



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 19, 2020 – 08:34 pm BST

PDB ID : 2G50
Title : The location of the allosteric amino acid binding site of muscle pyruvate kinase.
Authors : Holyoak, T.; Williams, R.; Fenton, A.W.
Deposited on : 2006-02-22
Resolution : 1.65 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

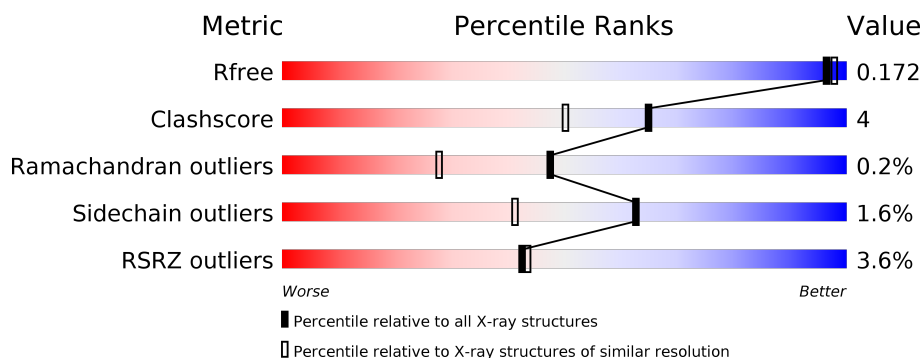
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 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}	130704	1827 (1.66-1.66)
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)
RSRZ outliers	127900	1791 (1.66-1.66)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	530	<div> <div>2%</div> <div>90%</div> <div>7%</div> <div>..</div> </div>
1	B	530	<div> <div>6%</div> <div>87%</div> <div>9%</div> <div>.</div> </div>
1	C	530	<div> <div>4%</div> <div>87%</div> <div>9%</div> <div>..</div> </div>
1	D	530	<div> <div>2%</div> <div>90%</div> <div>8%</div> <div>..</div> </div>
1	E	530	<div> <div>%</div> <div>90%</div> <div>8%</div> <div>.</div> </div>
1	F	530	<div> <div>4%</div> <div>89%</div> <div>8%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	530	
1	H	530	

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
7	EDO	D	6017	-	-	X	-
9	ETE	B	6018	-	-	X	-

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 38184 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 Pyruvate kinase isozymes M1/M2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	519	Total	C	N	O	S	0	26	0
			4134	2617	726	758	33			
1	B	511	Total	C	N	O	S	0	27	0
			4102	2598	720	755	29			
1	C	512	Total	C	N	O	S	0	26	0
			4116	2601	727	757	31			
1	D	521	Total	C	N	O	S	0	25	0
			4162	2627	737	769	29			
1	E	521	Total	C	N	O	S	0	30	0
			4187	2656	734	767	30			
1	F	515	Total	C	N	O	S	0	27	0
			4136	2617	729	761	29			
1	G	510	Total	C	N	O	S	0	15	0
			4015	2535	709	742	29			
1	H	519	Total	C	N	O	S	0	20	0
			4116	2599	727	760	30			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	29	LYS	MET	SEE REMARK 999	UNP P11974
A	400	ALA	SER	SEE REMARK 999	UNP P11974
A	403	GLN	HIS	SEE REMARK 999	UNP P11974
B	29	LYS	MET	SEE REMARK 999	UNP P11974
B	400	ALA	SER	SEE REMARK 999	UNP P11974
B	403	GLN	HIS	SEE REMARK 999	UNP P11974
C	29	LYS	MET	SEE REMARK 999	UNP P11974
C	400	ALA	SER	SEE REMARK 999	UNP P11974
C	403	GLN	HIS	SEE REMARK 999	UNP P11974
D	29	LYS	MET	SEE REMARK 999	UNP P11974
D	400	ALA	SER	SEE REMARK 999	UNP P11974
D	403	GLN	HIS	SEE REMARK 999	UNP P11974
E	29	LYS	MET	SEE REMARK 999	UNP P11974

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Chain	Residue	Modelled	Actual	Comment	Reference
E	400	ALA	SER	SEE REMARK 999	UNP P11974
E	403	GLN	HIS	SEE REMARK 999	UNP P11974
F	29	LYS	MET	SEE REMARK 999	UNP P11974
F	400	ALA	SER	SEE REMARK 999	UNP P11974
F	403	GLN	HIS	SEE REMARK 999	UNP P11974
G	29	LYS	MET	SEE REMARK 999	UNP P11974
G	400	ALA	SER	SEE REMARK 999	UNP P11974
G	403	GLN	HIS	SEE REMARK 999	UNP P11974
H	29	LYS	MET	SEE REMARK 999	UNP P11974
H	400	ALA	SER	SEE REMARK 999	UNP P11974
H	403	GLN	HIS	SEE REMARK 999	UNP P11974

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Mn 1 1	0	0
2	D	1	Total Mn 1 1	0	0
2	E	1	Total Mn 1 1	0	0
2	H	1	Total Mn 1 1	0	0
2	B	1	Total Mn 1 1	0	0
2	C	1	Total Mn 1 1	0	0
2	A	1	Total Mn 1 1	0	0
2	F	1	Total Mn 1 1	0	0

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	1	Total K 1 1	0	0
3	D	1	Total K 1 1	0	0
3	E	1	Total K 1 1	0	0

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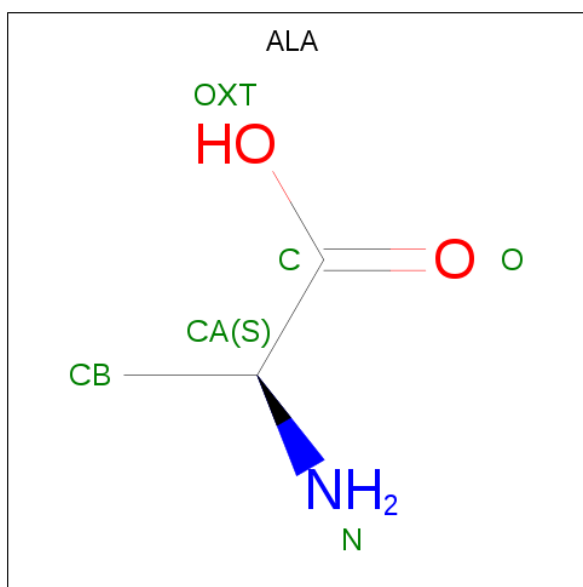
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	1	Total 1	K 1	0	0
3	B	1	Total 1	K 1	0	0
3	C	1	Total 1	K 1	0	0
3	A	1	Total 1	K 1	0	0
3	F	1	Total 1	K 1	0	0

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

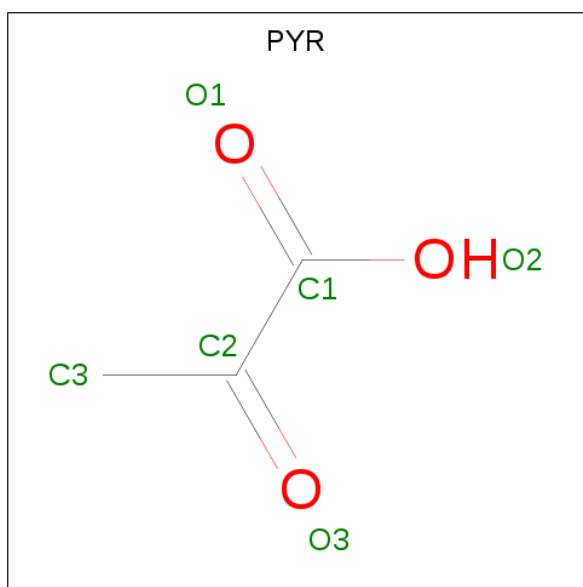
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	1	Total 1	Na 1	0	0
4	D	2	Total 2	Na 2	0	0
4	E	2	Total 2	Na 2	0	0
4	H	2	Total 2	Na 2	0	0
4	B	1	Total 1	Na 1	0	0
4	C	1	Total 1	Na 1	0	0
4	A	2	Total 2	Na 2	0	0
4	F	1	Total 1	Na 1	0	0

- Molecule 5 is ALANINE (three-letter code: ALA) (formula: C₃H₇NO₂).



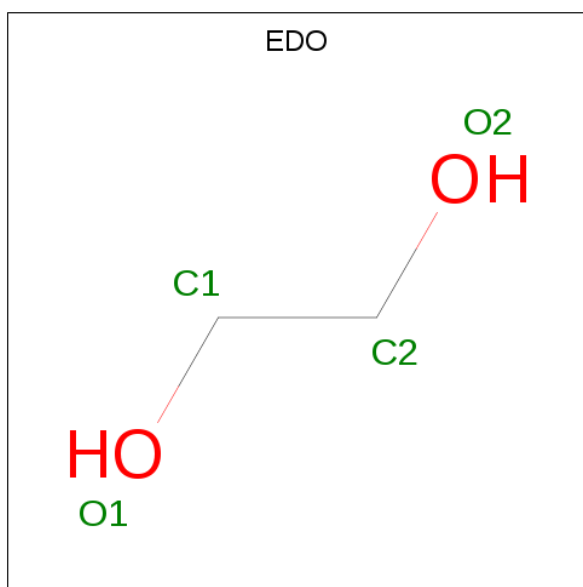
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			6	3	1	2		
5	B	1	Total	C	N	O	0	0
			6	3	1	2		
5	C	1	Total	C	N	O	0	0
			6	3	1	2		
5	D	1	Total	C	N	O	0	0
			6	3	1	2		
5	E	1	Total	C	N	O	0	0
			6	3	1	2		
5	F	1	Total	C	N	O	0	0
			6	3	1	2		
5	G	1	Total	C	N	O	0	0
			6	3	1	2		
5	H	1	Total	C	N	O	0	0
			6	3	1	2		

- Molecule 6 is PYRUVIC ACID (three-letter code: PYR) (formula: C₃H₄O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		
6	D	1	Total	C	O	0	0
			6	3	3		
6	E	1	Total	C	O	0	0
			6	3	3		
6	F	1	Total	C	O	0	0
			6	3	3		
6	G	1	Total	C	O	0	0
			6	3	3		
6	H	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



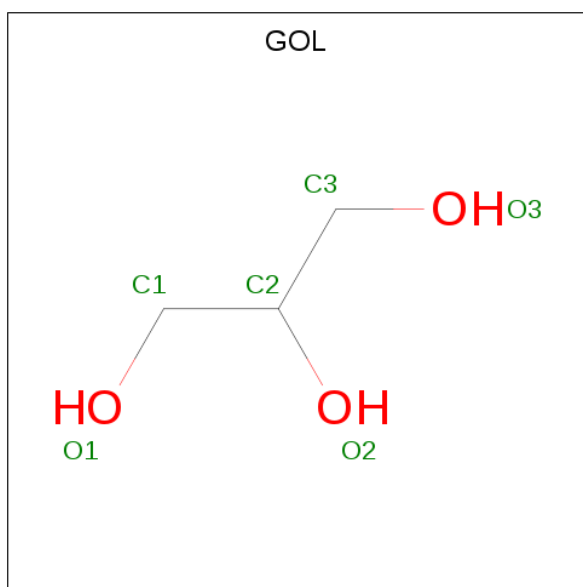
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	C	1	Total	C	O	0	0
			4	2	2		
7	C	1	Total	C	O	0	0
			4	2	2		
7	D	1	Total	C	O	0	0
			4	2	2		
7	D	1	Total	C	O	0	0
			4	2	2		
7	D	1	Total	C	O	0	0
			4	2	2		
7	E	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	E	1	Total	C	O	0	0
			4	2	2		
7	E	1	Total	C	O	0	0
			4	2	2		
7	E	1	Total	C	O	0	0
			4	2	2		
7	E	1	Total	C	O	0	0
			4	2	2		
7	E	1	Total	C	O	0	0
			4	2	2		
7	F	1	Total	C	O	0	0
			4	2	2		
7	F	1	Total	C	O	0	0
			4	2	2		
7	G	1	Total	C	O	0	0
			4	2	2		
7	G	1	Total	C	O	0	0
			4	2	2		
7	H	1	Total	C	O	0	0
			4	2	2		
7	H	1	Total	C	O	0	0
			4	2	2		
7	H	1	Total	C	O	0	0
			4	2	2		
7	H	1	Total	C	O	0	0
			4	2	2		
7	H	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



