,5,5	0.73	0
6	0YR	G	409	4	10,11,11	1.52	2 (20%)	12,14,14	2.34	6 (50%)
5	GOL	H	406	-	5,5,5	0.73	0	5,5,5	0.57	0
5	GOL	H	407	-	5,5,5	0.64	0	5,5,5	0.72	0
5	GOL	H	408	-	5,5,5	0.80	0	5,5,5	0.74	0
6	0YR	H	409	4	10,11,11	1.74	1 (10%)	12,14,14	2.53	7 (58%)
5	GOL	I	405	-	5,5,5	0.50	0	5,5,5	0.44	0
6	0YR	I	406	4	10,11,11	1.62	2 (20%)	12,14,14	1.48	3 (25%)
5	GOL	J	405	-	5,5,5	0.75	0	5,5,5	0.29	0
5	GOL	J	406	-	5,5,5	0.75	0	5,5,5	1.42	1 (20%)
5	GOL	J	407	-	5,5,5	0.52	0	5,5,5	0.47	0
6	0YR	J	408	4	10,11,11	1.44	1 (10%)	12,14,14	1.62	2 (16%)
5	GOL	K	406	-	5,5,5	0.44	0	5,5,5	0.65	0
5	GOL	K	407	-	5,5,5	0.53	0	5,5,5	0.98	0
5	GOL	K	408	-	5,5,5	0.52	0	5,5,5	1.89	2 (40%)
6	0YR	K	409	4	10,11,11	1.47	3 (30%)	12,14,14	2.27	4 (33%)
5	GOL	L	405	-	5,5,5	0.20	0	5,5,5	0.54	0
5	GOL	L	406	-	5,5,5	0.89	0	5,5,5	1.23	0
6	0YR	L	407	4	10,11,11	2.06	4 (40%)	12,14,14	2.56	8 (66%)
5	GOL	M	406	-	5,5,5	0.54	0	5,5,5	0.76	0
6	0YR	M	407	4	10,11,11	1.78	2 (20%)	12,14,14	1.73	3 (25%)
5	GOL	N	406	-	5,5,5	0.85	0	5,5,5	0.62	0
5	GOL	N	407	-	5,5,5	0.77	0	5,5,5	1.10	0
5	GOL	N	408	-	5,5,5	0.66	0	5,5,5	0.93	0
6	0YR	N	409	4	10,11,11	1.94	3 (30%)	12,14,14	1.72	3 (25%)
5	GOL	O	406	-	5,5,5	0.59	0	5,5,5	0.50	0
5	GOL	O	407	-	5,5,5	0.57	0	5,5,5	0.63	0
6	0YR	O	408	4	10,11,11	1.53	2 (20%)	12,14,14	2.30	4 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	GOL	P	405	-	5,5,5	0.70	0	5,5,5	0.77	0
5	GOL	P	406	-	5,5,5	0.62	0	5,5,5	0.72	0
5	GOL	P	407	-	5,5,5	0.62	0	5,5,5	1.29	0
5	GOL	P	408	-	5,5,5	0.39	0	5,5,5	1.18	0
6	0YR	P	409	4	10,11,11	0.95	0	12,14,14	2.15	5 (41%)

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
5	GOL	A	406	-	-	0/4/4/4	0/0/0/0
5	GOL	A	407	-	-	0/4/4/4	0/0/0/0
5	GOL	A	408	-	-	0/4/4/4	0/0/0/0
5	GOL	A	409	-	-	0/4/4/4	0/0/0/0
6	0YR	A	410	4	-	0/15/16/16	0/0/0/0
5	GOL	B	406	-	-	0/4/4/4	0/0/0/0
5	GOL	B	407	-	-	0/4/4/4	0/0/0/0
5	GOL	B	408	-	-	0/4/4/4	0/0/0/0
6	0YR	B	409	4	-	0/15/16/16	0/0/0/0
5	GOL	C	405	-	-	0/4/4/4	0/0/0/0
5	GOL	C	406	-	-	0/4/4/4	0/0/0/0
5	GOL	C	407	-	-	0/4/4/4	0/0/0/0
6	0YR	C	408	4	-	0/15/16/16	0/0/0/0
5	GOL	D	408	-	-	0/4/4/4	0/0/0/0
