



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 26, 2017 – 07:37 PM EDT

PDB ID : 5GUD
Title : Glutamate dehydrogenase from *Corynebacterium glutamicum* (alpha-iminoglutarate/NADP+ complex)
Authors : Tomita, T.; Nishiyama, M.
Deposited on : 2016-08-28
Resolution : 1.68 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029077
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029077

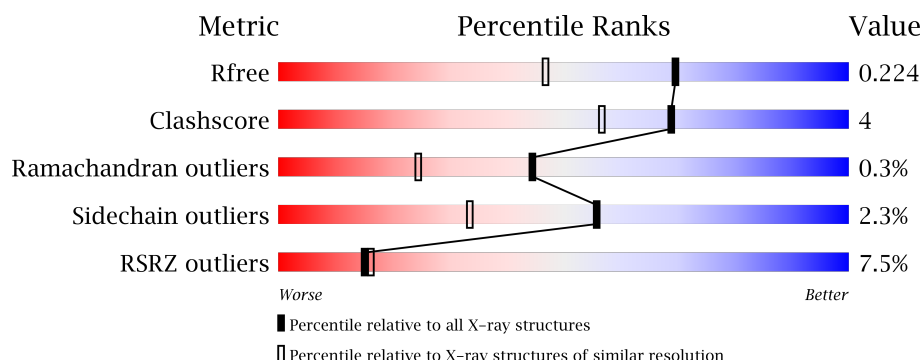
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.68 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	5252 (1.70-1.66)
Clashscore	112137	5803 (1.70-1.66)
Ramachandran outliers	110173	5704 (1.70-1.66)
Sidechain outliers	110143	5703 (1.70-1.66)
RSRZ outliers	101464	5298 (1.70-1.66)

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. 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	471	<div> <div>2%</div> <div>87%</div> <div>7%</div> <div>5%</div> </div>
1	B	471	<div> <div>18%</div> <div>81%</div> <div>12%</div> <div>5%</div> </div>
1	C	471	<div> <div>6%</div> <div>86%</div> <div>9%</div> <div>5%</div> </div>
1	D	471	<div> <div>10%</div> <div>85%</div> <div>9%</div> <div>5%</div> </div>
1	E	471	<div> <div>3%</div> <div>90%</div> <div>7%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	471	<div><div></div><div>3%</div><div>87%</div><div>7%</div><div>5%</div></div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 23954 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 Glutamate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	447	Total	C	N	O	S	0	0	0
			3449	2167	605	660	17			
1	B	446	Total	C	N	O	S	0	0	0
			3441	2162	604	659	16			
1	C	447	Total	C	N	O	S	0	1	0
			3458	2175	605	661	17			
1	D	447	Total	C	N	O	S	0	2	0
			3461	2176	607	661	17			
1	E	460	Total	C	N	O	S	0	3	0
			3559	2237	627	678	17			
1	F	447	Total	C	N	O	S	0	2	0
			3463	2177	609	660	17			

There are 156 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-23	MET	-	expression tag	UNP A0A0U4QBJ6
A	-22	LYS	-	expression tag	UNP A0A0U4QBJ6
A	-21	HIS	-	expression tag	UNP A0A0U4QBJ6
A	-20	HIS	-	expression tag	UNP A0A0U4QBJ6
A	-19	HIS	-	expression tag	UNP A0A0U4QBJ6
A	-18	HIS	-	expression tag	UNP A0A0U4QBJ6
A	-17	HIS	-	expression tag	UNP A0A0U4QBJ6
A	-16	HIS	-	expression tag	UNP A0A0U4QBJ6
A	-15	HIS	-	expression tag	UNP A0A0U4QBJ6
A	-14	HIS	-	expression tag	UNP A0A0U4QBJ6
A	-13	GLY	-	expression tag	UNP A0A0U4QBJ6
A	-12	GLY	-	expression tag	UNP A0A0U4QBJ6
A	-11	LEU	-	expression tag	UNP A0A0U4QBJ6
A	-10	VAL	-	expression tag	UNP A0A0U4QBJ6
A	-9	PRO	-	expression tag	UNP A0A0U4QBJ6
A	-8	ARG	-	expression tag	UNP A0A0U4QBJ6
A	-7	GLY	-	expression tag	UNP A0A0U4QBJ6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	SER	-	expression tag	UNP A0A0U4QBJ6
A	-5	HIS	-	expression tag	UNP A0A0U4QBJ6
A	-4	GLY	-	expression tag	UNP A0A0U4QBJ6
A	-3	GLY	-	expression tag	UNP A0A0U4QBJ6
A	-2	SER	-	expression tag	UNP A0A0U4QBJ6
A	-1	GLU	-	expression tag	UNP A0A0U4QBJ6
A	0	PHE	-	expression tag	UNP A0A0U4QBJ6
A	298	ILE	VAL	conflict	UNP A0A0U4QBJ6
A	299	GLU	ASP	conflict	UNP A0A0U4QBJ6
B	-23	MET	-	expression tag	UNP A0A0U4QBJ6
B	-22	LYS	-	expression tag	UNP A0A0U4QBJ6
B	-21	HIS	-	expression tag	UNP A0A0U4QBJ6
B	-20	HIS	-	expression tag	UNP A0A0U4QBJ6
B	-19	HIS	-	expression tag	UNP A0A0U4QBJ6
B	-18	HIS	-	expression tag	UNP A0A0U4QBJ6
B	-17	HIS	-	expression tag	UNP A0A0U4QBJ6
B	-16	HIS	-	expression tag	UNP A0A0U4QBJ6
B	-15	HIS	-	expression tag	UNP A0A0U4QBJ6
B	-14	HIS	-	expression tag	UNP A0A0U4QBJ6
B	-13	GLY	-	expression tag	UNP A0A0U4QBJ6
B	-12	GLY	-	expression tag	UNP A0A0U4QBJ6
B	-11	LEU	-	expression tag	UNP A0A0U4QBJ6
B	-10	VAL	-	expression tag	UNP A0A0U4QBJ6
B	-9	PRO	-	expression tag	UNP A0A0U4QBJ6
B	-8	ARG	-	expression tag	UNP A0A0U4QBJ6
B	-7	GLY	-	expression tag	UNP A0A0U4QBJ6
B	-6	SER	-	expression tag	UNP A0A0U4QBJ6
B	-5	HIS	-	expression tag	UNP A0A0U4QBJ6
B	-4	GLY	-	expression tag	UNP A0A0U4QBJ6
B	-3	GLY	-	expression tag	UNP A0A0U4QBJ6
B	-2	SER	-	expression tag	UNP A0A0U4QBJ6
B	-1	GLU	-	expression tag	UNP A0A0U4QBJ6
B	0	PHE	-	expression tag	UNP A0A0U4QBJ6
B	298	ILE	VAL	conflict	UNP A0A0U4QBJ6
B	299	GLU	ASP	conflict	UNP A0A0U4QBJ6
C	-23	MET	-	expression tag	UNP A0A0U4QBJ6
C	-22	LYS	-	expression tag	UNP A0A0U4QBJ6
C	-21	HIS	-	expression tag	UNP A0A0U4QBJ6
C	-20	HIS	-	expression tag	UNP A0A0U4QBJ6
C	-19	HIS	-	expression tag	UNP A0A0U4QBJ6
C	-18	HIS	-	expression tag	UNP A0A0U4QBJ6
C	-17	HIS	-	expression tag	UNP A0A0U4QBJ6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-16	HIS	-	expression tag	UNP A0A0U4QBJ6
C	-15	HIS	-	expression tag	UNP A0A0U4QBJ6
C	-14	HIS	-	expression tag	UNP A0A0U4QBJ6
C	-13	GLY	-	expression tag	UNP A0A0U4QBJ6
C	-12	GLY	-	expression tag	UNP A0A0U4QBJ6
C	-11	LEU	-	expression tag	UNP A0A0U4QBJ6
C	-10	VAL	-	expression tag	UNP A0A0U4QBJ6
C	-9	PRO	-	expression tag	UNP A0A0U4QBJ6
C	-8	ARG	-	expression tag	UNP A0A0U4QBJ6
C	-7	GLY	-	expression tag	UNP A0A0U4QBJ6
C	-6	SER	-	expression tag	UNP A0A0U4QBJ6
C	-5	HIS	-	expression tag	UNP A0A0U4QBJ6
C	-4	GLY	-	expression tag	UNP A0A0U4QBJ6
C	-3	GLY	-	expression tag	UNP A0A0U4QBJ6
C	-2	SER	-	expression tag	UNP A0A0U4QBJ6
C	-1	GLU	-	expression tag	UNP A0A0U4QBJ6
C	0	PHE	-	expression tag	UNP A0A0U4QBJ6
C	298	ILE	VAL	conflict	UNP A0A0U4QBJ6
C	299	GLU	ASP	conflict	UNP A0A0U4QBJ6
D	-23	MET	-	expression tag	UNP A0A0U4QBJ6
D	-22	LYS	-	expression tag	UNP A0A0U4QBJ6
D	-21	HIS	-	expression tag	UNP A0A0U4QBJ6
D	-20	HIS	-	expression tag	UNP A0A0U4QBJ6
D	-19	HIS	-	expression tag	UNP A0A0U4QBJ6
D	-18	HIS	-	expression tag	UNP A0A0U4QBJ6
D	-17	HIS	-	expression tag	UNP A0A0U4QBJ6
D	-16	HIS	-	expression tag	UNP A0A0U4QBJ6
D	-15	HIS	-	expression tag	UNP A0A0U4QBJ6
D	-14	HIS	-	expression tag	UNP A0A0U4QBJ6
D	-13	GLY	-	expression tag	UNP A0A0U4QBJ6
D	-12	GLY	-	expression tag	UNP A0A0U4QBJ6
D	-11	LEU	-	expression tag	UNP A0A0U4QBJ6
D	-10	VAL	-	expression tag	UNP A0A0U4QBJ6
D	-9	PRO	-	expression tag	UNP A0A0U4QBJ6
D	-8	ARG	-	expression tag	UNP A0A0U4QBJ6
D	-7	GLY	-	expression tag	UNP A0A0U4QBJ6
D	-6	SER	-	expression tag	UNP A0A0U4QBJ6
D	-5	HIS	-	expression tag	UNP A0A0U4QBJ6
D	-4	GLY	-	expression tag	UNP A0A0U4QBJ6
D	-3	GLY	-	expression tag	UNP A0A0U4QBJ6
D	-2	SER	-	expression tag	UNP A0A0U4QBJ6
D	-1	GLU	-	expression tag	UNP A0A0U4QBJ6