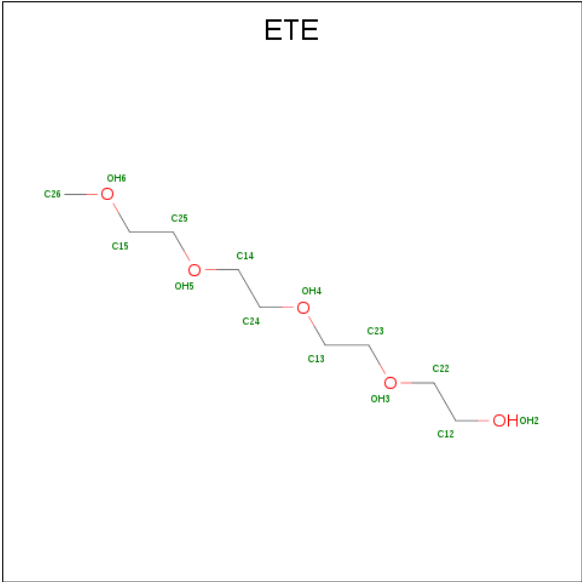
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		
8	C	1	Total	C	O	0	0
			6	3	3		
8	C	1	Total	C	O	0	0
			6	3	3		
8	C	1	Total	C	O	0	0
			6	3	3		
8	C	1	Total	C	O	0	0
			6	3	3		
8	D	1	Total	C	O	0	0
			6	3	3		
8	D	1	Total	C	O	0	0
			6	3	3		
8	E	1	Total	C	O	0	0
			6	3	3		
8	E	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	E	1	Total	C	O	0	0
			6	3	3		
8	F	1	Total	C	O	0	0
			6	3	3		
8	F	1	Total	C	O	0	0
			6	3	3		
8	F	1	Total	C	O	0	0
			6	3	3		
8	F	1	Total	C	O	0	0
			6	3	3		
8	F	1	Total	C	O	0	0
			6	3	3		
8	G	1	Total	C	O	0	0
			6	3	3		
8	G	1	Total	C	O	0	0
			6	3	3		
8	G	1	Total	C	O	0	0
			6	3	3		
8	H	1	Total	C	O	0	0
			6	3	3		
8	H	1	Total	C	O	0	0
			6	3	3		
8	H	1	Total	C	O	0	0
			6	3	3		

- Molecule 9 is 2-{2-[2-2-(METHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHANOL (three-letter code: ETE) (formula: C₉H₂₀O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			14	9	5		

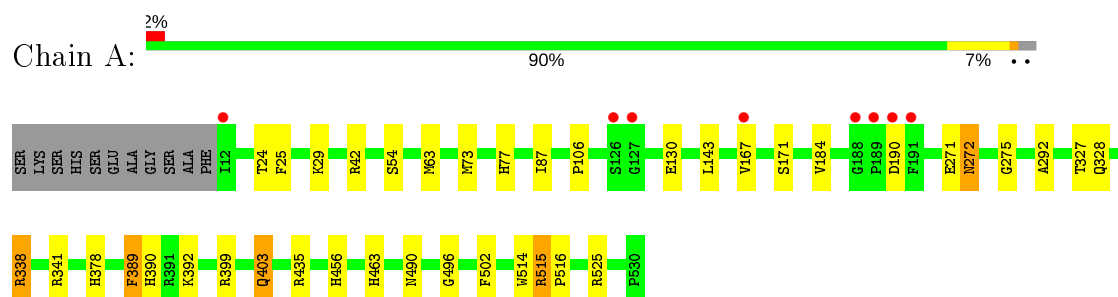
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	651	Total	O	0	0
			651	651		
10	B	517	Total	O	0	0
			517	517		
10	C	605	Total	O	0	0
			605	605		
10	D	649	Total	O	0	0
			649	649		
10	E	682	Total	O	0	0
			682	682		
10	F	605	Total	O	0	0
			605	605		
10	G	490	Total	O	0	0
			490	490		
10	H	595	Total	O	0	0
			595	595		

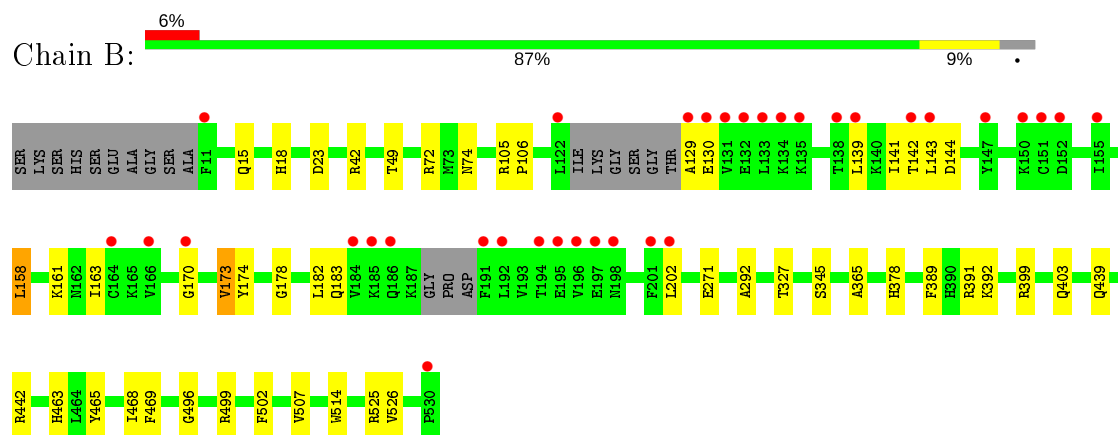
3 Residue-property plots [i](#)

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.

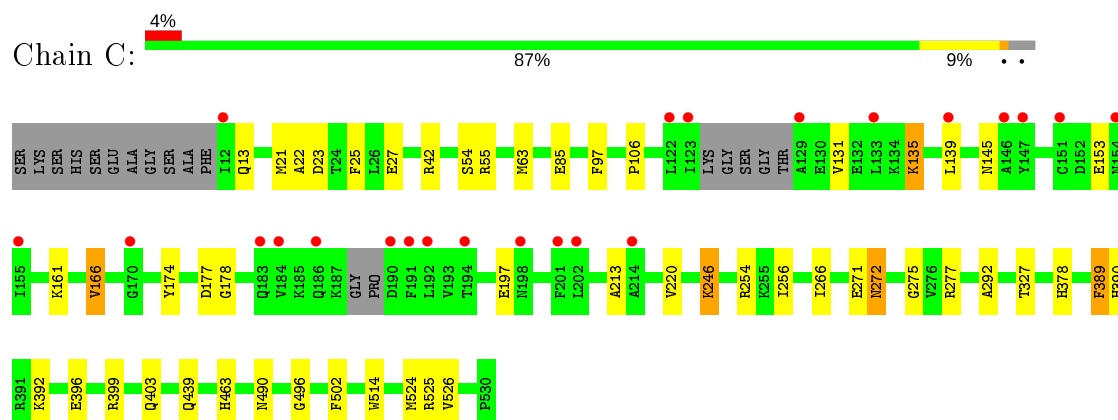
• Molecule 1: Pyruvate kinase isozymes M1/M2



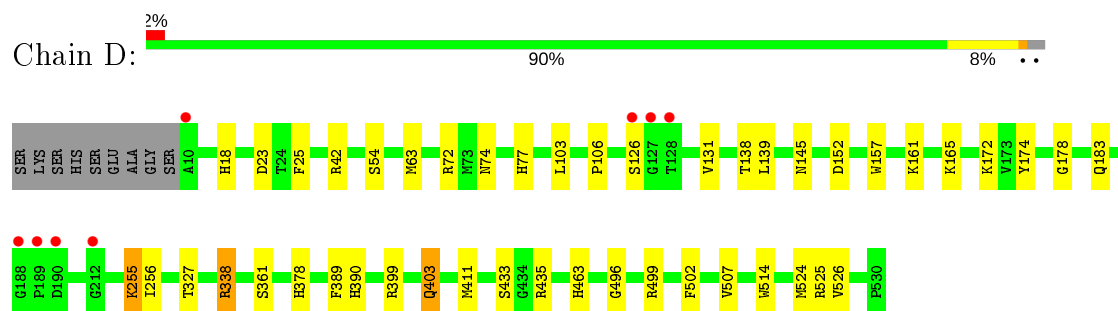
• Molecule 1: Pyruvate kinase isozymes M1/M2



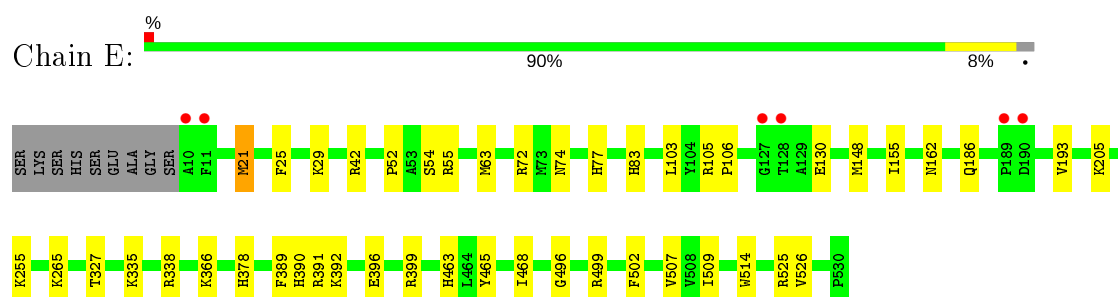
• Molecule 1: Pyruvate kinase isozymes M1/M2



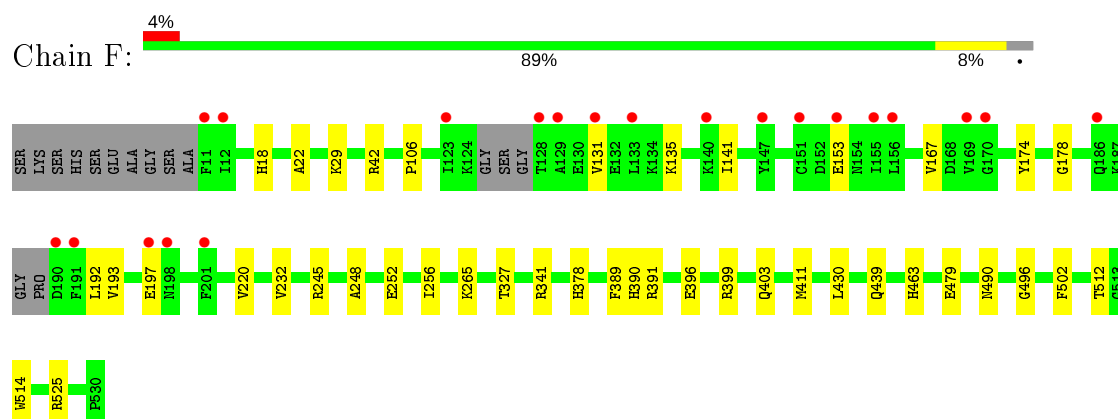
- Molecule 1: Pyruvate kinase isozymes M1/M2