5	GOL	D	409	-	-	0/4/4/4	0/0/0/0
5	GOL	D	410	-	-	0/4/4/4	0/0/0/0
6	0YR	D	411	4	-	0/15/16/16	0/0/0/0
5	GOL	E	405	-	-	0/4/4/4	0/0/0/0
5	GOL	E	406	-	-	0/4/4/4	0/0/0/0
5	GOL	E	407	-	-	0/4/4/4	0/0/0/0
6	0YR	E	408	4	-	0/15/16/16	0/0/0/0
5	GOL	F	405	-	-	0/4/4/4	0/0/0/0
5	GOL	F	406	-	-	0/4/4/4	0/0/0/0
5	GOL	F	407	-	-	0/4/4/4	0/0/0/0
6	0YR	F	408	4	-	0/15/16/16	0/0/0/0
5	GOL	G	406	-	-	0/4/4/4	0/0/0/0
5	GOL	G	407	-	-	0/4/4/4	0/0/0/0
5	GOL	G	408	-	-	0/4/4/4	0/0/0/0
6	0YR	G	409	4	-	0/15/16/16	0/0/0/0
5	GOL	H	406	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	H	407	-	-	0/4/4/4	0/0/0/0
5	GOL	H	408	-	-	0/4/4/4	0/0/0/0
6	0YR	H	409	4	-	0/15/16/16	0/0/0/0
5	GOL	I	405	-	-	0/4/4/4	0/0/0/0
6	0YR	I	406	4	-	0/15/16/16	0/0/0/0
5	GOL	J	405	-	-	0/4/4/4	0/0/0/0
5	GOL	J	406	-	-	0/4/4/4	0/0/0/0
5	GOL	J	407	-	-	0/4/4/4	0/0/0/0
6	0YR	J	408	4	-	0/15/16/16	0/0/0/0
5	GOL	K	406	-	-	0/4/4/4	0/0/0/0
5	GOL	K	407	-	-	0/4/4/4	0/0/0/0
5	GOL	K	408	-	-	0/4/4/4	0/0/0/0
6	0YR	K	409	4	-	0/15/16/16	0/0/0/0
5	GOL	L	405	-	-	0/4/4/4	0/0/0/0
5	GOL	L	406	-	-	0/4/4/4	0/0/0/0
6	0YR	L	407	4	-	0/15/16/16	0/0/0/0
5	GOL	M	406	-	-	0/4/4/4	0/0/0/0
6	0YR	M	407	4	-	0/15/16/16	0/0/0/0
5	GOL	N	406	-	-	0/4/4/4	0/0/0/0
5	GOL	N	407	-	-	0/4/4/4	0/0/0/0
5	GOL	N	408	-	-	0/4/4/4	0/0/0/0
6	0YR	N	409	4	-	0/15/16/16	0/0/0/0
5	GOL	O	406	-	-	0/4/4/4	0/0/0/0
5	GOL	O	407	-	-	0/4/4/4	0/0/0/0
6	0YR	O	408	4	-	0/15/16/16	0/0/0/0
5	GOL	P	405	-	-	0/4/4/4	0/0/0/0
5	GOL	P	406	-	-	0/4/4/4	0/0/0/0
5	GOL	P	407	-	-	0/4/4/4	0/0/0/0
5	GOL	P	408	-	-	0/4/4/4	0/0/0/0
6	0YR	P	409	4	-	0/15/16/16	0/0/0/0

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	407	0YR	OAC-NAH	-2.71	1.35	1.39
6	L	407	0YR	OAF-CAL	-2.51	1.36	1.43
6	G	409	0YR	OAC-NAH	-2.04	1.36	1.39
6	E	408	0YR	CAJ-CAL	2.02	1.57	1.53
6	K	409	0YR	CAK-CAI	2.05	1.57	1.52
6	G	409	0YR	CAK-CAI	2.23	1.57	1.52
6	N	409	0YR	OAC-NAH	2.24	1.43	1.39
6	K	409	0YR	CAJ-CAL	2.39	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	I	406	0YR	OAC-NAH	2.41	1.44	1.39
6	B	409	0YR	OAC-NAH	2.48	1.44	1.39
6	I	406	0YR	CAJ-CAL	2.48	1.58	1.53
6	O	408	0YR	CAG-CAJ	2.51	1.59	1.52