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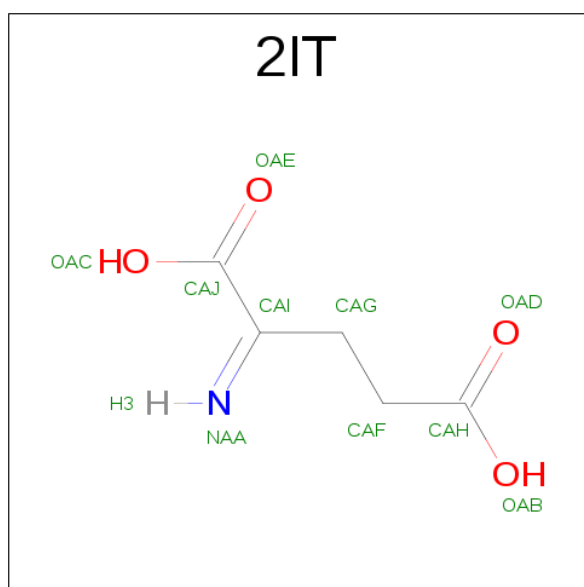
Chain	Residue	Modelled	Actual	Comment	Reference
D	0	PHE	-	expression tag	UNP A0A0U4QBJ6
D	298	ILE	VAL	conflict	UNP A0A0U4QBJ6
D	299	GLU	ASP	conflict	UNP A0A0U4QBJ6
E	-23	MET	-	expression tag	UNP A0A0U4QBJ6
E	-22	LYS	-	expression tag	UNP A0A0U4QBJ6
E	-21	HIS	-	expression tag	UNP A0A0U4QBJ6
E	-20	HIS	-	expression tag	UNP A0A0U4QBJ6
E	-19	HIS	-	expression tag	UNP A0A0U4QBJ6
E	-18	HIS	-	expression tag	UNP A0A0U4QBJ6
E	-17	HIS	-	expression tag	UNP A0A0U4QBJ6
E	-16	HIS	-	expression tag	UNP A0A0U4QBJ6
E	-15	HIS	-	expression tag	UNP A0A0U4QBJ6
E	-14	HIS	-	expression tag	UNP A0A0U4QBJ6
E	-13	GLY	-	expression tag	UNP A0A0U4QBJ6
E	-12	GLY	-	expression tag	UNP A0A0U4QBJ6
E	-11	LEU	-	expression tag	UNP A0A0U4QBJ6
E	-10	VAL	-	expression tag	UNP A0A0U4QBJ6
E	-9	PRO	-	expression tag	UNP A0A0U4QBJ6
E	-8	ARG	-	expression tag	UNP A0A0U4QBJ6
E	-7	GLY	-	expression tag	UNP A0A0U4QBJ6
E	-6	SER	-	expression tag	UNP A0A0U4QBJ6
E	-5	HIS	-	expression tag	UNP A0A0U4QBJ6
E	-4	GLY	-	expression tag	UNP A0A0U4QBJ6
E	-3	GLY	-	expression tag	UNP A0A0U4QBJ6
E	-2	SER	-	expression tag	UNP A0A0U4QBJ6
E	-1	GLU	-	expression tag	UNP A0A0U4QBJ6
E	0	PHE	-	expression tag	UNP A0A0U4QBJ6
E	298	ILE	VAL	conflict	UNP A0A0U4QBJ6
E	299	GLU	ASP	conflict	UNP A0A0U4QBJ6
F	-23	MET	-	expression tag	UNP A0A0U4QBJ6
F	-22	LYS	-	expression tag	UNP A0A0U4QBJ6
F	-21	HIS	-	expression tag	UNP A0A0U4QBJ6
F	-20	HIS	-	expression tag	UNP A0A0U4QBJ6
F	-19	HIS	-	expression tag	UNP A0A0U4QBJ6
F	-18	HIS	-	expression tag	UNP A0A0U4QBJ6
F	-17	HIS	-	expression tag	UNP A0A0U4QBJ6
F	-16	HIS	-	expression tag	UNP A0A0U4QBJ6
F	-15	HIS	-	expression tag	UNP A0A0U4QBJ6
F	-14	HIS	-	expression tag	UNP A0A0U4QBJ6
F	-13	GLY	-	expression tag	UNP A0A0U4QBJ6
F	-12	GLY	-	expression tag	UNP A0A0U4QBJ6
F	-11	LEU	-	expression tag	UNP A0A0U4QBJ6

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-10	VAL	-	expression tag	UNP A0A0U4QBJ6
F	-9	PRO	-	expression tag	UNP A0A0U4QBJ6
F	-8	ARG	-	expression tag	UNP A0A0U4QBJ6
F	-7	GLY	-	expression tag	UNP A0A0U4QBJ6
F	-6	SER	-	expression tag	UNP A0A0U4QBJ6
F	-5	HIS	-	expression tag	UNP A0A0U4QBJ6
F	-4	GLY	-	expression tag	UNP A0A0U4QBJ6
F	-3	GLY	-	expression tag	UNP A0A0U4QBJ6
F	-2	SER	-	expression tag	UNP A0A0U4QBJ6
F	-1	GLU	-	expression tag	UNP A0A0U4QBJ6
F	0	PHE	-	expression tag	UNP A0A0U4QBJ6
F	298	ILE	VAL	conflict	UNP A0A0U4QBJ6
F	299	GLU	ASP	conflict	UNP A0A0U4QBJ6