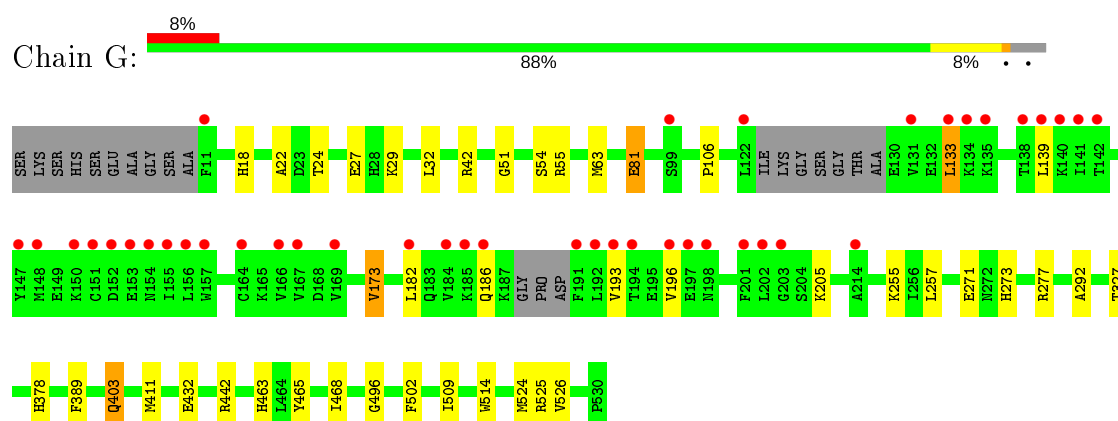
- Molecule 1: Pyruvate kinase isozymes M1/M2



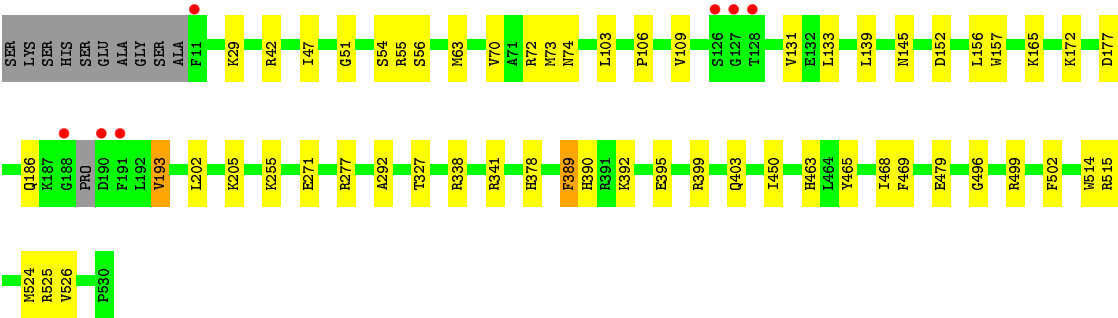
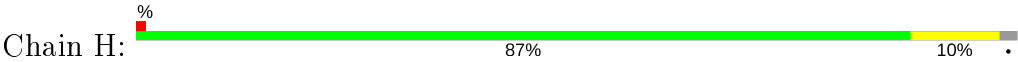
- Molecule 1: Pyruvate kinase isozymes M1/M2



- Molecule 1: Pyruvate kinase isozymes M1/M2



● Molecule 1: Pyruvate kinase isozymes M1/M2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	82.63Å 109.01Å 144.46Å 95.15° 93.45° 112.26°	Depositor
Resolution (Å)	76.47 – 1.65 76.46 – 1.65	Depositor EDS
% Data completeness (in resolution range)	92.1 (76.47-1.65) 92.1 (76.46-1.65)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.23 (at 1.65Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.148 , 0.174 0.146 , 0.172	Depositor DCC
R_{free} test set	25590 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	18.1	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 52.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	38184	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, NA, PYR, MN, EDO, ETE, K

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.46	0/4278	0.60	0/5760
1	B	0.48	2/4240 (0.0%)	0.57	0/5708
1	C	0.49	1/4235 (0.0%)	0.59	0/5701
1	D	0.45	0/4285	0.58	0/5774
1	E	0.46	0/4328	0.58	0/5829
1	F	0.48	0/4268	0.59	0/5748
1	G	0.42	0/4119	0.54	0/5549
1	H	0.46	0/4224	0.58	0/5688
All	All	0.46	3/33977 (0.0%)	0.58	0/45757

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	142	THR	C-N	8.55	1.53	1.34
1	B	144	ASP	C-O	5.59	1.33	1.23
1	C	135	LYS	CE-NZ	5.16	1.61	1.49

There are no bond angle outliers.

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	4134	0	4316	32	0
1	B	4102	0	4250	39	0
1	C	4116	0	4253	41	0
1	D	4162	0	4294	35	0
1	E	4187	0	4356	47	0
1	F	4136	0	4284	34	0
1	G	4015	0	4132	28	0
1	H	4116	0	4245	42	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	2	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	2	0	0	0	0
4	E	2	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	2	0	0	0	0
5	A	6	0	4	1	0
5	B	6	0	4	1	0
5	C	6	0	4	1	0
5	D	6	0	4	1	0
5	E	6	0	4	1	0
5	F	6	0	4	1	0
5	G	6	0	4	1	0
5	H	6	0	4	1	0
6	A	6	0	3	0	0
6	B	6	0	3	0	0
6	C	6	0	3	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	D	6	0	3	0	0
6	E	6	0	3	0	0
6	F	6	0	3	0	0
6	G	6	0	3	0	0
6	H	6	0	3	0	0
7	A	12	0	18	0	0
7	B	16	0	24	3	0
7	C	8	0	12	2	0
7	D	16	0	24	4	0
7	E	24	0	36	6	0
7	F	8	0	12	2	0
7	G	8	0	12	0	0
7	H	24	0	36	3	0
8	A	18	0	24	1	0
8	B	18	0	24	0	0
8	C	24	0	32	1	0
8	D	12	0	16	0	0
8	E	18	0	24	2	0
8	F	36	0	48	4	0
8	G	18	0	24	0	0
8	H	24	0	32	3	0
9	B	14	0	20	8	0
10	A	651	0	0	4	0
10	B	517	0	0	9	0
10	C	605	0	0	9	0
10	D	649	0	0	6	0
10	E	682	0	0	10	0
10	F	605	0	0	7	0
10	G	490	0	0	1	0
10	H	595	0	0	7	0
All	All	38184	0	34604	278	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 4.