6	O	408	0YR	CAK-CAI	2.51	1.58	1.52
6	N	409	0YR	OAE-CAK	2.55	1.47	1.42
6	B	409	0YR	CAK-CAI	2.61	1.58	1.52
6	C	408	0YR	CAK-CAI	2.69	1.58	1.52
6	C	408	0YR	CAJ-CAL	2.73	1.59	1.53
6	A	410	0YR	CAJ-CAL	2.97	1.59	1.53
6	J	408	0YR	CAK-CAI	3.02	1.59	1.52
6	K	409	0YR	OAD-CAJ	3.02	1.50	1.43
6	L	407	0YR	CAK-CAI	3.08	1.59	1.52
6	L	407	0YR	OAD-CAJ	3.18	1.50	1.43
6	M	407	0YR	CAK-CAI	3.21	1.59	1.52
6	F	408	0YR	CAK-CAI	3.26	1.59	1.52
6	A	410	0YR	CAK-CAI	3.28	1.59	1.52
6	B	409	0YR	CAJ-CAL	3.41	1.60	1.53
6	B	409	0YR	OAE-CAK	3.49	1.48	1.42
6	N	409	0YR	CAK-CAI	3.60	1.60	1.52
6	M	407	0YR	OAC-NAH	3.68	1.46	1.39
6	C	408	0YR	OAE-CAK	3.73	1.49	1.42
6	F	408	0YR	OAC-NAH	3.78	1.46	1.39
6	D	411	0YR	OAC-NAH	4.13	1.47	1.39
6	E	408	0YR	CAK-CAI	4.16	1.61	1.52
6	H	409	0YR	OAC-NAH	4.34	1.47	1.39
6	D	411	0YR	CAK-CAI	4.52	1.62	1.52

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	O	408	0YR	OAE-CAK-CAL	-5.42	99.11	110.41
6	H	409	0YR	OAC-NAH-CAI	-4.92	112.91	119.86
6	L	407	0YR	OAE-CAK-CAL	-4.86	100.28	110.41
6	K	409	0YR	OAE-CAK-CAL	-4.55	100.92	110.41
6	G	409	0YR	OAC-NAH-CAI	-4.32	113.75	119.86
5	A	407	GOL	O3-C3-C2	-4.12	90.19	110.18
6	F	408	0YR	OAE-CAK-CAL	-3.60	102.91	110.41
6	P	409	0YR	OAE-CAK-CAI	-3.54	102.23	110.47
6	M	407	0YR	OAC-NAH-CAI	-3.36	115.11	119.86
6	L	407	0YR	OAE-CAK-CAI	-3.35	102.68	110.47
6	P	409	0YR	OAE-CAK-CAL	-3.24	103.65	110.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	H	409	0YR	CAK-CAI-NAH	-3.17	111.75	116.26
6	E	408	0YR	OAE-CAK-CAL	-3.10	103.95	110.41
6	J	408	0YR	OAE-CAK-CAL	-3.05	104.05	110.41
6	H	409	0YR	OAE-CAK-CAI	-3.00	103.50	110.47
6	H	409	0YR	OAE-CAK-CAL	-2.92	104.32	110.41
5	K	408	GOL	C3-C2-C1	-2.88	99.83	111.12
6	B	409	0YR	OAE-CAK-CAI	-2.83	103.89	110.47
6	G	409	0YR	OAF-CAL-CAK	-2.78	104.25	109.28
6	F	408	0YR	OAE-CAK-CAI	-2.76	104.05	110.47
6	N	409	0YR	CAK-CAI-NAH	-2.75	112.35	116.26
6	O	408	0YR	CAK-CAI-NAH	-2.74	112.36	116.26
6	C	408	0YR	CAK-CAI-NAH	-2.73	112.38	116.26
6	D	411	0YR	CAK-CAI-NAH	-2.67	112.47	116.26
6	L	407	0YR	OAB-CAG-CAJ	-2.65	105.33	111.10
6	K	409	0YR	CAK-CAI-NAH	-2.65	112.49	116.26