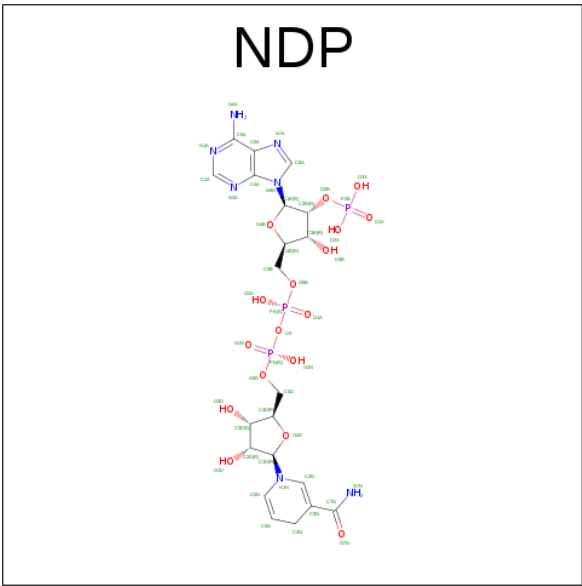
- Molecule 2 is (2Z)-2-iminopentanedioic acid (three-letter code: 2IT) (formula: C₅H₇NO₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			10	5	1	4		
2	B	1	Total	C	N	O	0	0
			10	5	1	4		
2	C	1	Total	C	N	O	0	0
			10	5	1	4		
2	F	1	Total	C	N	O	0	0
			10	5	1	4		

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE

PHOSPHATE (three-letter code: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	F	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

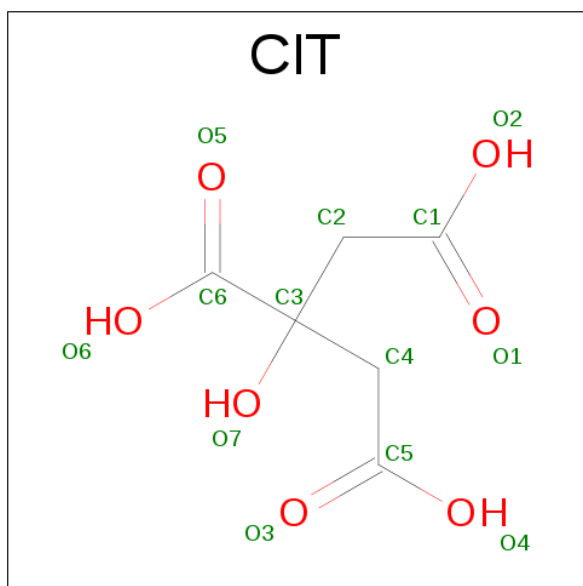
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	2	Total	K	0	0
			2	2		
4	E	4	Total	K	0	0
			4	4		
4	B	1	Total	K	0	0
			1	1		
4	C	2	Total	K	0	0
			2	2		
4	A	3	Total	K	0	0
			3	3		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	F	2	Total	K	0	0
			2	2		

- Molecule 5 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	E	1	Total	C	O	0	0
			13	6	7		

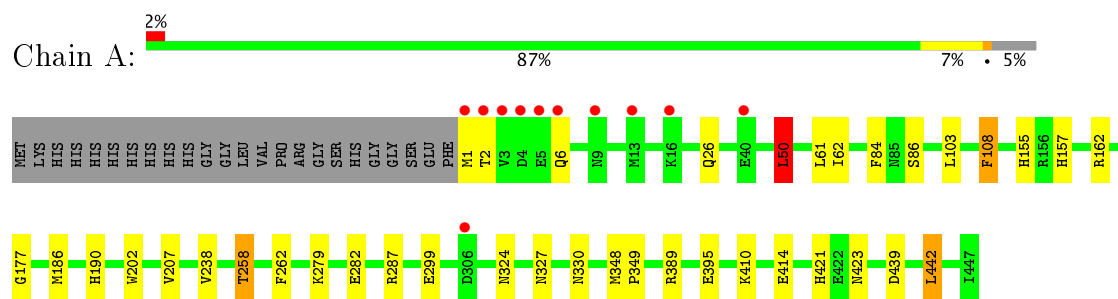
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	525	Total	O	0	0
			525	525		
6	B	355	Total	O	0	0
			355	355		
6	C	429	Total	O	0	0
			429	429		
6	D	401	Total	O	0	0
			401	401		
6	E	583	Total	O	0	0
			583	583		
6	F	475	Total	O	0	0
			475	475		

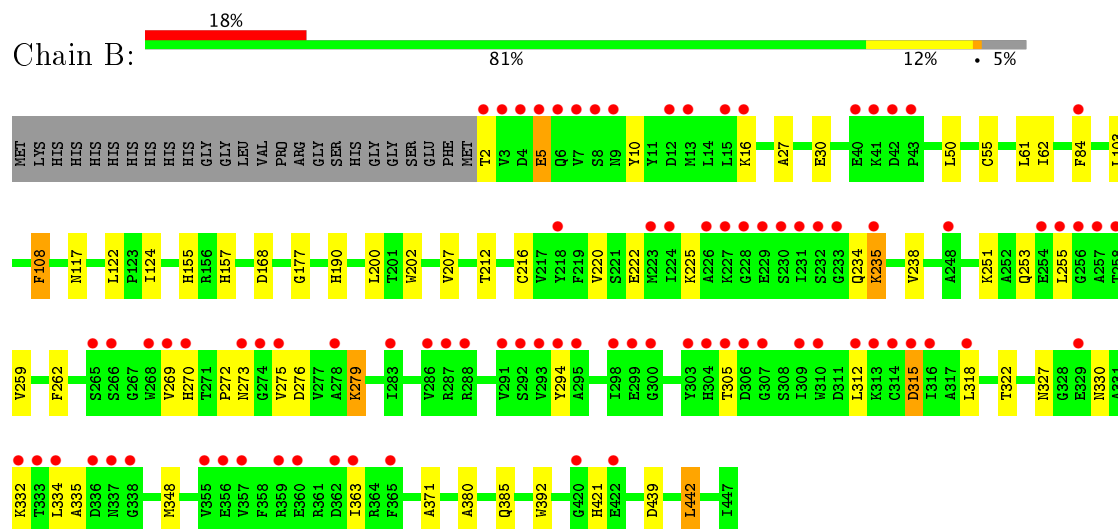
3 Residue-property plots

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 ($\text{RSRZ} > 2$). 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.

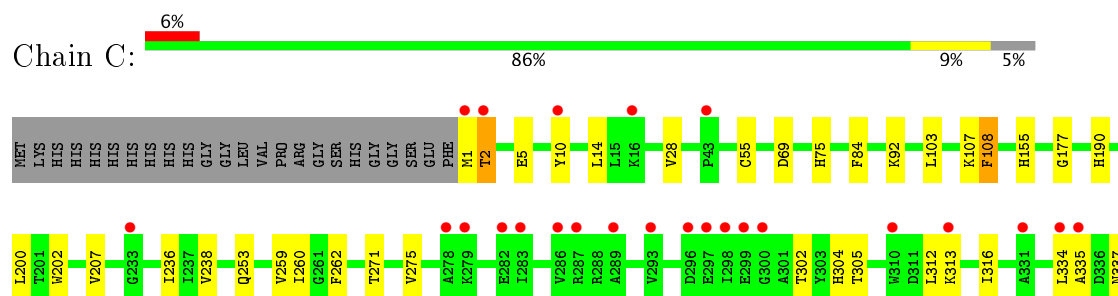
- Molecule 1: Glutamate dehydrogenase

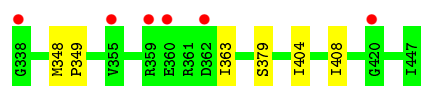


- Molecule 1: Glutamate dehydrogenase

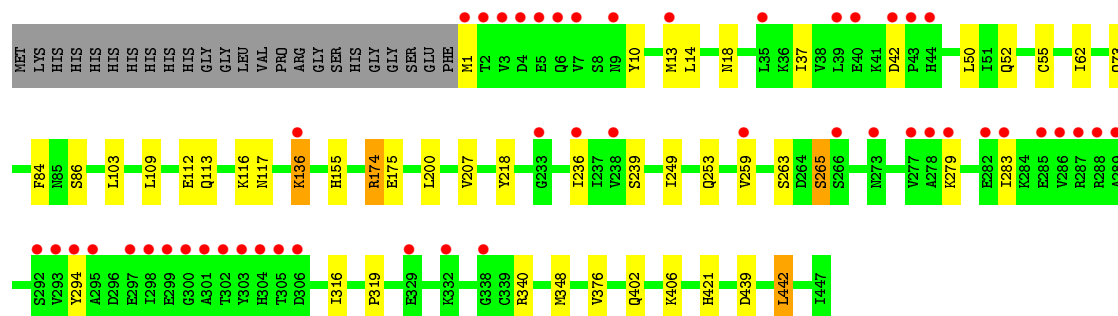
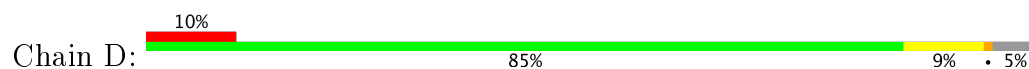