All (278) 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:B:469[B]:PHE:HZ	10:B:6759:HOH:O	1.32	1.12
1:E:391[B]:ARG:NH1	1:F:399[B]:ARG:HG2	1.64	1.10
1:E:186:GLN:HB3	1:E:193[B]:VAL:HG13	1.46	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:55:ARG:HH11	7:E:6045:EDO:H11	1.34	0.93
1:B:469[B]:PHE:CE2	1:B:499:ARG:NH1	2.38	0.91
1:D:42:ARG:HE	1:D:378:HIS:HD2	1.15	0.90
1:C:42:ARG:HE	1:C:378:HIS:HD2	1.15	0.89
1:E:42:ARG:HE	1:E:378:HIS:HD2	1.14	0.88
8:F:6010:GOL:H32	1:H:341:ARG:HH12	1.36	0.88
1:B:72:ARG:HH12	9:B:6018:ETE:H222	1.36	0.88
1:F:42:ARG:HE	1:F:378:HIS:HD2	1.19	0.88
1:C:439[B]:GLN:NE2	10:C:6624:HOH:O	1.96	0.87
1:B:42:ARG:HE	1:B:378:HIS:HD2	1.18	0.87
1:G:42:ARG:HE	1:G:378:HIS:HD2	1.20	0.86
1:A:42:ARG:HE	1:A:378:HIS:HD2	1.20	0.85
1:H:338[A]:ARG:NH2	10:H:7070:HOH:O	2.08	0.84
1:E:52:PRO:HB3	8:E:6031:GOL:H2	1.60	0.83
1:C:220:VAL:HG11	1:C:256[A]:ILE:CD1	2.09	0.83
1:B:469[B]:PHE:CZ	10:B:6759:HOH:O	2.14	0.82
1:B:365:ALA:HB1	9:B:6018:ETE:H142	1.59	0.82
1:F:220:VAL:HG11	1:F:256[A]:ILE:CD1	2.10	0.82
1:H:42:ARG:HE	1:H:378:HIS:HD2	1.25	0.81
1:H:186:GLN:HB3	1:H:193:VAL:HG13	1.61	0.81
1:A:73[B]:MET:SD	1:A:87:ILE:HD11	2.21	0.80
1:C:399[A]:ARG:NH1	10:C:7100:HOH:O	2.15	0.79
1:E:338[A]:ARG:NH2	10:E:2698:HOH:O	2.16	0.78
1:H:72:ARG:HH12	7:H:6034:EDO:H22	1.49	0.78
1:B:129:ALA:HA	1:B:130:GLU:HB3	1.64	0.78
1:F:245[A]:ARG:NH2	10:F:6928:HOH:O	2.17	0.77
1:H:499:ARG:HH22	8:H:6006:GOL:H2	1.49	0.76
1:D:72:ARG:HH12	7:D:6017:EDO:H22	1.50	0.75
1:B:72:ARG:HH12	9:B:6018:ETE:C22	2.00	0.75
1:G:186:GLN:HB3	1:G:193:VAL:HB	1.69	0.74
1:D:433:SER:OG	1:D:435[B]:ARG:HG2	1.88	0.73
1:F:341:ARG:HH22	7:F:6036:EDO:H22	1.53	0.72
1:B:105:ARG:HG2	7:B:6032:EDO:H12	1.71	0.72
1:B:42:ARG:HE	1:B:378:HIS:CD2	2.06	0.71
1:E:21:MET:CE	1:E:391[B]:ARG:NH2	2.53	0.71
1:E:21:MET:HE1	1:E:391[B]:ARG:HH21	1.55	0.71
1:E:526[A]:VAL:HG23	1:F:411:MET:SD	2.31	0.70
1:E:72:ARG:HH12	7:E:6038:EDO:H11	1.57	0.69
1:F:439[A]:GLN:NE2	10:F:7065:HOH:O	2.25	0.69
1:E:42:ARG:HE	1:E:378:HIS:CD2	2.04	0.69
1:C:42:ARG:HE	1:C:378:HIS:CD2	2.05	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:469[B]:PHE:HE2	1:B:499:ARG:NH1	1.91	0.68
1:D:42:ARG:HE	1:D:378:HIS:CD2	2.06	0.68
1:E:52:PRO:CB	8:E:6031:GOL:H2	2.22	0.68
1:C:463:HIS:HD2	5:C:6103:ALA:N	1.93	0.67
1:E:25[B]:PHE:CZ	1:E:392:LYS:HG2	2.30	0.66
1:E:391[B]:ARG:HH12	1:F:399[B]:ARG:HG2	1.60	0.66
1:B:173:VAL:HG13	1:B:182:LEU:HB2	1.75	0.66
1:B:129:ALA:HA	1:B:130:GLU:CB	2.25	0.66
1:E:55:ARG:NH1	7:E:6045:EDO:H11	2.09	0.66
1:B:399[A]:ARG:HG3	10:B:6848:HOH:O	1.96	0.66
1:A:42:ARG:HE	1:A:378:HIS:CD2	2.08	0.66
1:F:399[B]:ARG:HG3	10:F:6715:HOH:O	1.96	0.65
1:D:399[A]:ARG:NH1	10:D:6908:HOH:O	2.29	0.65
1:F:42:ARG:HE	1:F:378:HIS:CD2	2.09	0.64
1:E:399:ARG:NH1	10:E:3220:HOH:O	2.30	0.64
1:B:141:ILE:HG23	1:B:158:LEU:HD11	1.80	0.64
1:G:173:VAL:HG13	1:G:182:LEU:HB2	1.79	0.64
1:A:463:HIS:HD2	5:A:6101:ALA:N	1.96	0.63
1:G:463:HIS:HD2	5:G:6107:ALA:N	1.97	0.62
1:D:463:HIS:HD2	5:D:6104:ALA:N	1.96	0.62
1:F:463:HIS:HD2	5:F:6106:ALA:N	1.98	0.61
1:B:463:HIS:HD2	5:B:6102:ALA:N	1.98	0.61
1:B:106:PRO:O	1:B:463:HIS:HE1	1.83	0.61
1:C:526[B]:VAL:HG23	1:D:411:MET:SD	2.40	0.61
1:F:479:GLU:H	1:F:479:GLU:CD	2.02	0.61
1:C:97:PHE:CD1	8:C:6055:GOL:H2	2.36	0.61
1:D:338[A]:ARG:NH1	10:D:7092:HOH:O	2.34	0.60
1:H:106:PRO:O	1:H:463:HIS:HE1	1.84	0.60
1:E:21:MET:CE	1:E:391[B]:ARG:HH21	2.15	0.60
1:H:42:ARG:HE	1:H:378:HIS:CD2	2.13	0.60
1:C:524[A]:MET:HE2	1:D:524[A]:MET:HB3	1.84	0.59
1:E:463:HIS:HD2	5:E:6105:ALA:N	2.00	0.59
1:E:205[B]:LYS:NZ	10:E:3396:HOH:O	2.34	0.59
1:A:399[A]:ARG:NH1	1:B:23:ASP:OD1	2.36	0.59
1:C:220:VAL:HG11	1:C:256[A]:ILE:HD13	1.82	0.58
1:H:389:PHE:CE1	1:H:392:LYS:HG3	2.38	0.58
1:A:106:PRO:O	1:A:463:HIS:HE1	1.86	0.58
1:E:21:MET:HA	1:E:21:MET:CE	2.33	0.58
1:H:463:HIS:HD2	5:H:6108:ALA:N	2.01	0.58
1:G:42:ARG:HE	1:G:378:HIS:CD2	2.11	0.58
1:G:273[B]:HIS:CE1	1:G:277:ARG:NE	2.72	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:21:MET:HE1	1:E:391[B]:ARG:NH2	2.17	0.57
1:F:106:PRO:O	1:F:463:HIS:HE1	1.86	0.57
1:G:106:PRO:O	1:G:463:HIS:HE1	1.87	0.57
1:E:83:HIS:HD2	10:E:3460:HOH:O	1.87	0.57
7:E:6038:EDO:H12	7:E:6046:EDO:O2	2.04	0.57
1:C:135:LYS:HD3	1:C:197:GLU:O	2.03	0.57
1:A:272:ASN:HD22	1:A:275:GLY:H	1.52	0.57
1:A:390:HIS:HD2	10:A:6607:HOH:O	1.88	0.56
10:F:7087:HOH:O	1:H:177:ASP:HB3	2.05	0.56
1:D:72:ARG:NH1	7:D:6017:EDO:H22	2.21	0.56
1:E:21:MET:HE2	1:E:391[B]:ARG:NH2	2.21	0.56
1:A:167[B]:VAL:HG11	1:A:184:VAL:HG21	1.88	0.56
1:E:106:PRO:O	1:E:463:HIS:HE1	1.89	0.56
1:E:186:GLN:HB3	1:E:193[B]:VAL:CG1	2.30	0.55
1:H:255:LYS:HE2	10:H:7063:HOH:O	2.06	0.55
1:D:361:SER:HB3	7:D:6017:EDO:H11	1.88	0.55
1:C:106:PRO:O	1:C:463:HIS:HE1	1.89	0.55
1:D:106:PRO:O	1:D:463:HIS:HE1	1.90	0.55
1:B:496:GLY:HA3	1:B:502:PHE:CZ	2.42	0.54
1:D:145:ASN:HD22	1:D:157:TRP:HE1	1.55	0.54
1:F:141:ILE:HB	1:F:192:LEU:HB2	1.89	0.54
1:G:273[B]:HIS:HE1	1:G:277:ARG:NE	2.06	0.54
1:C:525:ARG:HD3	1:D:514:TRP:CE3	2.42	0.54
1:H:145:ASN:HD22	1:H:157:TRP:HE1	1.55	0.54
1:G:81:GLU:CD	1:G:81:GLU:H	2.10	0.53
1:G:18:HIS:HD2	10:G:3340:HOH:O	1.92	0.53
1:D:138[A]:THR:HG22	10:D:6766:HOH:O	2.09	0.53
1:D:255[A]:LYS:HE2	1:D:256:ILE:HD13	1.91	0.53
1:F:341:ARG:HH22	7:F:6036:EDO:C2	2.21	0.53
1:A:525:ARG:HD3	1:B:514:TRP:CE3	2.44	0.53
1:E:509:ILE:CD1	1:E:526[B]:VAL:HG12	2.38	0.53
1:A:272:ASN:ND2	1:A:275:GLY:H	2.07	0.53
1:A:73[B]:MET:SD	1:A:87:ILE:CD1	2.94	0.53
1:B:170:GLY:HA2	1:B:183:GLN:HE21	1.74	0.53
1:C:22:ALA:HB1	1:C:27[B]:GLU:HB3	1.91	0.53
1:C:131:VAL:HG13	1:C:153:GLU:HG3	1.90	0.53
1:C:55[A]:ARG:NH2	1:C:85:GLU:HB3	2.24	0.53
1:B:15:GLN:NE2	10:B:6886:HOH:O	2.42	0.52
1:H:399[A]:ARG:NH1	10:H:7074:HOH:O	2.42	0.52
1:A:496:GLY:HA3	1:A:502:PHE:CZ	2.45	0.52
7:B:6032:EDO:C1	10:B:6758:HOH:O	2.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:18:HIS:HD2	10:D:6587:HOH:O	1.93	0.52
1:E:105:ARG:NE	10:E:4823:HOH:O	2.35	0.52
1:B:72:ARG:NH1	9:B:6018:ETE:H222	2.15	0.52
1:F:174:TYR:HB3	1:F:178:GLY:HA2	1.92	0.52
1:H:277[B]:ARG:NH1	10:H:7038:HOH:O	2.42	0.51
1:E:21:MET:HA	1:E:21:MET:HE3	1.93	0.51
1:F:390:HIS:HD2	10:F:7004:HOH:O	1.93	0.51
1:G:496:GLY:HA3	1:G:502:PHE:CZ	2.45	0.51
1:H:496:GLY:HA3	1:H:502:PHE:CZ	2.46	0.51
1:C:496:GLY:HA3	1:C:502:PHE:CZ	2.46	0.51
1:D:390:HIS:HD2	10:D:6942:HOH:O	1.93	0.51
1:A:77:HIS:HD2	10:A:6678:HOH:O	1.93	0.51
1:F:220:VAL:HG11	1:F:256[A]:ILE:HD11	1.92	0.50
1:G:514:TRP:CE3	1:H:525:ARG:HD3	2.45	0.50
1:E:390:HIS:HD2	10:E:2682:HOH:O	1.93	0.50
1:E:525:ARG:HD3	1:F:514:TRP:CE3	2.47	0.50
1:H:390:HIS:HD2	10:H:6538:HOH:O	1.95	0.50
1:E:77:HIS:O	1:E:83:HIS:HE1	1.94	0.50
1:B:507[A]:VAL:CG1	1:B:526[A]:VAL:HG13	2.42	0.50
1:H:74:ASN:HD22	7:H:6034:EDO:H21	1.77	0.50
1:C:166:VAL:HG13	1:C:213:ALA:HB1	1.94	0.50
1:C:220:VAL:HG11	1:C:256[A]:ILE:HD11	1.93	0.50
1:F:479:GLU:N	1:F:479:GLU:CD	2.65	0.50
1:G:271:GLU:HB3	1:G:292:ALA:HB3	1.94	0.50
1:B:465:TYR:HB2	1:B:468:ILE:HD12	1.93	0.50
1:C:177:ASP:HB3	10:C:7056:HOH:O	2.12	0.50
1:C:490[B]:ASN:ND2	10:C:6992:HOH:O	2.44	0.50
1:C:272:ASN:ND2	1:C:275:GLY:H	2.10	0.49
1:G:54:SER:HB2	1:G:63[B]:MET:SD	2.53	0.49
1:C:390:HIS:HD2	10:C:6579:HOH:O	1.95	0.49
1:E:514:TRP:CE3	1:F:525:ARG:HD3	2.47	0.49
1:F:496:GLY:HA3	1:F:502:PHE:CZ	2.48	0.49
1:A:167[B]:VAL:HG13	1:A:171:SER:HB2	1.95	0.49
1:A:73[B]:MET:SD	1:A:87:ILE:CG1	3.01	0.49
1:B:143:LEU:HD11	1:B:163:ILE:HG22	1.94	0.49
7:B:6032:EDO:H11	10:B:6758:HOH:O	2.13	0.49
1:H:271:GLU:HB3	1:H:292:ALA:HB3	1.94	0.48
1:G:411:MET:SD	1:H:526[B]:VAL:HG23	2.53	0.48
1:D:496:GLY:HA3	1:D:502:PHE:CZ	2.47	0.48
1:B:18:HIS:HD2	10:B:6798:HOH:O	1.97	0.48
1:F:135:LYS:HG3	1:F:197:GLU:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:525:ARG:HD3	1:H:514:TRP:CE3	2.49	0.48
1:B:74:ASN:HB3	9:B:6018:ETE:H131	1.96	0.48
1:A:378:HIS:CD2	8:A:6002:GOL:H32	2.49	0.48
1:A:514:TRP:CE3	1:B:525:ARG:HD3	2.49	0.47
1:E:52:PRO:HD2	1:E:366[B]:LYS:HZ2	1.79	0.47
1:D:54:SER:HB2	1:D:63[A]:MET:SD	2.55	0.47
1:E:496:GLY:HA3	1:E:502:PHE:CZ	2.49	0.47
1:H:131:VAL:HG21	1:H:152:ASP:HA	1.96	0.47
1:C:174:TYR:HB3	1:C:178:GLY:HA2	1.96	0.47
1:E:509:ILE:HD13	1:E:526[B]:VAL:HG12	1.96	0.47
1:C:54:SER:HB2	1:C:63[B]:MET:SD	2.55	0.46
1:C:399[B]:ARG:HD3	1:D:23:ASP:OD1	2.15	0.46
1:A:167[B]:VAL:CG1	1:A:184:VAL:HG21	2.45	0.46
1:B:143:LEU:HD13	1:B:161:LYS:HA	1.97	0.46
1:D:174:TYR:HB3	1:D:178:GLY:HA2	1.98	0.46
1:E:105:ARG:NH1	10:E:4823:HOH:O	2.45	0.46
1:C:272:ASN:HD22	1:C:275:GLY:H	1.63	0.46
1:E:366[B]:LYS:NZ	7:E:6046:EDO:O1	2.27	0.46
1:H:51:GLY:O	1:H:55:ARG:HG3	2.16	0.46
1:D:403:GLN:H	1:D:403:GLN:NE2	2.14	0.45
1:G:524[A]:MET:HB3	1:H:524[A]:MET:HE2	1.97	0.45
1:F:490:ASN:ND2	10:F:6858:HOH:O	2.47	0.45
1:F:430:LEU:HD22	1:F:512:THR:HG22	1.98	0.45
1:D:507[B]:VAL:CG1	1:D:526[B]:VAL:CG2	2.94	0.45
1:B:271:GLU:HB3	1:B:292:ALA:HB3	1.99	0.45
1:D:255[A]:LYS:HG3	1:D:256:ILE:N	2.32	0.45
1:A:143[B]:LEU:HD13	1:A:190:ASP:O	2.16	0.45
1:C:246[B]:LYS:NZ	10:C:6723:HOH:O	2.46	0.45
1:A:435:ARG:NH2	10:A:7127:HOH:O	2.50	0.45
1:A:29[B]:LYS:HE3	1:A:29[B]:LYS:HB3	1.82	0.44
1:C:271:GLU:HB3	1:C:292:ALA:HB3	1.98	0.44
1:B:439[B]:GLN:HE22	1:B:442:ARG:HH11	1.65	0.44
1:G:133:LEU:HB3	1:G:196:VAL:HG21	1.99	0.44
1:G:273[B]:HIS:CE1	1:G:277:ARG:HE	2.35	0.44
1:G:465:TYR:HB2	1:G:468:ILE:HD12	1.99	0.44
1:C:389:PHE:CE1	1:C:392:LYS:HG3	2.51	0.44
1:E:265:LYS:HD3	1:E:265:LYS:HA	1.90	0.44
1:A:54:SER:HB2	1:A:63[A]:MET:SD	2.58	0.44
1:C:23:ASP:CG	1:D:399[B]:ARG:HH11	2.20	0.44
1:G:524[A]:MET:HE2	1:H:524[A]:MET:HB3	1.99	0.44
1:C:13:GLN:HE22	1:C:21[B]:MET:CE	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:29:LYS:HE3	1:F:29:LYS:HB3	1.82	0.44
1:H:465:TYR:HB2	1:H:468:ILE:HD12	2.00	0.44
1:A:490[A]:ASN:ND2	10:A:7138:HOH:O	2.51	0.43
1:C:390:HIS:HE1	10:C:6524:HOH:O	1.99	0.43
1:G:51:GLY:O	1:G:55:ARG:HB2	2.18	0.43
1:H:73:MET:CE	1:H:109:VAL:HG13	2.49	0.43
7:C:6044:EDO:H12	10:C:6891:HOH:O	2.18	0.43
1:H:205:LYS:NZ	10:H:6762:HOH:O	2.51	0.43
1:B:74:ASN:CB	9:B:6018:ETE:H131	2.49	0.43
1:B:74:ASN:HD22	9:B:6018:ETE:H221	1.83	0.43
1:C:23:ASP:OD1	1:D:399[B]:ARG:NE	2.50	0.43
1:A:25[A]:PHE:CZ	1:C:25[A]:PHE:CG	2.80	0.43
1:H:103:LEU:O	8:H:6006:GOL:H31	2.18	0.43
1:B:391[A]:ARG:HH22	1:B:392:LYS:HE2	1.84	0.43
1:D:74:ASN:HD22	7:D:6017:EDO:H21	1.83	0.43
1:G:403:GLN:H	1:G:403:GLN:NE2	2.17	0.43
1:E:148[B]:MET:HG2	10:E:3397:HOH:O	2.18	0.42
1:F:232:VAL:HG21	8:F:6001:GOL:H32	1.99	0.42
1:H:156:LEU:HD13	1:H:202:LEU:HD21	2.01	0.42
1:A:271:GLU:HB3	1:A:292:ALA:HB3	1.99	0.42
1:G:509:ILE:CD1	1:G:526[A]:VAL:HG12	2.49	0.42
1:E:29[A]:LYS:HE2	10:E:3655:HOH:O	2.18	0.42
1:H:378:HIS:CD2	8:H:6008:GOL:H32	2.54	0.42
1:D:161:LYS:HA	1:D:161:LYS:HD3	1.91	0.42
8:F:6010:GOL:H32	1:H:341:ARG:NH1	2.19	0.42
1:A:389:PHE:CE1	1:A:392:LYS:HG3	2.55	0.42
1:G:22:ALA:HB1	1:G:27[A]:GLU:HB3	2.01	0.42
1:D:77:HIS:HD2	10:D:6564:HOH:O	2.02	0.42
1:E:465:TYR:HB2	1:E:468:ILE:HD12	2.02	0.42
1:B:345[B]:SER:HB2	10:B:6597:HOH:O	2.18	0.42
1:F:248:ALA:O	1:F:252:GLU:HG3	2.20	0.42
1:G:273[B]:HIS:HE1	1:G:277:ARG:HE	1.66	0.42
1:B:174:TYR:HB3	1:B:178:GLY:HA2	2.02	0.42
1:B:391[B]:ARG:HD3	10:B:6784:HOH:O	2.20	0.42
1:C:145:ASN:HD21	1:C:161:LYS:NZ	2.18	0.42
1:C:514:TRP:CE3	1:D:525:ARG:HD3	2.54	0.42
1:E:54:SER:HB2	1:E:63[B]:MET:SD	2.60	0.42
1:F:131:VAL:HB	1:F:153:GLU:HG3	2.02	0.41
1:F:22:ALA:O	1:F:391:ARG:NH2	2.42	0.41
1:A:328:GLN:HE22	7:C:6044:EDO:H11	1.85	0.41
1:F:378:HIS:CD2	8:F:6005:GOL:H32	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:THR:HB	1:C:396:GLU:CD	2.41	0.41
1:A:338[B]:ARG:HH22	1:A:341:ARG:HH12	1.68	0.41
1:H:133:LEU:HD11	1:H:202:LEU:HD22	2.02	0.41
1:H:395:GLU:HG3	10:H:6844:HOH:O	2.21	0.41
1:C:277:ARG:NH2	10:C:7101:HOH:O	2.54	0.41
1:C:524[A]:MET:HE1	1:D:524[A]:MET:SD	2.60	0.41
1:C:254:ARG:CZ	1:C:266:ILE:HD12	2.50	0.41
1:D:131:VAL:HG11	1:D:152:ASP:HA	2.02	0.41
1:D:172:LYS:HE2	1:D:183[B]:GLN:NE2	2.36	0.41
1:H:54:SER:HB2	1:H:63[B]:MET:SD	2.60	0.41
1:E:507[A]:VAL:CG1	1:E:526[A]:VAL:HG13	2.51	0.41
1:G:29[A]:LYS:HE2	1:G:32:LEU:HD11	2.03	0.41
1:A:515:ARG:HB2	1:A:516:PRO:HD2	2.02	0.41
1:F:18:HIS:HD2	10:F:7002:HOH:O	2.03	0.41
1:F:265:LYS:HD3	1:F:265:LYS:HA	1.90	0.41
1:H:47:ILE:HG12	1:H:70:VAL:HB	2.03	0.41
1:H:56:SER:OG	7:H:6054:EDO:H22	2.20	0.41
1:H:450[B]:ILE:HD13	1:H:469:PHE:HB3	2.03	0.41
1:A:403:GLN:H	1:A:403:GLN:NE2	2.18	0.40
1:E:103:LEU:O	1:E:499:ARG:NH1	2.52	0.40
1:E:396:GLU:CD	1:G:24:THR:HB	2.41	0.40
1:H:29[B]:LYS:HB3	1:H:29[B]:LYS:HE3	1.87	0.40
1:H:515:ARG:HD3	1:H:515:ARG:HA	1.95	0.40
1:E:74:ASN:HD22	7:E:6038:EDO:H12	1.87	0.40
1:H:186:GLN:HB3	1:H:193:VAL:CG1	2.43	0.40
1:B:49:THR:HG21	9:B:6018:ETE:H132	2.03	0.40
1:D:103:LEU:O	1:D:499:ARG:NH2	2.51	0.40
1:E:255:LYS:HE2	10:E:3316:HOH:O	2.21	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	544/530 (103%)	538 (99%)	5 (1%)	1 (0%)	47	28
1	B	532/530 (100%)	524 (98%)	7 (1%)	1 (0%)	47	28
1	C	532/530 (100%)	524 (98%)	7 (1%)	1 (0%)	47	28
1	D	544/530 (103%)	537 (99%)	6 (1%)	1 (0%)	47	28
1	E	549/530 (104%)	541 (98%)	7 (1%)	1 (0%)	47	28
1	F	536/530 (101%)	527 (98%)	8 (2%)	1 (0%)	47	28
1	G	519/530 (98%)	509 (98%)	9 (2%)	1 (0%)	47	28
1	H	535/530 (101%)	527 (98%)	7 (1%)	1 (0%)	47	28
All	All	4291/4240 (101%)	4227 (98%)	56 (1%)	8 (0%)	47	28