6	L	407	0YR	OAC-NAH-CAI	-2.57	116.22	119.86
5	G	407	GOL	O1-C1-C2	-2.57	97.74	110.18
6	G	409	0YR	CAK-CAI-NAH	-2.56	112.62	116.26
6	M	407	0YR	OAE-CAK-CAL	-2.54	105.12	110.41
6	F	408	0YR	CAK-CAI-NAH	-2.53	112.66	116.26
6	B	409	0YR	OAB-CAG-CAJ	-2.52	105.61	111.10
6	N	409	0YR	OAE-CAK-CAL	-2.51	105.17	110.41
6	L	407	0YR	CAK-CAI-NAH	-2.49	112.72	116.26
6	O	408	0YR	OAE-CAK-CAI	-2.46	104.74	110.47
6	D	411	0YR	OAE-CAK-CAI	-2.44	104.79	110.47
6	F	408	0YR	OAF-CAL-CAK	-2.43	104.89	109.28
6	A	410	0YR	CAK-CAI-NAH	-2.34	112.94	116.26
6	A	410	0YR	OAE-CAK-CAL	-2.32	105.57	110.41
6	E	408	0YR	OAD-CAJ-CAG	-2.32	103.80	109.22
6	A	410	0YR	OAE-CAK-CAI	-2.31	105.09	110.47
6	A	410	0YR	OAC-NAH-CAI	-2.29	116.63	119.86
6	P	409	0YR	CAK-CAI-NAH	-2.26	113.06	116.26
6	I	406	0YR	OAC-NAH-CAI	-2.21	116.74	119.86
6	G	409	0YR	OAE-CAK-CAL	-2.21	105.81	110.41
6	I	406	0YR	OAF-CAL-CAK	-2.20	105.31	109.28
6	H	409	0YR	OAB-CAG-CAJ	-2.18	106.36	111.10
5	G	407	GOL	C3-C2-C1	-2.16	102.66	111.12
6	G	409	0YR	OAE-CAK-CAI	-2.14	105.49	110.47
6	A	410	0YR	OAB-CAG-CAJ	-2.11	106.51	111.10
6	E	408	0YR	OAC-NAH-CAI	-2.11	116.89	119.86
6	K	409	0YR	OAF-CAL-CAK	-2.10	105.48	109.28
6	P	409	0YR	CAG-CAJ-CAL	-2.10	107.55	112.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	L	407	0YR	OAF-CAL-CAK	-2.09	105.50	109.28
6	B	409	0YR	OAD-CAJ-CAL	-2.01	103.97	109.02
6	C	408	0YR	CAL-CAK-CAI	2.02	114.90	110.05
5	D	409	GOL	O2-C2-C3	2.12	118.38	108.65
5	C	406	GOL	O1-C1-C2	2.14	120.58	110.18
6	N	409	0YR	CAL-CAK-CAI	2.28	115.53	110.05
5	D	409	GOL	O3-C3-C2	2.30	121.31	110.18
6	A	410	0YR	CAL-CAK-CAI	2.30	115.58	110.05
6	L	407	0YR	OAF-CAL-CAJ	2.33	114.61	108.75
5	K	408	GOL	O1-C1-C2	2.34	121.51	110.18
5	J	406	GOL	O3-C3-C2	2.38	121.73	110.18
5	C	406	GOL	O3-C3-C2	2.38	121.73	110.18
6	I	406	0YR	CAL-CAK-CAI	2.48	116.01	110.05
6	A	410	0YR	OAF-CAL-CAJ	2.50	115.05	108.75
5	G	407	GOL	O2-C2-C3	2.60	120.58	108.65
5	E	407	GOL	O3-C3-C2	2.69	123.21	110.18
6	E	408	0YR	CAL-CAK-CAI	2.71	116.56	110.05
6	F	408	0YR	OAF-CAL-CAJ	2.74	115.66	108.75
6	M	407	0YR	CAL-CAK-CAI	2.79	116.77	110.05