- Molecule 1: Glutamate dehydrogenase

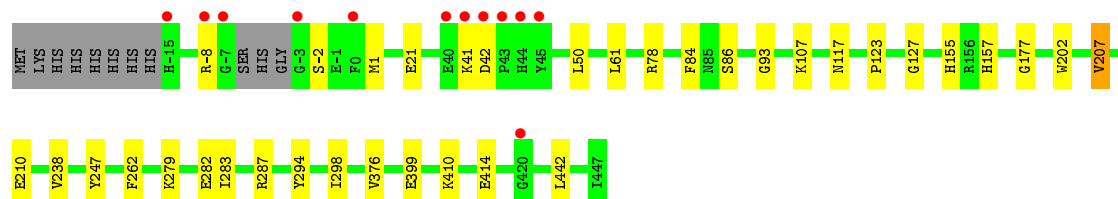
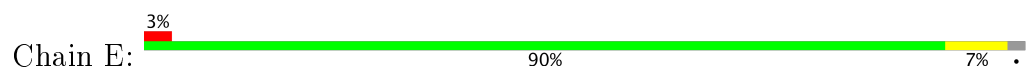




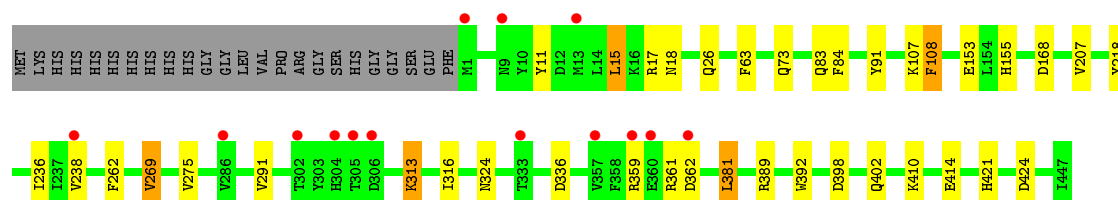
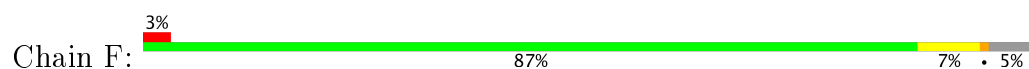
- Molecule 1: Glutamate dehydrogenase



- Molecule 1: Glutamate dehydrogenase



- Molecule 1: Glutamate dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	92.59Å 127.67Å 126.63Å 90.00° 106.70° 90.00°	Depositor
Resolution (Å)	30.83 – 1.68 30.83 – 1.68	Depositor EDS
% Data completeness (in resolution range)	96.9 (30.83-1.68) 96.9 (30.83-1.68)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 1.68Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, R_{free}	0.192 , 0.226 0.190 , 0.224	Depositor DCC
R_{free} test set	15636 reflections (5.32%)	DCC
Wilson B-factor (Å ²)	19.9	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 54.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	23954	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NDP, 2IT, K, CIT