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	327	THR
1	D	327	THR
1	E	327	THR
1	F	327	THR
1	A	327	THR
1	B	327	THR
1	G	327	THR
1	H	327	THR

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	452/433 (104%)	444 (98%)	8 (2%)	59	36
1	B	447/433 (103%)	441 (99%)	6 (1%)	69	50
1	C	447/433 (103%)	439 (98%)	8 (2%)	59	36
1	D	451/433 (104%)	440 (98%)	11 (2%)	49	23
1	E	456/433 (105%)	449 (98%)	7 (2%)	65	44
1	F	451/433 (104%)	446 (99%)	5 (1%)	73	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	435/433 (100%)	424 (98%)	11 (2%)	47	22
1	H	445/433 (103%)	438 (98%)	7 (2%)	62	41
All	All	3584/3464 (104%)	3521 (98%)	63 (2%)	62	36

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	130	GLU
1	A	272	ASN
1	A	338[A]	ARG
1	A	338[B]	ARG
1	A	389	PHE
1	A	403	GLN
1	A	456	HIS
1	A	515	ARG
1	B	139	LEU
1	B	158	LEU
1	B	173	VAL
1	B	202	LEU
1	B	389	PHE
1	B	403	GLN
1	C	139	LEU
1	C	166	VAL
1	C	246[A]	LYS
1	C	246[B]	LYS
1	C	272	ASN
1	C	389	PHE
1	C	403[A]	GLN
1	C	403[B]	GLN
1	D	25[A]	PHE
1	D	25[B]	PHE
1	D	126	SER
1	D	139	LEU
1	D	165	LYS
1	D	255[A]	LYS
1	D	255[B]	LYS
1	D	338[A]	ARG
1	D	338[B]	ARG
1	D	389	PHE
1	D	403	GLN
1	E	21	MET