6	H	409	0YR	OAA-CAI-CAK	2.81	125.78	120.05
6	B	409	0YR	CAL-CAK-CAI	2.99	117.24	110.05
6	H	409	0YR	CAL-CAK-CAI	3.03	117.34	110.05
6	D	411	0YR	CAL-CAK-CAI	3.09	117.48	110.05
6	J	408	0YR	CAL-CAK-CAI	3.14	117.60	110.05
6	F	408	0YR	CAL-CAK-CAI	3.31	118.00	110.05
6	L	407	0YR	CAL-CAK-CAI	3.31	118.02	110.05
6	K	409	0YR	CAL-CAK-CAI	3.36	118.13	110.05
6	O	408	0YR	CAL-CAK-CAI	3.50	118.48	110.05
6	P	409	0YR	CAL-CAK-CAI	3.70	118.95	110.05
6	G	409	0YR	CAL-CAK-CAI	4.05	119.80	110.05

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	409	GOL	1	0
5	E	406	GOL	2	0
5	E	407	GOL	1	0
5	G	407	GOL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	K	406	GOL	1	0
5	M	406	GOL	1	0
5	P	407	GOL	1	0
5	P	408	GOL	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{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	372/372 (100%)	-0.73	0 100 100	7, 12, 26, 42	0
1	B	372/372 (100%)	-0.71	0 100 100	8, 14, 27, 50	1 (0%)
1	C	372/372 (100%)	-0.72	0 100 100	8, 14, 28, 47	2 (0%)
1	D	372/372 (100%)	-0.75	0 100 100	7, 12, 24, 43	2 (0%)
1	E	372/372 (100%)	-0.75	0 100 100	8, 13, 25, 45	2 (0%)
1	F	372/372 (100%)	-0.75	0 100 100	8, 14, 27, 46	1 (0%)
1	G	372/372 (100%)	-0.76	0 100 100	7, 13, 25, 47	1 (0%)
1	H	372/372 (100%)	-0.70	0 100 100	8, 14, 29, 51	1 (0%)
1	I	372/372 (100%)	-0.68	0 100 100	9, 15, 30, 46	0
1	J	372/372 (100%)	-0.65	0 100 100	9, 16, 31, 58	1 (0%)
1	K	372/372 (100%)	-0.66	0 100 100	7, 15, 29, 54	1 (0%)
1	L	372/372 (100%)	-0.65	1 (0%) 94 92	8, 16, 30, 52	2 (0%)
1	M	372/372 (100%)	-0.68	0 100 100	9, 16, 29, 49	1 (0%)
1	N	372/372 (100%)	-0.75	0 100 100	8, 14, 25, 50	3 (0%)
1	O	372/372 (100%)	-0.68	0 100 100	8, 15, 30, 56	1 (0%)
1	P	372/372 (100%)	-0.70	0 100 100	9, 16, 31, 50	1 (0%)
All	All	5952/5952 (100%)	-0.71	1 (0%) 100 100	7, 14, 29, 58	20 (0%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	364	PHE	2.7

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (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
5	GOL	N	407	6/6	0.93	0.15	15.68	16,22,26,33	0
5	GOL	C	407	6/6	0.94	0.16	15.27	14,22,26,31	0