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	0.63	0/3519	0.69	1/4749 (0.0%)
1	B	0.55	0/3511	0.64	0/4739
1	C	0.55	0/3532	0.65	0/4767
1	D	0.55	0/3537	0.63	1/4772 (0.0%)
1	E	0.62	0/3641	0.68	0/4910
1	F	0.60	0/3539	0.67	0/4774
All	All	0.59	0/21279	0.66	2/28711 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	50	LEU	CA-CB-CG	5.24	127.35	115.30
1	D	174	ARG	NE-CZ-NH2	-5.20	117.70	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3449	0	3357	28	0
1	B	3441	0	3345	40	0
1	C	3458	0	3366	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3461	0	3378	30	0
1	E	3559	0	3470	26	0
1	F	3463	0	3383	35	0
2	A	10	0	0	2	0
2	B	10	0	0	1	0
2	C	10	0	0	1	0
2	F	10	0	0	1	0
3	A	48	0	26	1	0
3	B	48	0	26	3	0
3	C	48	0	26	1	0
3	D	48	0	26	1	0
3	E	48	0	26	0	0
3	F	48	0	26	2	0
4	A	3	0	0	0	0
4	B	1	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
4	E	4	0	0	0	0
4	F	2	0	0	0	0
5	E	13	0	5	0	0
6	A	525	0	0	9	0
6	B	355	0	0	13	0
6	C	429	0	0	2	0
6	D	401	0	0	5	0
6	E	583	0	0	4	0
6	F	475	0	0	5	0
All	All	23954	0	20460	178	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 (178) 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)
3:F:502:NDP:H8A	6:F:950:HOH:O	1.37	1.20
1:B:225:LYS:HB2	6:B:785:HOH:O	1.54	1.05
1:C:2:THR:HG22	1:C:5:GLU:H	1.35	0.91
1:E:-8:ARG:H	1:F:73:GLN:HE22	1.23	0.84
1:C:253:GLN:HE22	1:C:275:VAL:H	1.24	0.82
1:D:340:ARG:HG3	1:D:340:ARG:HH11	1.46	0.80
1:E:78:ARG:NH2	6:E:601:HOH:O	2.14	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:253:GLN:HE22	1:B:275:VAL:H	1.34	0.76
1:F:269:VAL:HG11	1:F:291:VAL:HG22	1.66	0.76
1:E:282:GLU:OE2	1:E:287:ARG:HD2	1.87	0.74
1:B:253:GLN:HE21	1:B:259:VAL:H	1.34	0.74
1:F:269:VAL:CG1	1:F:291:VAL:CG2	2.66	0.74
1:C:253:GLN:HE21	1:C:259:VAL:H	1.33	0.73
1:A:327:ASN:H	1:A:330:ASN:HD22	1.35	0.73
2:F:501:2IT:CAI	3:F:502:NDP:H41N	2.17	0.73
1:F:313:LYS:N	1:F:313:LYS:HD3	2.04	0.72
1:F:269:VAL:CG1	1:F:291:VAL:HG22	2.21	0.70
1:C:69:ASP:OD2	1:C:75:HIS:HE1	1.74	0.70
1:A:421:HIS:HD2	6:A:621:HOH:O	1.75	0.69
1:B:50:LEU:HD22	1:B:442:LEU:HD13	1.75	0.67
1:F:402:GLN:NE2	6:F:602:HOH:O	2.28	0.67
1:F:269:VAL:HG11	1:F:291:VAL:CG2	2.25	0.66
1:F:313:LYS:HD3	1:F:313:LYS:H	1.59	0.66
1:A:282:GLU:OE2	1:A:287:ARG:NH1	2.28	0.66
1:B:222:GLU:HA	6:B:785:HOH:O	1.95	0.65
1:B:2:THR:HG23	1:B:5:GLU:HB3	1.77	0.65
1:F:26:GLN:HE22	1:F:324:ASN:HD21	1.45	0.65
1:E:410:LYS:HE2	1:E:414:GLU:OE1	1.97	0.65
1:B:273:ASN:O	6:B:601:HOH:O	2.14	0.64
1:B:190:HIS:HE1	6:B:666:HOH:O	1.79	0.64
1:F:389:ARG:NH2	6:F:603:HOH:O	2.31	0.64
1:D:50:LEU:HD12	1:D:442:LEU:HD13	1.80	0.63
1:A:439:ASP:HB2	6:A:613:HOH:O	1.99	0.63
1:E:399:GLU:HG3	6:E:647:HOH:O	1.99	0.62
1:E:78:ARG:HH22	1:F:18:ASN:HD21	1.46	0.62
2:B:501:2IT:CAI	3:B:502:NDP:H41N	2.30	0.62
1:B:385:GLN:NE2	1:B:392:TRP:H	1.98	0.62
1:D:253:GLN:HE21	1:D:259:VAL:H	1.47	0.61
1:F:313:LYS:CD	1:F:313:LYS:H	2.13	0.61
1:F:269:VAL:CG1	1:F:291:VAL:HG21	2.30	0.61
1:F:381:LEU:HG	1:F:392:TRP:HZ3	1.66	0.61
1:A:190:HIS:HE1	6:A:635:HOH:O	1.83	0.61
1:B:327:ASN:H	1:B:330:ASN:HD22	1.49	0.61
1:A:50:LEU:HD23	1:A:442:LEU:HD13	1.83	0.60
1:A:258:THR:HG22	6:A:663:HOH:O	2.01	0.60
1:B:385:GLN:HE21	1:B:392:TRP:H	1.50	0.60
1:C:190:HIS:HE1	6:C:652:HOH:O	1.84	0.59
1:D:174:ARG:HD2	1:D:175:GLU:OE2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MET:HA	6:A:981:HOH:O	2.02	0.58
1:E:61:LEU:HD22	1:E:157:HIS:CD2	2.38	0.58
1:A:62:ILE:HD11	1:A:103:LEU:HD22	1.86	0.58
1:B:27:ALA:HA	1:B:348:MET:HE1	1.85	0.58
1:B:276:ASP:HB3	1:B:279:LYS:HB3	1.86	0.57
2:C:501:2IT:CAI	3:C:502:NDP:H41N	2.35	0.56
1:B:238:VAL:O	1:B:262:PHE:HA	2.05	0.56
1:D:37:ILE:H	1:D:37:ILE:HD12	1.70	0.56
1:F:218:TYR:CE2	1:F:402:GLN:HG2	2.40	0.56
1:D:265:SER:HB2	3:D:502:NDP:O1X	2.06	0.55
1:D:340:ARG:NH1	1:D:340:ARG:HG3	2.19	0.55
1:A:26:GLN:HE22	1:A:324:ASN:HD21	1.54	0.55
1:D:62:ILE:HD11	1:D:103:LEU:HD22	1.89	0.55
1:F:398:ASP:O	1:F:402:GLN:HG3	2.08	0.54
1:D:348:MET:HE2	6:D:844:HOH:O	2.06	0.54
1:F:313:LYS:N	1:F:313:LYS:CD	2.69	0.54
2:A:501:2IT:CAI	3:A:502:NDP:H41N	2.38	0.54
1:E:-8:ARG:H	1:F:73:GLN:NE2	2.01	0.53
1:F:262:PHE:HE1	1:F:291:VAL:HG23	1.74	0.53
1:D:14:LEU:HG	1:D:18:ASN:HD22	1.74	0.53
1:B:234:GLN:HA	1:B:234:GLN:HE21	1.74	0.53
1:D:73:GLN:NE2	6:D:601:HOH:O	2.18	0.53
1:D:218:TYR:CD1	1:D:402:GLN:HG3	2.45	0.52
1:A:155:HIS:CE1	1:A:186:MET:HE3	2.44	0.52
1:C:155:HIS:HD2	6:C:946:HOH:O	1.93	0.52
1:E:117:ASN:OD1	1:E:376:VAL:HG21	2.10	0.52
1:A:190:HIS:HD2	1:E:86:SER:O	1.92	0.51
1:F:336:ASP:OD1	1:F:361:ARG:NH1	2.41	0.51
1:A:238:VAL:O	1:A:262:PHE:HA	2.12	0.50
1:B:155:HIS:HD2	6:B:908:HOH:O	1.94	0.50
1:B:439:ASP:HB2	6:B:622:HOH:O	2.12	0.50
1:B:108:PHE:C	1:B:108:PHE:CD1	2.83	0.50
1:B:190:HIS:HD2	1:D:86:SER:O	1.95	0.50
1:A:61:LEU:HD22	1:A:157:HIS:CD2	2.47	0.49
1:B:220:VAL:HB	6:B:611:HOH:O	2.13	0.49
1:F:421:HIS:HE1	6:F:975:HOH:O	1.96	0.49
1:A:155:HIS:HD2	6:A:1017:HOH:O	1.94	0.49
1:C:108:PHE:CD1	1:C:108:PHE:C	2.86	0.49
1:E:282:GLU:OE2	1:E:287:ARG:CD	2.58	0.49
1:B:50:LEU:HD22	1:B:442:LEU:CD1	2.43	0.49
1:F:359:ARG:NH2	1:F:424:ASP:OD2	2.31	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:18:ASN:HD22	1:F:107:LYS:NZ	2.11	0.48
1:B:421:HIS:HE1	6:B:894:HOH:O	1.95	0.48
1:F:155:HIS:HD2	6:F:978:HOH:O	1.95	0.48
1:A:86:SER:O	1:C:190:HIS:HD2	1.96	0.48
1:E:41:LYS:NZ	6:E:607:HOH:O	2.47	0.48
1:B:177:GLY:HA2	1:B:202:TRP:CH2	2.48	0.48
1:F:262:PHE:CE1	1:F:291:VAL:HG23	2.47	0.48
1:E:238:VAL:O	1:E:262:PHE:HA	2.14	0.48
1:F:381:LEU:HG	1:F:392:TRP:CZ3	2.49	0.48
1:A:155:HIS:CE1	1:A:186:MET:CE	2.97	0.47
1:D:10:TYR:OH	1:D:55:CYS:HB2	2.14	0.47
1:C:348:MET:N	1:C:349:PRO:CD	2.78	0.47
1:A:389:ARG:NH1	1:E:123:PRO:HG2	2.29	0.47
1:B:30:GLU:HG3	6:B:714:HOH:O	2.14	0.47
1:B:10:TYR:OH	1:B:55:CYS:HB2	2.15	0.47
1:B:235:LYS:HD2	1:B:315:ASP:OD2	2.14	0.46
1:C:260:ILE:HA	1:C:271:THR:O	2.14	0.46
1:B:212:THR:OG1	3:B:502:NDP:H42N	2.15	0.46
1:C:14:LEU:HD13	1:C:28:VAL:HG11	1.97	0.46
1:A:395:GLU:CD	1:A:395:GLU:H	2.19	0.46
1:A:162:ARG:CZ	6:A:771:HOH:O	2.64	0.46
1:C:335:ALA:HB2	1:C:363:ILE:HD11	1.97	0.46
1:D:236:ILE:HG12	1:D:316:ILE:HB	1.98	0.46
1:C:404:ILE:O	1:C:408:ILE:HG13	2.16	0.46
1:F:262:PHE:CE1	1:F:291:VAL:CG2	2.99	0.45
1:A:410:LYS:HE3	1:A:414:GLU:OE2	2.16	0.45
1:E:279:LYS:HG2	1:E:298:ILE:HD11	1.98	0.45
1:F:11:TYR:CZ	1:F:15:LEU:HD21	2.50	0.45
1:C:177:GLY:HA2	1:C:202:TRP:CH2	2.51	0.45
1:C:313:LYS:HG3	1:C:337:ASN:O	2.17	0.45
1:D:283:ILE:HD13	1:D:294:TYR:HB2	1.97	0.45
1:D:117:ASN:OD1	1:D:376:VAL:HG21	2.17	0.45
1:B:270:HIS:CE1	1:B:272:PRO:HG3	2.51	0.45
1:E:50:LEU:HD12	1:E:442:LEU:HG	1.98	0.45
1:B:318:LEU:HD22	6:B:611:HOH:O	2.16	0.44
1:B:332:LYS:HG2	6:B:693:HOH:O	2.16	0.44
1:B:61:LEU:HD22	1:B:157:HIS:CD2	2.51	0.44
1:E:21:GLU:CD	1:E:107:LYS:HZ3	2.21	0.44
1:A:327:ASN:H	1:A:330:ASN:ND2	2.06	0.44
1:D:340:ARG:CG	1:D:340:ARG:HH11	2.23	0.44
1:F:291:VAL:O	1:F:291:VAL:HG22	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:PHE:CD1	1:A:108:PHE:C	2.90	0.44
1:F:236:ILE:HG12	1:F:316:ILE:HB	2.00	0.44
1:D:109:LEU:O	1:D:113:GLN:HG2	2.18	0.44
1:D:73:GLN:HB3	6:D:601:HOH:O	2.18	0.44
1:F:108:PHE:CD1	1:F:108:PHE:C	2.90	0.44
1:B:117:ASN:HB3	1:B:124:ILE:HG13	2.00	0.44
1:B:322:THR:HG21	3:B:502:NDP:C6A	2.48	0.44
1:B:62:ILE:HD11	1:B:103:LEU:HD22	2.00	0.44
1:A:190:HIS:CD2	1:E:86:SER:O	2.72	0.43
1:A:2:THR:O	1:A:6:GLN:HG3	2.18	0.43
1:D:10:TYR:CE1	1:D:52:GLN:HG3	2.54	0.43
1:A:177:GLY:HA2	1:A:202:TRP:CH2	2.53	0.43
1:C:10[A]:TYR:OH	1:C:55:CYS:HB2	2.19	0.43
1:D:421:HIS:HD2	6:D:709:HOH:O	2.02	0.43
1:E:93:GLY:HA3	1:E:127:GLY:O	2.18	0.43
1:C:103:LEU:HG	1:C:107:LYS:HD2	2.00	0.43
1:B:251:LYS:O	1:B:255:LEU:HG	2.19	0.43
1:E:210:GLU:HG3	1:E:247:TYR:CD1	2.54	0.42
1:D:155:HIS:HD2	6:D:940:HOH:O	2.01	0.42
1:C:236:ILE:HG12	1:C:316:ILE:HB	2.01	0.42
1:B:225:LYS:HE3	6:B:785:HOH:O	2.19	0.42
1:C:238:VAL:O	1:C:262:PHE:HA	2.20	0.42
1:E:207:VAL:O	1:E:207:VAL:HG12	2.19	0.42
1:F:238:VAL:O	1:F:262:PHE:HA	2.20	0.42
1:F:410:LYS:HE2	1:F:414:GLU:OE1	2.19	0.42
6:B:627:HOH:O	1:D:439:ASP:HB2	2.19	0.42
1:B:216:CYS:HA	1:B:371:ALA:O	2.19	0.41
1:D:402:GLN:NE2	1:D:406:LYS:HD2	2.35	0.41
1:A:423:ASN:ND2	6:A:610:HOH:O	2.52	0.41
1:C:92:LYS:HE3	1:C:379:SER:HB3	2.03	0.41
1:A:348:MET:N	1:A:349:PRO:CD	2.84	0.41
1:B:122:LEU:HD13	1:B:380:ALA:HB3	2.01	0.41
1:C:302:THR:OG1	1:C:304:HIS:HE1	2.03	0.41
1:D:136:LYS:N	1:D:136:LYS:HE3	2.35	0.41
1:D:249:ILE:HG12	1:D:259:VAL:HG11	2.03	0.41
1:D:239:SER:OG	1:D:319:PRO:HA	2.20	0.41
1:B:335:ALA:HB2	1:B:363:ILE:HD11	2.03	0.41
1:E:-2:SER:O	1:E:1:MET:HE2	2.20	0.41
1:D:402:GLN:HE21	1:D:406:LYS:HD2	1.85	0.41
1:E:1:MET:HE2	1:E:1:MET:HB2	1.79	0.41
1:F:63:PHE:CG	1:F:153:GLU:HG2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:155:HIS:HD2	6:E:1051:HOH:O	2.04	0.41
1:E:177:GLY:HA2	1:E:202:TRP:CH2	2.56	0.41
1:F:83:GLN:HB3	1:F:91:TYR:CE2	2.55	0.40
1:B:279:LYS:HG2	1:B:294:TYR:CE1	2.56	0.40
1:D:112:GLU:O	1:D:116[B]:LYS:HG3	2.22	0.40
2:A:501:2IT:CAI	6:A:601:HOH:O	2.70	0.40
1:E:283:ILE:CD1	1:E:294:TYR:HA	2.51	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	445/471 (94%)	435 (98%)	9 (2%)	1 (0%)	51	30
1	B	444/471 (94%)	432 (97%)	10 (2%)	2 (0%)	32	14
1	C	446/471 (95%)	435 (98%)	10 (2%)	1 (0%)	51	30
1	D	447/471 (95%)	435 (97%)	11 (2%)	1 (0%)	51	30
1	E	459/471 (98%)	449 (98%)	9 (2%)	1 (0%)	51	30
1	F	447/471 (95%)	437 (98%)	8 (2%)	2 (0%)	38	18
All	All	2688/2826 (95%)	2623 (98%)	57 (2%)	8 (0%)	44	24