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Mol	Chain	Res	Type
1	E	130	GLU
1	E	155[A]	ILE
1	E	155[B]	ILE
1	E	162	ASN
1	E	335	LYS
1	E	389	PHE
1	F	167	VAL
1	F	193	VAL
1	F	389	PHE
1	F	403[A]	GLN
1	F	403[B]	GLN
1	G	81	GLU
1	G	133	LEU
1	G	139	LEU
1	G	173	VAL
1	G	205	LYS
1	G	255	LYS
1	G	257	LEU
1	G	389	PHE
1	G	403	GLN
1	G	432	GLU
1	G	442	ARG
1	H	139	LEU
1	H	165	LYS
1	H	172	LYS
1	H	193	VAL
1	H	389	PHE
1	H	403	GLN
1	H	479	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (88) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	43	ASN
1	A	234	GLN
1	A	272	ASN
1	A	377	GLN
1	A	378	HIS
1	A	390	HIS
1	A	403	GLN
1	A	456	HIS

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Mol	Chain	Res	Type
1	A	457	GLN
1	A	463	HIS
1	A	494	ASN
1	B	15	GLN
1	B	18	HIS
1	B	43	ASN
1	B	145	ASN
1	B	183	GLN
1	B	377	GLN
1	B	378	HIS
1	B	463	HIS
1	B	494	ASN
1	C	13	GLN
1	C	15	GLN
1	C	18	HIS
1	C	43	ASN
1	C	145	ASN
1	C	234	GLN
1	C	251	HIS
1	C	263	ASN
1	C	272	ASN
1	C	377	GLN
1	C	378	HIS
1	C	390	HIS
1	C	463	HIS
1	C	494	ASN
1	D	18	HIS
1	D	43	ASN
1	D	145	ASN
1	D	198	ASN
1	D	234	GLN
1	D	377	GLN
1	D	378	HIS
1	D	390	HIS
1	D	403	GLN
1	D	456	HIS
1	D	463	HIS
1	D	494	ASN
1	E	18	HIS
1	E	43	ASN
1	E	83	HIS
1	E	162	ASN

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Mol	Chain	Res	Type
1	E	198	ASN
1	E	234	GLN
1	E	377	GLN
1	E	378	HIS
1	E	390	HIS
1	E	463	HIS
1	E	494	ASN
1	F	15	GLN
1	F	18	HIS
1	F	43	ASN
1	F	145	ASN
1	F	377	GLN
1	F	378	HIS
1	F	390	HIS
1	F	463	HIS
1	F	494	ASN
1	G	18	HIS
1	G	43	ASN
1	G	145	ASN
1	G	263	ASN
1	G	377	GLN
1	G	378	HIS
1	G	403	GLN
1	G	463	HIS
1	G	494	ASN
1	H	15	GLN
1	H	18	HIS
1	H	43	ASN
1	H	145	ASN
1	H	234	GLN
1	H	263	ASN
1	H	377	GLN
1	H	378	HIS
1	H	390	HIS
1	H	403	GLN
1	H	463	HIS
1	H	494	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 102 ligands modelled in this entry, 28 are monoatomic - leaving 74 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	$\# Z > 2$
8	GOL	G	6307	-	5,5,5	0.33	0	5,5,5	0.51	0
8	GOL	B	6007	-	5,5,5	0.33	0	5,5,5	0.33	0
8	GOL	F	6010	-	5,5,5	0.34	0	5,5,5	0.57	0
8	GOL	F	6001	-	5,5,5	0.37	0	5,5,5	0.49	0
8	GOL	G	6207	-	5,5,5	0.31	0	5,5,5	0.28	0
7	EDO	H	6041	-	3,3,3	0.47	0	2,2,2	0.29	0
8	GOL	E	6305	-	5,5,5	0.28	0	5,5,5	0.58	0
7	EDO	E	6045	-	3,3,3	0.40	0	2,2,2	0.32	0
9	ETE	B	6018	-	13,13,13	0.47	0	12,12,12	0.36	0
7	EDO	H	6042	-	3,3,3	0.45	0	2,2,2	0.35	0
7	EDO	E	6015	-	3,3,3	0.43	0	2,2,2	0.47	0
8	GOL	C	6056	-	5,5,5	0.37	0	5,5,5	0.38	0
7	EDO	D	6017	-	3,3,3	0.60	0	2,2,2	0.17	0
7	EDO	B	6013	-	3,3,3	0.48	0	2,2,2	0.37	0
8	GOL	A	6002	-	5,5,5	0.28	0	5,5,5	0.30	0
8	GOL	H	6006	-	5,5,5	0.41	0	5,5,5	0.48	0
6	PYR	C	600	2	2,5,5	2.27	1 (50%)	2,6,6	1.47	1 (50%)
7	EDO	E	6046	-	3,3,3	0.30	0	2,2,2	0.53	0
7	EDO	B	6047	-	3,3,3	0.45	0	2,2,2	0.35	0
7	EDO	G	6052	-	3,3,3	0.45	0	2,2,2	0.36	0
7	EDO	A	6043	-	3,3,3	0.46	0	2,2,2	0.36	0
8	GOL	H	6208	-	5,5,5	0.21	0	5,5,5	0.61	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	EDO	D	6011	-	3,3,3	0.52	0	2,2,2	0.32	0
6	PYR	B	600	2	2,5,5	1.93	1 (50%)	2,6,6	1.15	0
8	GOL	H	6008	-	5,5,5	0.30	0	5,5,5	0.35	0
7	EDO	B	6048	-	3,3,3	0.48	0	2,2,2	0.29	0
7	EDO	H	6037	-	3,3,3	0.48	0	2,2,2	0.17	0
8	GOL	B	6202	-	5,5,5	0.31	0	5,5,5	0.34	0
8	GOL	F	6306	-	5,5,5	0.31	0	5,5,5	0.64	0
6	PYR	H	600	2	2,5,5	2.31	1 (50%)	2,6,6	1.69	1 (50%)
8	GOL	C	6055	-	5,5,5	0.34	0	5,5,5	0.69	0
8	GOL	A	6201	-	5,5,5	0.29	0	5,5,5	0.54	0
8	GOL	E	6031	-	5,5,5	0.45	0	5,5,5	0.34	0
7	EDO	H	6053	-	3,3,3	0.45	0	2,2,2	0.32	0
8	GOL	G	6004	-	5,5,5	0.33	0	5,5,5	0.41	0
7	EDO	E	6039	-	3,3,3	0.47	0	2,2,2	0.31	0
7	EDO	F	6012	-	3,3,3	0.55	0	2,2,2	0.37	0
8	GOL	D	6204	-	5,5,5	0.27	0	5,5,5	0.58	0
8	GOL	D	6304	-	5,5,5	0.32	0	5,5,5	0.80	0
7	EDO	H	6054	-	3,3,3	0.41	0	2,2,2	0.45	0
7	EDO	H	6034	-	3,3,3	0.57	0	2,2,2	0.05	0
8	GOL	F	6057	-	5,5,5	0.37	0	5,5,5	0.24	0
8	GOL	F	6206	-	5,5,5	0.28	0	5,5,5	0.57	0
7	EDO	D	6040	-	3,3,3	0.50	0	2,2,2	0.28	0
6	PYR	E	600	2	2,5,5	2.14	1 (50%)	2,6,6	1.51	1 (50%)
6	PYR	D	600	2	2,5,5	2.26	1 (50%)	2,6,6	1.82	1 (50%)
7	EDO	E	6038	-	3,3,3	0.61	0	2,2,2	0.06	0
7	EDO	C	6014	-	3,3,3	0.48	0	2,2,2	0.43	0
8	GOL	E	6205	-	5,5,5	0.33	0	5,5,5	0.44	0
6	PYR	F	600	2	2,5,5	2.04	1 (50%)	2,6,6	1.31	0
8	GOL	C	6303	-	5,5,5	0.29	0	5,5,5	0.68	0
7	EDO	A	6050	-	3,3,3	0.48	0	2,2,2	0.15	0
7	EDO	F	6036	-	3,3,3	0.51	0	2,2,2	0.16	0
7	EDO	G	6016	-	3,3,3	0.48	0	2,2,2	0.32	0
8	GOL	H	6308	-	5,5,5	0.34	0	5,5,5	0.87	0
7	EDO	A	6051	-	3,3,3	0.42	0	2,2,2	0.34	0
7	EDO	D	6033	-	3,3,3	0.48	0	2,2,2	0.30	0
7	EDO	E	6049	-	3,3,3	0.47	0	2,2,2	0.28	0
6	PYR	A	600	2	2,5,5	2.07	1 (50%)	2,6,6	1.51	1 (50%)
8	GOL	C	6203	-	5,5,5	0.31	0	5,5,5	0.27	0
7	EDO	B	6032	-	3,3,3	0.27	0	2,2,2	0.77	0
8	GOL	A	6301	-	5,5,5	0.32	0	5,5,5	0.67	0
8	GOL	F	6005	-	5,5,5	0.27	0	5,5,5	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	PYR	G	600	2	2,5,5	2.09	1 (50%)	2,6,6	1.05	0
8	GOL	B	6302	-	5,5,5	0.33	0	5,5,5	0.54	0
7	EDO	C	6044	-	3,3,3	0.46	0	2,2,2	0.46	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
8	GOL	G	6307	-	-	2/4/4/4	-
8	GOL	B	6007	-	-	2/4/4/4	-
8	GOL	F	6010	-	-	2/4/4/4	-
8	GOL	F	6001	-	-	2/4/4/4	-
8	GOL	G	6207	-	-	2/4/4/4	-
7	EDO	H	6041	-	-	0/1/1/1	-
8	GOL	E	6305	-	-	1/4/4/4	-
7	EDO	E	6045	-	-	0/1/1/1	-
9	ETE	B	6018	-	-	7/11/11/11	-
7	EDO	H	6042	-	-	0/1/1/1	-
7	EDO	E	6015	-	-	0/1/1/1	-
8	GOL	C	6056	-	-	4/4/4/4	-
7	EDO	D	6017	-	-	0/1/1/1	-
7	EDO	B	6013	-	-	1/1/1/1	-
8	GOL	A	6002	-	-	4/4/4/4	-
8	GOL	H	6006	-	-	4/4/4/4	-
6	PYR	C	600	2	-	0/0/4/4	-
7	EDO	E	6046	-	-	1/1/1/1	-
7	EDO	B	6047	-	-	0/1/1/1	-
7	EDO	G	6052	-	-	1/1/1/1	-
7	EDO	A	6043	-	-	1/1/1/1	-
8	GOL	H	6208	-	-	3/4/4/4	-
7	EDO	D	6011	-	-	1/1/1/1	-
6	PYR	B	600	2	-	0/0/4/4	-
8	GOL	H	6008	-	-	4/4/4/4	-
7	EDO	B	6048	-	-	0/1/1/1	-
7	EDO	H	6037	-	-	1/1/1/1	-
8	GOL	B	6202	-	-	0/4/4/4	-
8	GOL	F	6306	-	-	1/4/4/4	-
6	PYR	H	600	2	-	0/0/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	GOL	C	6055	-	-	3/4/4/4	-
8	GOL	A	6201	-	-	1/4/4/4	-
8	GOL	E	6031	-	-	3/4/4/4	-
7	EDO	H	6053	-	-	1/1/1/1	-
8	GOL	G	6004	-	-	2/4/4/4	-
7	EDO	E	6039	-	-	1/1/1/1	-
7	EDO	F	6012	-	-	0/1/1/1	-
8	GOL	D	6204	-	-	3/4/4/4	-
8	GOL	D	6304	-	-	1/4/4/4	-
7	EDO	H	6054	-	-	1/1/1/1	-
7	EDO	H	6034	-	-	1/1/1/1	-
8	GOL	F	6057	-	-	2/4/4/4	-
8	GOL	F	6206	-	-	4/4/4/4	-
7	EDO	D	6040	-	-	1/1/1/1	-
6	PYR	E	600	2	-	0/0/4/4	-
6	PYR	D	600	2	-	0/0/4/4	-
7	EDO	E	6038	-	-	0/1/1/1	-
7	EDO	C	6014	-	-	1/1/1/1	-
8	GOL	E	6205	-	-	0/4/4/4	-
6	PYR	F	600	2	-	0/0/4/4	-
8	GOL	C	6303	-	-	2/4/4/4	-
7	EDO	A	6050	-	-	0/1/1/1	-
7	EDO	F	6036	-	-	1/1/1/1	-
7	EDO	G	6016	-	-	1/1/1/1	-
8	GOL	H	6308	-	-	2/4/4/4	-
7	EDO	A	6051	-	-	1/1/1/1	-
7	EDO	D	6033	-	-	0/1/1/1	-
7	EDO	E	6049	-	-	0/1/1/1	-
6	PYR	A	600	2	-	0/0/4/4	-
8	GOL	C	6203	-	-	2/4/4/4	-
7	EDO	B	6032	-	-	1/1/1/1	-
8	GOL	A	6301	-	-	2/4/4/4	-
8	GOL	F	6005	-	-	4/4/4/4	-
6	PYR	G	600	2	-	0/0/4/4	-
8	GOL	B	6302	-	-	2/4/4/4	-
7	EDO	C	6044	-	-	0/1/1/1	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	600	PYR	O3-C2	3.24	1.32	1.22
6	C	600	PYR	O3-C2	3.14	1.32	1.22
6	D	600	PYR	O3-C2	3.09	1.32	1.22
6	E	600	PYR	O3-C2	2.98	1.32	1.22
6	G	600	PYR	O3-C2	2.90	1.31	1.22
6	F	600	PYR	O3-C2	2.87	1.31	1.22
6	A	600	PYR	O3-C2	2.84	1.31	1.22
6	B	600	PYR	O3-C2	2.69	1.31	1.22