3	CL	A	404	1/1	0.99	0.16	14.52	29,29,29,29	0
3	CL	N	403	1/1	0.99	0.16	13.69	28,28,28,28	0
5	GOL	F	406	6/6	0.95	0.14	13.19	14,20,24,29	0
5	GOL	P	408	6/6	0.94	0.14	12.94	26,30,36,38	0
5	GOL	A	408	6/6	0.92	0.14	12.38	25,32,36,43	0
3	CL	O	403	1/1	0.99	0.19	12.37	31,31,31,31	0
3	CL	J	403	1/1	0.99	0.14	11.97	31,31,31,31	0
5	GOL	E	406	6/6	0.95	0.16	11.83	16,25,26,33	0
3	CL	F	403	1/1	0.99	0.15	11.39	32,32,32,32	0
3	CL	M	403	1/1	0.99	0.17	11.36	33,33,33,33	0
5	GOL	K	408	6/6	0.93	0.13	11.11	18,25,29,33	0
5	GOL	F	407	6/6	0.94	0.24	10.25	20,34,35,39	0
3	CL	G	403	1/1	0.99	0.14	10.10	27,27,27,27	0
3	CL	F	402	1/1	0.99	0.15	8.81	29,29,29,29	0
3	CL	P	403	1/1	0.98	0.14	8.19	36,36,36,36	0
5	GOL	D	409	6/6	0.95	0.12	8.01	16,27,31,38	0
3	CL	D	404	1/1	0.99	0.17	7.88	29,29,29,29	0
3	CL	I	402	1/1	0.99	0.12	7.44	30,30,30,30	0
5	GOL	A	407	6/6	0.93	0.16	7.36	15,22,25,38	0
3	CL	E	402	1/1	0.99	0.14	7.09	29,29,29,29	0
5	GOL	A	406	6/6	0.96	0.09	6.53	13,17,19,19	0
3	CL	E	403	1/1	0.99	0.12	6.40	29,29,29,29	0
5	GOL	G	407	6/6	0.96	0.12	6.37	17,26,29,34	0
5	GOL	P	407	6/6	0.92	0.11	6.13	20,27,29,39	0
3	CL	D	405	1/1	0.99	0.12	6.11	26,26,26,26	0
3	CL	B	403	1/1	0.99	0.12	6.07	28,28,28,28	0
5	GOL	B	408	6/6	0.94	0.11	5.82	30,34,37,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	CL	L	403	1/1	0.99	0.10	5.80	29,29,29,29	0
3	CL	K	403	1/1	0.99	0.12	5.64	28,28,28,28	0
5	GOL	P	405	6/6	0.96	0.11	5.61	16,19,20,24	0
6	0YR	N	409	12/12	0.94	0.15	5.50	16,27,32,33	0
3	CL	P	402	1/1	0.98	0.10	5.41	29,29,29,29	0
5	GOL	N	406	6/6	0.97	0.09	5.20	15,16,17,18	0
5	GOL	J	406	6/6	0.96	0.12	5.19	18,30,32,36	0
3	CL	C	403	1/1	0.99	0.12	5.15	31,31,31,31	0
3	CL	I	403	1/1	0.98	0.12	5.12	33,33,33,33	0
3	CL	O	404	1/1	0.97	0.12	4.94	35,35,35,35	0
3	CL	H	404	1/1	0.99	0.13	4.25	31,31,31,31	0
3	CL	A	403	1/1	0.99	0.11	4.25	29,29,29,29	0
6	0YR	L	407	12/12	0.94	0.15	4.19	17,27,32,35	0
5	GOL	E	405	6/6	0.98	0.10	4.14	15,16,18,19	0
6	0YR	F	408	12/12	0.93	0.14	3.94	18,28,31,31	0
6	0YR	H	409	12/12	0.95	0.15	3.26	16,27,29,31	0
3	CL	B	404	1/1	1.00	0.11	3.13	35,35,35,35	0
6	0YR	K	409	12/12	0.95	0.15	3.03	20,28,39,45	0