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	207	VAL
1	B	207	VAL
1	D	207	VAL
1	E	207	VAL
1	F	207	VAL

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Mol	Chain	Res	Type
1	C	207	VAL
1	F	168	ASP
1	B	168	ASP

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	358/377 (95%)	351 (98%)	7 (2%)	60	40
1	B	357/377 (95%)	344 (96%)	13 (4%)	40	16
1	C	359/377 (95%)	351 (98%)	8 (2%)	57	35
1	D	360/377 (96%)	350 (97%)	10 (3%)	49	25
1	E	370/377 (98%)	368 (100%)	2 (0%)	91	86
1	F	360/377 (96%)	350 (97%)	10 (3%)	49	25
All	All	2164/2262 (96%)	2114 (98%)	50 (2%)	56	33

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	LEU
1	A	84	PHE
1	A	108	PHE
1	A	258	THR
1	A	279	LYS
1	A	299	GLU
1	A	442	LEU
1	B	5	GLU
1	B	16	LYS
1	B	84	PHE
1	B	108	PHE
1	B	200	LEU
1	B	235	LYS
1	B	269	VAL
1	B	279	LYS

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Mol	Chain	Res	Type
1	B	305	THR
1	B	312	LEU
1	B	315	ASP
1	B	334	LEU
1	B	442	LEU
1	C	1	MET
1	C	2	THR
1	C	84	PHE
1	C	108	PHE
1	C	200	LEU
1	C	305	THR
1	C	312	LEU
1	C	334	LEU
1	D	1	MET
1	D	13	MET
1	D	42	ASP
1	D	84	PHE
1	D	136	LYS
1	D	200	LEU
1	D	263	SER
1	D	265	SER
1	D	279	LYS
1	D	442	LEU
1	E	42	ASP
1	E	84	PHE
1	F	15	LEU
1	F	17[A]	ARG
1	F	17[B]	ARG
1	F	84	PHE
1	F	108	PHE
1	F	269	VAL
1	F	275	VAL
1	F	313	LYS
1	F	362	ASP
1	F	381	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	73	GLN
1	A	155	HIS

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Mol	Chain	Res	Type
1	A	190	HIS
1	A	304	HIS
1	A	330	ASN
1	A	384	GLN
1	A	423	ASN
1	B	73	GLN
1	B	155	HIS
1	B	190	HIS
1	B	234	GLN
1	B	253	GLN
1	B	270	HIS
1	B	330	ASN
1	B	385	GLN
1	B	402	GLN
1	B	421	HIS
1	C	75	HIS
1	C	155	HIS
1	C	182	HIS
1	C	190	HIS
1	C	253	GLN
1	C	270	HIS
1	C	304	HIS
1	D	60	GLN
1	D	155	HIS
1	D	182	HIS
1	D	253	GLN
1	D	402	GLN
1	D	421	HIS
1	E	73	GLN
1	E	155	HIS
1	E	182	HIS
1	E	304	HIS
1	E	421	HIS
1	F	18	ASN
1	F	26	GLN
1	F	60	GLN
1	F	73	GLN
1	F	155	HIS
1	F	182	HIS
1	F	402	GLN
1	F	421	HIS