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	600	PYR	O3-C2-C3	2.53	125.87	120.17
6	H	600	PYR	O3-C2-C3	2.39	125.55	120.17
6	E	600	PYR	O3-C2-C3	2.07	124.83	120.17
6	C	600	PYR	O3-C2-C3	2.05	124.79	120.17
6	A	600	PYR	O3-C2-C3	2.04	124.77	120.17

There are no chirality outliers.

All (87) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	6002	GOL	O1-C1-C2-C3
8	A	6002	GOL	C1-C2-C3-O3
8	F	6005	GOL	O1-C1-C2-C3
8	F	6005	GOL	C1-C2-C3-O3
8	H	6006	GOL	C1-C2-C3-O3
8	C	6203	GOL	C1-C2-C3-O3
8	B	6007	GOL	O1-C1-C2-C3
8	C	6056	GOL	C1-C2-C3-O3
8	H	6208	GOL	O1-C1-C2-C3
8	E	6031	GOL	C1-C2-C3-O3
8	D	6204	GOL	C1-C2-C3-O3
8	H	6006	GOL	O2-C2-C3-O3
8	C	6055	GOL	C1-C2-C3-O3
8	C	6303	GOL	C1-C2-C3-O3
8	H	6006	GOL	O1-C1-C2-C3
8	F	6306	GOL	O1-C1-C2-C3
8	G	6307	GOL	C1-C2-C3-O3
8	H	6308	GOL	C1-C2-C3-O3
8	B	6302	GOL	O1-C1-C2-C3
8	A	6301	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
8	F	6001	GOL	O1-C1-C2-C3
8	C	6056	GOL	O1-C1-C2-C3
8	D	6304	GOL	C1-C2-C3-O3
8	F	6057	GOL	C1-C2-C3-O3
9	B	6018	ETE	OH4-C13-C23-OH3
8	C	6055	GOL	O2-C2-C3-O3
8	B	6007	GOL	O1-C1-C2-O2
8	C	6056	GOL	O2-C2-C3-O3
8	D	6204	GOL	O2-C2-C3-O3
7	C	6014	EDO	O1-C1-C2-O2
7	G	6016	EDO	O1-C1-C2-O2
7	E	6046	EDO	O1-C1-C2-O2
8	A	6002	GOL	O1-C1-C2-O2
8	A	6002	GOL	O2-C2-C3-O3
8	F	6005	GOL	O1-C1-C2-O2
8	F	6005	GOL	O2-C2-C3-O3
8	C	6203	GOL	O2-C2-C3-O3
8	F	6001	GOL	O1-C1-C2-O2
8	H	6208	GOL	O1-C1-C2-O2
9	B	6018	ETE	OH5-C14-C24-OH4
7	G	6052	EDO	O1-C1-C2-O2
9	B	6018	ETE	OH6-C15-C25-OH5
8	F	6206	GOL	O2-C2-C3-O3
8	G	6004	GOL	O2-C2-C3-O3
8	H	6308	GOL	O2-C2-C3-O3
7	B	6032	EDO	O1-C1-C2-O2
9	B	6018	ETE	C14-C24-OH4-C13
8	H	6008	GOL	O1-C1-C2-O2
8	H	6008	GOL	O2-C2-C3-O3
8	F	6206	GOL	O1-C1-C2-O2
8	C	6055	GOL	O1-C1-C2-O2
8	C	6303	GOL	O2-C2-C3-O3
8	F	6010	GOL	O2-C2-C3-O3
8	G	6207	GOL	O2-C2-C3-O3
8	G	6307	GOL	O2-C2-C3-O3
8	B	6302	GOL	O1-C1-C2-O2
8	A	6301	GOL	O1-C1-C2-O2
8	C	6056	GOL	O1-C1-C2-O2
8	H	6208	GOL	O2-C2-C3-O3
8	E	6031	GOL	O2-C2-C3-O3
8	D	6204	GOL	O1-C1-C2-O2
8	H	6008	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
7	H	6053	EDO	O1-C1-C2-O2
9	B	6018	ETE	C23-C13-OH4-C24
9	B	6018	ETE	C24-C14-OH5-C25
7	D	6040	EDO	O1-C1-C2-O2
7	H	6054	EDO	O1-C1-C2-O2
8	E	6305	GOL	O1-C1-C2-C3
8	E	6031	GOL	O1-C1-C2-C3
8	H	6006	GOL	O1-C1-C2-O2
7	B	6013	EDO	O1-C1-C2-O2
7	H	6037	EDO	O1-C1-C2-O2
9	B	6018	ETE	C25-C15-OH6-C26
7	A	6043	EDO	O1-C1-C2-O2
8	H	6008	GOL	O1-C1-C2-C3
8	F	6206	GOL	C1-C2-C3-O3
8	G	6207	GOL	C1-C2-C3-O3
8	G	6004	GOL	C1-C2-C3-O3
7	F	6036	EDO	O1-C1-C2-O2
7	H	6034	EDO	O1-C1-C2-O2
7	D	6011	EDO	O1-C1-C2-O2
7	A	6051	EDO	O1-C1-C2-O2
8	A	6201	GOL	O2-C2-C3-O3
8	F	6057	GOL	O2-C2-C3-O3
8	F	6206	GOL	O1-C1-C2-C3
8	F	6010	GOL	C1-C2-C3-O3
7	E	6039	EDO	O1-C1-C2-O2

There are no ring outliers.

18 monomers are involved in 39 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	F	6010	GOL	2	0
8	F	6001	GOL	1	0
7	E	6045	EDO	2	0
9	B	6018	ETE	8	0
7	D	6017	EDO	4	0
8	A	6002	GOL	1	0
8	H	6006	GOL	2	0
7	E	6046	EDO	2	0
8	H	6008	GOL	1	0
8	C	6055	GOL	1	0
8	E	6031	GOL	2	0
7	H	6054	EDO	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	H	6034	EDO	2	0
7	E	6038	EDO	3	0
7	F	6036	EDO	2	0
7	B	6032	EDO	3	0
8	F	6005	GOL	1	0
7	C	6044	EDO	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	519/530 (97%)	-0.49	8 (1%) 73 77	7, 10, 17, 26	1 (0%)
1	B	511/530 (96%)	-0.15	34 (6%) 17 16	7, 11, 41, 63	0
1	C	512/530 (96%)	0.01	23 (4%) 33 32	7, 10, 25, 31	0
1	D	521/530 (98%)	-0.47	8 (1%) 73 77	5, 10, 18, 26	0
1	E	521/530 (98%)	-0.47	6 (1%) 79 81	5, 10, 18, 25	0
1	F	515/530 (97%)	0.02	21 (4%) 37 37	7, 10, 24, 34	0
1	G	510/530 (96%)	-0.10	41 (8%) 12 12	7, 11, 36, 43	0
1	H	519/530 (97%)	-0.47	7 (1%) 77 80	6, 11, 18, 29	0
All	All	4128/4240 (97%)	-0.27	148 (3%) 42 43	5, 10, 25, 63	1 (0%)

All (148) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	201	PHE	9.7
1	F	129	ALA	6.7
1	G	191	PHE	6.7
1	G	155	ILE	6.7
1	H	11	PHE	6.5
1	F	11	PHE	6.4
1	G	201	PHE	6.4
1	D	189	PRO	6.1
1	C	201	PHE	5.9
1	G	11	PHE	5.6
1	G	147	TYR	5.5
1	B	191	PHE	5.4
1	B	155	ILE	5.3
1	C	191	PHE	5.2
1	F	201	PHE	5.1
1	G	151	CYS	4.9

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Mol	Chain	Res	Type	RSRZ
1	F	147	TYR	4.9
1	G	186	GLN	4.8
1	B	122	LEU	4.7
1	F	133	LEU	4.7
1	G	131	VAL	4.6
1	C	129	ALA	4.5
1	E	10	ALA	4.5
1	B	133	LEU	4.4
1	A	191	PHE	4.4
1	B	129	ALA	4.4
1	B	11	PHE	4.4
1	C	133	LEU	4.3
1	G	133	LEU	4.3
1	A	189	PRO	4.3
1	B	131	VAL	4.3
1	B	202	LEU	4.2
1	D	128	THR	4.1
1	B	192	LEU	4.1
1	C	155	ILE	4.0
1	F	155	ILE	4.0
1	C	122	LEU	3.9
1	F	191	PHE	3.8
1	A	188	GLY	3.8
1	G	134	LYS	3.8
1	G	150	LYS	3.7
1	B	151	CYS	3.7
1	F	151	CYS	3.6
1	H	191	PHE	3.6
1	E	128	THR	3.5
1	F	123	ILE	3.5
1	E	189	PRO	3.5
1	G	122	LEU	3.5
1	C	190	ASP	3.4
1	G	192	LEU	3.4
1	H	190	ASP	3.4
1	G	139	LEU	3.4
1	B	147	TYR	3.3
1	B	166	VAL	3.3
1	A	190	ASP	3.3
1	C	147	TYR	3.3
1	B	186	GLN	3.2
1	C	186	GLN	3.2