6	0YR	G	409	12/12	0.96	0.13	3.02	13,25,28,33	0
3	CL	H	403	1/1	1.00	0.10	2.97	27,27,27,27	0
5	GOL	I	405	6/6	0.98	0.08	2.75	15,16,17,18	0
6	0YR	P	409	12/12	0.94	0.14	2.72	19,27,37,39	0
5	GOL	M	406	6/6	0.97	0.09	2.60	16,18,19,21	0
3	CL	K	404	1/1	0.98	0.09	2.59	32,32,32,32	0
5	GOL	L	405	6/6	0.97	0.09	2.58	15,17,19,19	0
6	0YR	C	408	12/12	0.95	0.12	2.53	20,27,32,36	0
5	GOL	B	406	6/6	0.97	0.09	2.37	15,17,19,21	0
6	0YR	E	408	12/12	0.94	0.13	2.07	17,25,28,29	0
6	0YR	O	408	12/12	0.95	0.12	2.05	17,26,34,36	0
5	GOL	J	405	6/6	0.96	0.08	2.01	16,18,19,22	0
6	0YR	J	408	12/12	0.94	0.15	1.97	19,30,35,36	0
6	0YR	A	410	12/12	0.94	0.12	1.90	14,24,27,31	0
6	0YR	I	406	12/12	0.94	0.13	1.83	16,27,32,35	0
6	0YR	M	407	12/12	0.92	0.12	1.75	19,29,31,35	0
6	0YR	B	409	12/12	0.95	0.12	1.63	17,27,30,33	0
5	GOL	H	406	6/6	0.97	0.07	1.34	14,15,16,18	0
6	0YR	D	411	12/12	0.94	0.10	1.33	14,24,29,29	0
5	GOL	C	405	6/6	0.97	0.07	1.20	13,17,17,22	0
5	GOL	F	405	6/6	0.98	0.07	1.13	14,16,17,19	0
5	GOL	O	406	6/6	0.97	0.07	1.08	15,17,17,19	0
3	CL	G	402	1/1	1.00	0.07	0.98	13,13,13,13	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	CL	D	403	1/1	0.99	0.07	0.93	26,26,26,26	0
3	CL	C	402	1/1	0.97	0.08	0.81	35,35,35,35	0
5	GOL	K	406	6/6	0.98	0.07	0.57	14,15,16,18	0
5	GOL	D	408	6/6	0.98	0.07	0.47	13,14,15,16	0
3	CL	L	402	1/1	0.98	0.07	0.46	34,34,34,34	0
3	CL	J	402	1/1	0.99	0.06	0.20	15,15,15,15	0
5	GOL	G	406	6/6	0.98	0.06	0.02	14,16,18,19	0
2	CA	B	401	1/1	0.99	0.07	-0.02	24,24,24,24	0
3	CL	N	404	1/1	0.99	0.07	-0.10	30,30,30,30	0
3	CL	G	404	1/1	0.99	0.06	-0.34	30,30,30,30	0
3	CL	H	402	1/1	0.99	0.06	-0.37	15,15,15,15	0
3	CL	M	404	1/1	0.95	0.07	-0.53	28,28,28,28	0
3	CL	C	401	1/1	1.00	0.06	-0.97	13,13,13,13	0
3	CL	L	401	1/1	0.99	0.05	-1.37	16,16,16,16	0
4	MG	H	405	1/1	1.00	0.05	-1.40	12,12,12,12	0
3	CL	I	401	1/1	0.99	0.05	-1.73	15,15,15,15	0
3	CL	K	402	1/1	0.99	0.05	-1.84	14,14,14,14	0
3	CL	N	402	1/1	1.00	0.05	-2.28	16,16,16,16	0
3	CL	M	402	1/1	0.99	0.05	-2.40	16,16,16,16	0
3	CL	B	402	1/1	0.99	0.06	-2.52	14,14,14,14	0
3	CL	A	402	1/1	1.00	0.05	-2.69	13,13,13,13	0