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 25 ligands modelled in this entry, 14 are monoatomic - leaving 11 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	$\# Z > 2$
2	2IT	A	501	-	4,9,9	2.37	2 (50%)	2,11,11	1.88	1 (50%)
3	NDP	A	502	-	43,52,52	1.68	8 (18%)	49,80,80	2.12	3 (6%)
2	2IT	B	501	-	4,9,9	2.12	2 (50%)	2,11,11	1.34	0
3	NDP	B	502	-	43,52,52	1.93	10 (23%)	49,80,80	2.04	2 (4%)
2	2IT	C	501	-	4,9,9	2.18	2 (50%)	2,11,11	1.58	0
3	NDP	C	502	-	43,52,52	1.83	10 (23%)	49,80,80	2.17	8 (16%)
3	NDP	D	502	-	43,52,52	1.80	8 (18%)	49,80,80	2.30	6 (12%)
5	CIT	E	502	-	3,12,12	0.73	0	3,17,17	2.21	2 (66%)
3	NDP	E	503	-	43,52,52	1.92	10 (23%)	49,80,80	2.43	4 (8%)
2	2IT	F	501	-	4,9,9	1.98	2 (50%)	2,11,11	1.46	1 (50%)
3	NDP	F	502	-	43,52,52	1.72	8 (18%)	49,80,80	2.18	5 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means

no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	2IT	A	501	-	-	0/2/9/9	0/0/0/0
3	NDP	A	502	-	-	0/30/77/77	0/5/5/5
2	2IT	B	501	-	-	0/2/9/9	0/0/0/0
3	NDP	B	502	-	-	0/30/77/77	0/5/5/5
2	2IT	C	501	-	-	0/2/9/9	0/0/0/0
3	NDP	C	502	-	-	0/30/77/77	0/5/5/5
3	NDP	D	502	-	-	0/30/77/77	0/5/5/5
5	CIT	E	502	-	-	0/6/16/16	0/0/0/0
3	NDP	E	503	-	-	0/30/77/77	0/5/5/5
2	2IT	F	501	-	-	0/2/9/9	0/0/0/0
3	NDP	F	502	-	-	0/30/77/77	0/5/5/5

All (62) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	502	NDP	C4N-C5N	-4.60	1.39	1.49
3	D	502	NDP	C4N-C5N	-4.29	1.39	1.49
3	B	502	NDP	C4N-C5N	-4.05	1.40	1.49
3	E	503	NDP	C4N-C5N	-4.05	1.40	1.49
3	F	502	NDP	C4N-C5N	-3.98	1.40	1.49
3	E	503	NDP	C5A-C4A	-3.62	1.32	1.40
3	A	502	NDP	C4N-C5N	-3.37	1.41	1.49
2	A	501	2IT	CAJ-CAI	-3.33	1.46	1.52
2	C	501	2IT	CAJ-CAI	-3.07	1.47	1.52
2	B	501	2IT	CAJ-CAI	-3.03	1.47	1.52
3	D	502	NDP	C5A-C4A	-2.85	1.34	1.40
3	F	502	NDP	C5A-C4A	-2.78	1.34	1.40
3	A	502	NDP	C5A-C4A	-2.73	1.34	1.40
2	F	501	2IT	CAJ-CAI	-2.52	1.48	1.52
3	B	502	NDP	C5A-C4A	-2.51	1.34	1.40
3	C	502	NDP	C5A-C4A	-2.42	1.35	1.40
3	E	503	NDP	O4D-C1D	2.01	1.46	1.42
3	F	502	NDP	PA-O1A	2.03	1.58	1.50
3	C	502	NDP	C2N-C3N	2.07	1.40	1.34
3	A	502	NDP	C2N-C3N	2.07	1.40	1.34
3	C	502	NDP	P2B-O2B	2.18	1.63	1.59
3	B	502	NDP	C2N-C3N	2.25	1.41	1.34
3	E	503	NDP	PN-O1N	2.27	1.59	1.50
3	B	502	NDP	O3B-C3B	2.27	1.48	1.43
3	F	502	NDP	C2A-N1A	2.44	1.38	1.33
3	E	503	NDP	P2B-O1X	2.46	1.59	1.50
3	A	502	NDP	P2B-O1X	2.61	1.59	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	NDP	C6N-C5N	2.71	1.38	1.33
3	F	502	NDP	O4B-C1B	2.82	1.45	1.41
3	A	502	NDP	P2B-O2B	2.90	1.64	1.59
3	C	502	NDP	O3B-C3B	2.90	1.49	1.43
3	C	502	NDP	PN-O1N	2.96	1.62	1.50
2	B	501	2IT	CAI-NAA	2.96	1.35	1.27
3	D	502	NDP	PA-O1A	2.97	1.62	1.50
2	F	501	2IT	CAI-NAA	3.04	1.35	1.27
3	E	503	NDP	C2A-N1A	3.06	1.39	1.33
3	D	502	NDP	P2B-O1X	3.06	1.61	1.50
2	C	501	2IT	CAI-NAA	3.09	1.35	1.27
3	C	502	NDP	C6N-C5N	3.17	1.39	1.33
3	B	502	NDP	PN-O1N	3.34	1.63	1.50
3	F	502	NDP	C6N-C5N	3.37	1.39	1.33
2	A	501	2IT	CAI-NAA	3.37	1.36	1.27
3	F	502	NDP	P2B-O1X	3.38	1.62	1.50
3	C	502	NDP	C2A-N1A	3.42	1.40	1.33
3	D	502	NDP	O4B-C1B	3.54	1.46	1.41
3	D	502	NDP	C6N-C5N	3.57	1.39	1.33
3	B	502	NDP	C2A-N1A	3.61	1.40	1.33
3	E	503	NDP	C6N-C5N	3.63	1.40	1.33
3	D	502	NDP	C2A-N1A	3.67	1.40	1.33
3	B	502	NDP	C6N-C5N	3.70	1.40	1.33
3	B	502	NDP	O4B-C1B	3.75	1.46	1.41
3	B	502	NDP	P2B-O1X	3.96	1.64	1.50
3	E	503	NDP	O4B-C1B	4.17	1.47	1.41
3	A	502	NDP	C2A-N1A	4.44	1.42	1.33
3	C	502	NDP	O4B-C1B	4.59	1.47	1.41
3	E	503	NDP	C2A-N3A	4.78	1.40	1.32
3	C	502	NDP	C2A-N3A	4.98	1.40	1.32
3	A	502	NDP	C2A-N3A	5.06	1.40	1.32
3	D	502	NDP	C2A-N3A	5.08	1.40	1.32
3	E	503	NDP	P2B-O2B	5.20	1.68	1.59
3	B	502	NDP	C2A-N3A	5.46	1.41	1.32
3	F	502	NDP	C2A-N3A	5.90	1.42	1.32

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	503	NDP	N3A-C2A-N1A	-14.59	116.16	128.86
3	D	502	NDP	N3A-C2A-N1A	-13.56	117.05	128.86
3	F	502	NDP	N3A-C2A-N1A	-12.99	117.54	128.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	502	NDP	N3A-C2A-N1A	-12.79	117.72	128.86
3	A	502	NDP	N3A-C2A-N1A	-12.57	117.91	128.86
3	C	502	NDP	N3A-C2A-N1A	-12.08	118.33	128.86
3	E	503	NDP	C1B-N9A-C4A	-6.18	115.96	126.64
3	C	502	NDP	C4B-O4B-C1B	-4.13	105.37	109.77
3	A	502	NDP	C3N-C2N-N1N	-3.85	117.49	123.08
3	F	502	NDP	C4B-O4B-C1B	-3.18	106.38	109.77
3	D	502	NDP	C3N-C2N-N1N	-3.17	118.48	123.08
3	D	502	NDP	C4B-O4B-C1B	-3.15	106.41	109.77
3	C	502	NDP	O4D-C1D-N1N	-3.14	101.73	108.07
3	D	502	NDP	O4B-C1B-C2B	-3.12	101.14	106.59
3	B	502	NDP	C3N-C2N-N1N	-2.96	118.79	123.08
3	E	503	NDP	C4B-O4B-C1B	-2.57	107.03	109.77
3	A	502	NDP	O4D-C1D-N1N	-2.56	102.92	108.07
5	E	502	CIT	C3-C4-C5	-2.52	111.01	114.95
3	C	502	NDP	O4B-C1B-C2B	-2.50	102.22	106.59
2	A	501	2IT	CAG-CAF-CAH	-2.50	108.40	112.66
3	C	502	NDP	C3B-C2B-C1B	-2.44	97.97	102.75
3	C	502	NDP	C3N-C2N-N1N	-2.39	119.60	123.08
5	E	502	CIT	C3-C2-C1	-2.36	111.27	114.95
3	F	502	NDP	O4B-C1B-C2B	-2.34	102.50	106.59
3	C	502	NDP	C1D-N1N-C6N	-2.23	115.93	120.77
3	C	502	NDP	C4A-C5A-N7A	-2.15	107.34	109.41
3	F	502	NDP	O4D-C1D-N1N	-2.11	103.81	108.07
3	E	503	NDP	O2B-P2B-O1X	-2.11	101.00	109.26
2	F	501	2IT	CAG-CAI-NAA	-2.04	118.30	125.34
3	D	502	NDP	C3B-C2B-C1B	-2.01	98.81	102.75
3	D	502	NDP	O3X-P2B-O2B	2.47	117.23	106.00
3	F	502	NDP	O3X-P2B-O2B	2.48	117.25	106.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	2IT	2	0
3	A	502	NDP	1	0
2	B	501	2IT	1	0
3	B	502	NDP	3	0
2	C	501	2IT	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	502	NDP	1	0
3	D	502	NDP	1	0
2	F	501	2IT	1	0
3	F	502	NDP	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	447/471 (94%)	-0.06	11 (2%) 58 61	11, 17, 31, 50	0
1	B	446/471 (94%)	0.92	86 (19%) 1 1	14, 27, 45, 55	0
1	C	447/471 (94%)	0.28	30 (6%) 19 20	12, 22, 38, 47	0
1	D	447/471 (94%)	0.56	49 (10%) 6 6	13, 23, 47, 64	0
1	E	460/471 (97%)	-0.01	12 (2%) 56 60	11, 17, 31, 45	0
1	F	447/471 (94%)	0.13	14 (3%) 49 53	11, 19, 34, 44	0
All	All	2694/2826 (95%)	0.30	202 (7%) 15 16	11, 20, 42, 64	0