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Mol	Chain	Res	Type	RSRZ
1	F	12	ILE	3.2
1	G	166	VAL	3.2
1	G	164	CYS	3.2
1	C	123	ILE	3.1
1	A	127	GLY	3.1
1	B	142	THR	3.1
1	D	126	SER	3.1
1	H	188	GLY	3.1
1	G	156	LEU	3.1
1	G	135	LYS	3.0
1	C	202	LEU	3.0
1	B	139	LEU	3.0
1	B	198	ASN	2.9
1	D	190	ASP	2.9
1	C	170	GLY	2.9
1	G	138	THR	2.9
1	G	184	VAL	2.8
1	H	128	THR	2.8
1	A	12	ILE	2.8
1	G	141	ILE	2.8
1	B	164	CYS	2.8
1	G	194	THR	2.7
1	B	184	VAL	2.7
1	G	185	LYS	2.7
1	F	131	VAL	2.7
1	F	128	THR	2.7
1	D	188	GLY	2.6
1	F	186	GLN	2.6
1	G	140	LYS	2.6
1	G	193	VAL	2.6
1	B	130	GLU	2.6
1	B	143	LEU	2.6
1	C	198	ASN	2.6
1	B	152	ASP	2.5
1	B	196	VAL	2.5
1	G	197	GLU	2.5
1	B	150	LYS	2.5
1	B	138	THR	2.5
1	G	167	VAL	2.5
1	G	182	LEU	2.5
1	C	12	ILE	2.4
1	C	184	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	202	LEU	2.4
1	F	190	ASP	2.4
1	F	169	VAL	2.4
1	C	192	LEU	2.4
1	G	198	ASN	2.3
1	B	194	THR	2.3
1	B	195	GLU	2.3
1	B	530	PRO	2.3
1	G	142	THR	2.3
1	E	11	PHE	2.3
1	G	203	GLY	2.3
1	G	196	VAL	2.2
1	D	10	ALA	2.2
1	B	132	GLU	2.2
1	B	197	GLU	2.2
1	F	197	GLU	2.2
1	G	169	VAL	2.2
1	D	127	GLY	2.2
1	G	152	ASP	2.2
1	B	170	GLY	2.2
1	B	134	LYS	2.2
1	F	140	LYS	2.2
1	C	214	ALA	2.2
1	F	198	ASN	2.1
1	B	185	LYS	2.1
1	C	139	LEU	2.1
1	E	190	ASP	2.1
1	D	212	GLY	2.1
1	C	183	GLN	2.1
1	C	194	THR	2.1
1	F	153	GLU	2.1
1	E	127	GLY	2.1
1	G	157	TRP	2.1
1	G	214	ALA	2.1
1	G	148	MET	2.1
1	H	127	GLY	2.1
1	C	154	ASN	2.1
1	G	153	GLU	2.1
1	C	151	CYS	2.1
1	G	99	SER	2.1
1	C	146	ALA	2.0
1	A	167[A]	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	126	SER	2.0
1	H	126	SER	2.0
1	G	154	ASN	2.0
1	B	135	LYS	2.0
1	F	156	LEU	2.0
1	F	170	GLY	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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	EDO	D	6040	4/4	0.68	0.26	40,41,42,43	0
8	GOL	F	6010	6/6	0.69	0.24	47,48,49,49	0
7	EDO	A	6043	4/4	0.71	0.21	67,68,68,68	0
8	GOL	G	6307	6/6	0.72	0.32	35,37,38,38	0
8	GOL	F	6005	6/6	0.74	0.19	23,33,34,35	0
8	GOL	G	6004	6/6	0.74	0.38	49,51,51,52	0
8	GOL	B	6007	6/6	0.74	0.26	35,40,41,42	0
7	EDO	H	6054	4/4	0.74	0.28	34,34,36,37	0
7	EDO	B	6048	4/4	0.76	0.20	51,51,51,51	0
7	EDO	D	6017	4/4	0.76	0.23	26,28,30,31	0
8	GOL	F	6001	6/6	0.77	0.24	32,35,37,38	0
7	EDO	D	6033	4/4	0.78	0.14	53,53,53,53	0
8	GOL	H	6006	6/6	0.79	0.23	39,43,44,46	0
9	ETE	B	6018	14/14	0.79	0.26	35,40,43,44	0
8	GOL	H	6008	6/6	0.79	0.28	30,37,38,39	0
8	GOL	A	6002	6/6	0.79	0.21	29,36,38,38	0
8	GOL	B	6302	6/6	0.79	0.26	36,38,38,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	GOL	F	6306	6/6	0.81	0.19	23,30,30,30	0
7	EDO	C	6044	4/4	0.82	0.15	35,37,38,39	0
7	EDO	F	6036	4/4	0.83	0.14	33,33,35,36	0
8	GOL	G	6207	6/6	0.83	0.17	39,40,41,41	0
8	GOL	C	6056	6/6	0.83	0.19	42,44,44,44	0
8	GOL	C	6303	6/6	0.83	0.18	23,29,29,30	0
8	GOL	F	6206	6/6	0.84	0.15	22,28,29,29	0
7	EDO	H	6053	4/4	0.84	0.23	37,40,41,43	0
8	GOL	F	6057	6/6	0.84	0.20	67,67,67,67	0
8	GOL	A	6301	6/6	0.84	0.20	18,27,28,31	0
7	EDO	E	6038	4/4	0.85	0.21	27,28,30,31	0
8	GOL	C	6203	6/6	0.85	0.16	26,31,31,33	0
8	GOL	C	6055	6/6	0.86	0.19	21,25,29,31	0
7	EDO	B	6047	4/4	0.86	0.11	42,44,44,45	0
8	GOL	H	6208	6/6	0.86	0.14	23,28,29,30	0
7	EDO	G	6052	4/4	0.87	0.14	36,39,39,40	0
8	GOL	H	6308	6/6	0.87	0.17	18,27,28,30	0
8	GOL	B	6202	6/6	0.87	0.14	35,37,37,38	0
7	EDO	E	6039	4/4	0.87	0.13	49,49,49,50	0
8	GOL	E	6305	6/6	0.88	0.18	17,25,26,28	0
7	EDO	H	6041	4/4	0.88	0.10	46,46,46,47	0
8	GOL	D	6304	6/6	0.88	0.20	20,27,28,30	0
7	EDO	E	6049	4/4	0.89	0.12	30,34,35,37	0
7	EDO	H	6037	4/4	0.89	0.09	34,35,35,37	0
7	EDO	F	6012	4/4	0.89	0.15	27,29,30,30	0
8	GOL	E	6031	6/6	0.90	0.28	36,37,37,38	0
7	EDO	H	6042	4/4	0.90	0.09	42,42,43,44	0
8	GOL	A	6201	6/6	0.90	0.12	17,23,24,25	0
7	EDO	H	6034	4/4	0.90	0.15	28,28,29,30	0
7	EDO	E	6015	4/4	0.90	0.15	35,37,38,38	0
6	PYR	G	600	6/6	0.90	0.18	11,11,15,15	0
7	EDO	A	6051	4/4	0.90	0.23	40,42,42,42	0
7	EDO	C	6014	4/4	0.91	0.10	29,31,31,33	0
8	GOL	D	6204	6/6	0.92	0.11	19,27,27,27	0
6	PYR	B	600	6/6	0.92	0.13	10,12,14,14	0
7	EDO	B	6032	4/4	0.92	0.20	23,23,24,27	0
7	EDO	E	6046	4/4	0.92	0.28	25,29,30,32	0
7	EDO	G	6016	4/4	0.92	0.18	29,32,32,34	0
7	EDO	B	6013	4/4	0.92	0.13	32,34,35,36	0
8	GOL	E	6205	6/6	0.93	0.11	18,23,24,25	0
7	EDO	A	6050	4/4	0.93	0.09	28,32,32,35	0
5	ALA	G	6107	6/6	0.94	0.11	10,10,10,11	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	PYR	D	600	6/6	0.94	0.10	8,9,11,12	0
7	EDO	E	6045	4/4	0.94	0.26	33,34,34,34	0
5	ALA	D	6104	6/6	0.94	0.09	11,12,12,12	0
6	PYR	A	600	6/6	0.95	0.12	6,7,9,9	0
7	EDO	D	6011	4/4	0.95	0.09	28,30,31,32	0
6	PYR	E	600	6/6	0.95	0.10	6,9,11,12	0
6	PYR	F	600	6/6	0.95	0.09	5,6,9,10	0
6	PYR	H	600	6/6	0.95	0.11	5,8,9,9	0
5	ALA	C	6103	6/6	0.96	0.07	9,11,11,11	0
6	PYR	C	600	6/6	0.96	0.07	9,9,10,10	0
4	NA	D	6020	1/1	0.97	0.04	23,23,23,23	0
5	ALA	B	6102	6/6	0.97	0.07	11,12,12,12	0
5	ALA	F	6106	6/6	0.97	0.06	8,10,10,10	0
5	ALA	E	6105	6/6	0.97	0.08	11,12,12,12	0
3	K	G	6507	1/1	0.97	0.05	22,22,22,22	0
5	ALA	A	6101	6/6	0.97	0.07	9,10,10,11	0
4	NA	D	6026	1/1	0.98	0.08	19,19,19,19	0
4	NA	A	6019	1/1	0.98	0.05	21,21,21,21	0
4	NA	H	6022	1/1	0.98	0.05	21,21,21,21	0
2	MN	G	640	1/1	0.98	0.03	18,18,18,18	0
5	ALA	H	6108	6/6	0.98	0.08	10,11,11,11	0
4	NA	E	6021	1/1	0.98	0.05	21,21,21,21	0
2	MN	B	640	1/1	0.98	0.04	14,14,14,14	0
3	K	D	6504	1/1	0.99	0.02	14,14,14,14	0
3	K	H	6508	1/1	0.99	0.03	14,14,14,14	0
3	K	B	6502	1/1	0.99	0.04	18,18,18,18	0
4	NA	B	6024	1/1	0.99	0.06	21,21,21,21	0
4	NA	G	6028	1/1	0.99	0.04	21,21,21,21	0
3	K	E	6505	1/1	0.99	0.02	13,13,13,13	0
4	NA	E	6030	1/1	0.99	0.11	16,16,16,16	0
4	NA	C	6025	1/1	0.99	0.08	18,18,18,18	0
4	NA	A	6023	1/1	0.99	0.06	14,14,14,14	0
4	NA	F	6027	1/1	0.99	0.12	17,17,17,17	0
4	NA	H	6029	1/1	0.99	0.07	20,20,20,20	0
3	K	C	6503	1/1	1.00	0.03	13,13,13,13	0
3	K	A	6501	1/1	1.00	0.02	14,14,14,14	0
2	MN	F	640	1/1	1.00	0.02	10,10,10,10	0
2	MN	C	640	1/1	1.00	0.02	10,10,10,10	0
2	MN	E	640	1/1	1.00	0.02	11,11,11,11	0
2	MN	D	640	1/1	1.00	0.02	11,11,11,11	0
2	MN	A	640	1/1	1.00	0.01	10,10,10,10	0
3	K	F	6506	1/1	1.00	0.02	13,13,13,13	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MN	H	640	1/1	1.00	0.02	11,11,11,11	0

6.5 Other polymers [i](#)

There are no such residues in this entry.