3	CL	F	401	1/1	1.00	0.05	-2.77	13,13,13,13	0
3	CL	P	401	1/1	0.99	0.04	-2.85	15,15,15,15	0
4	MG	O	405	1/1	0.99	0.04	-2.92	11,11,11,11	0
3	CL	E	401	1/1	1.00	0.05	-2.97	14,14,14,14	0
4	MG	M	405	1/1	0.99	0.03	-3.37	13,13,13,13	0
3	CL	O	402	1/1	0.99	0.05	-3.38	13,13,13,13	0
4	MG	P	404	1/1	1.00	0.04	-3.48	13,13,13,13	0
2	CA	N	401	1/1	1.00	0.04	-4.21	20,20,20,20	0
4	MG	N	405	1/1	0.99	0.04	-4.22	13,13,13,13	0
4	MG	L	404	1/1	0.99	0.05	-4.41	14,14,14,14	0
2	CA	G	401	1/1	0.99	0.04	-4.50	20,20,20,20	0
4	MG	D	407	1/1	1.00	0.03	-4.71	11,11,11,11	0
4	MG	I	404	1/1	0.99	0.03	-4.80	13,13,13,13	0
4	MG	C	404	1/1	0.99	0.03	-4.85	12,12,12,12	0
4	MG	B	405	1/1	0.99	0.04	-4.89	12,12,12,12	0
4	MG	F	404	1/1	1.00	0.04	-5.01	11,11,11,11	0
2	CA	M	401	1/1	1.00	0.05	-5.08	21,21,21,21	0
4	MG	A	405	1/1	1.00	0.04	-5.21	12,12,12,12	0
3	CL	D	402	1/1	1.00	0.04	-5.51	14,14,14,14	0
4	MG	E	404	1/1	1.00	0.03	-5.69	11,11,11,11	0
2	CA	H	401	1/1	1.00	0.03	-5.95	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	MG	G	405	1/1	1.00	0.02	-6.61	11,11,11,11	0
4	MG	K	405	1/1	0.99	0.03	-6.68	12,12,12,12	0
2	CA	D	401	1/1	0.99	0.03	-10.31	21,21,21,21	0
4	MG	J	404	1/1	0.99	0.04	-10.39	14,14,14,14	0
5	GOL	N	408	6/6	0.85	0.13	-	34,37,39,39	0
5	GOL	O	407	6/6	0.92	0.12	-	36,36,39,40	0
5	GOL	C	406	6/6	0.91	0.09	-	29,34,35,35	0
5	GOL	A	409	6/6	0.93	0.08	-	32,36,37,38	0
5	GOL	B	407	6/6	0.94	0.11	-	32,34,35,38	0
5	GOL	D	410	6/6	0.95	0.10	-	32,34,37,37	0
2	CA	A	401	1/1	0.99	0.04	-	26,26,26,26	1
5	GOL	P	406	6/6	0.92	0.11	-	33,35,36,37	0
5	GOL	K	407	6/6	0.93	0.08	-	30,32,34,35	0
5	GOL	H	407	6/6	0.94	0.10	-	31,33,35,36	0
3	CL	D	406	1/1	0.94	0.08	-	27,27,27,27	1
2	CA	K	401	1/1	0.99	0.03	-	22,22,22,22	1
2	CA	J	401	1/1	1.00	0.05	-	21,21,21,21	1
5	GOL	G	408	6/6	0.94	0.11	-	33,34,36,36	0
5	GOL	L	406	6/6	0.94	0.14	-	32,36,38,38	0
5	GOL	E	407	6/6	0.95	0.08	-	32,33,33,34	0
5	GOL	J	407	6/6	0.94	0.10	-	37,37,40,42	0
5	GOL	H	408	6/6	0.91	0.12	-	34,35,36,38	0
2	CA	O	401	1/1	0.99	0.06	-	22,22,22,22	1

6.5 Other polymers (i)

There are no such residues in this entry.