All (202) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	3	VAL	10.2
1	D	1	MET	9.0
1	D	286	VAL	7.5
1	B	298	ILE	7.1
1	E	-3	GLY	6.4
1	C	1	MET	6.2
1	D	300	GLY	6.2
1	D	2	THR	6.0
1	A	1	MET	5.8
1	B	295	ALA	5.8
1	B	300	GLY	5.3
1	B	303	TYR	5.2
1	D	295	ALA	5.1
1	C	286	VAL	5.0
1	B	360	GLU	4.9
1	D	44	HIS	4.8
1	B	305	THR	4.7
1	D	299	GLU	4.7
1	B	286	VAL	4.7

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Mol	Chain	Res	Type	RSRZ
1	B	3	VAL	4.7
1	B	338	GLY	4.7
1	D	6	GLN	4.7
1	B	2	THR	4.6
1	B	233	GLY	4.6
1	B	269	VAL	4.5
1	B	293	VAL	4.5
1	D	288	ARG	4.5
1	B	310	TRP	4.4
1	D	301	ALA	4.4
1	B	334	LEU	4.4
1	B	4	ASP	4.3
1	B	299	GLU	4.3
1	B	362	ASP	4.3
1	D	42	ASP	4.2
1	D	40	GLU	4.2
1	D	289	ALA	4.2
1	B	230	SER	4.1
1	B	278	ALA	4.1
1	B	337	ASN	4.1
1	D	302	THR	4.1
1	E	-7	GLY	4.1
1	D	278	ALA	4.0
1	B	291	VAL	4.0
1	C	420	GLY	4.0
1	B	235	LYS	4.0
1	B	359	ARG	3.9
1	B	13	MET	3.9
1	F	362	ASP	3.9
1	D	293	VAL	3.9
1	E	44	HIS	3.9
1	B	227	LYS	3.8
1	B	5	GLU	3.8
1	B	420	GLY	3.8
1	F	1	MET	3.8
1	C	10[A]	TYR	3.7
1	E	-8	ARG	3.6
1	B	294	TYR	3.6
1	A	2	THR	3.6
1	B	8	SER	3.6
1	B	318	LEU	3.6
1	D	283	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	255	LEU	3.6
1	B	6	GLN	3.5
1	B	268	TRP	3.4
1	E	40	GLU	3.4
1	D	292	SER	3.4
1	B	224	ILE	3.3
1	B	15	LEU	3.3
1	D	39	LEU	3.3
1	B	314	CYS	3.3
1	B	422	GLU	3.3
1	C	299	GLU	3.3
1	D	5	GLU	3.3
1	B	287	ARG	3.2
1	D	4	ASP	3.2
1	B	223	MET	3.2
1	F	359	ARG	3.2
1	B	288	ARG	3.2
1	B	275	VAL	3.2
1	C	283	ILE	3.1
1	B	231	ILE	3.1
1	B	306	ASP	3.1
1	B	333	THR	3.1
1	D	273	ASN	3.1
1	B	226	ALA	3.1
1	D	305	THR	3.0
1	B	304	HIS	3.0
1	B	273	ASN	3.0
1	D	279	LYS	3.0
1	D	287	ARG	3.0
1	F	302	THR	3.0
1	C	2	THR	3.0
1	D	13	MET	3.0
1	B	266	SER	3.0
1	B	40	GLU	3.0
1	F	360	GLU	2.9
1	B	270	HIS	2.9
1	C	279	LYS	2.9
1	B	355	VAL	2.8
1	D	35	LEU	2.8
1	B	256	GLY	2.8
1	D	43	PRO	2.8
1	A	40	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	298	ILE	2.8
1	C	282	GLU	2.8
1	C	296	ASP	2.8
1	B	363	ILE	2.8
1	D	259	VAL	2.8
1	C	233	GLY	2.8
1	B	248	ALA	2.8
1	C	43	PRO	2.8
1	B	316	ILE	2.7
1	A	4	ASP	2.7
1	B	365	PHE	2.7
1	B	16	LYS	2.7
1	D	282	GLU	2.7
1	F	305	THR	2.7
1	C	287	ARG	2.7
1	D	277	VAL	2.7
1	F	9	ASN	2.7
1	B	229	GLU	2.6
1	B	336	ASP	2.6
1	D	136	LYS	2.6
1	B	232	SER	2.6
1	B	329	GLU	2.6
1	C	297	GLU	2.6
1	B	9	ASN	2.6
1	C	278	ALA	2.6
1	A	13	MET	2.6
1	B	42	ASP	2.5
1	D	238	VAL	2.5
1	F	357	VAL	2.5
1	B	312	LEU	2.5
1	B	228	GLY	2.5
1	D	303	TYR	2.5
1	C	300	GLY	2.5
1	B	309	ILE	2.5
1	C	331	ALA	2.5
1	B	332	LYS	2.5
1	C	298	ILE	2.5
1	D	233	GLY	2.5
1	F	333	THR	2.5
1	C	293	VAL	2.5
1	B	307	GLY	2.5
1	F	304	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	42	ASP	2.4
1	A	16	LYS	2.4
1	B	41	LYS	2.4
1	B	292	SER	2.4
1	C	355	VAL	2.4
1	E	0	PHE	2.4
1	D	306	ASP	2.4
1	C	16	LYS	2.4
1	C	359	ARG	2.4
1	D	9	ASN	2.4
1	A	306	ASP	2.4
1	F	306	ASP	2.4
1	E	-15	HIS	2.4
1	D	266	SER	2.4
1	D	7	VAL	2.4
1	C	310	TRP	2.4
1	B	313	LYS	2.4
1	C	335	ALA	2.4
1	A	5	GLU	2.4
1	B	7	VAL	2.3
1	F	13	MET	2.3
1	E	420	GLY	2.3
1	B	258	THR	2.3
1	A	3	VAL	2.3
1	D	332	LYS	2.3
1	E	43	PRO	2.3
1	D	297	GLU	2.3
1	C	338	GLY	2.3
1	B	12	ASP	2.3
1	D	294	TYR	2.3
1	E	45	TYR	2.3
1	C	360	GLU	2.2
1	B	265	SER	2.2
1	C	289	ALA	2.2
1	B	357	VAL	2.2
1	D	236	ILE	2.2
1	B	218	TYR	2.2
1	B	257	ALA	2.2
1	D	285	GLU	2.2
1	D	304	HIS	2.2
1	B	43	PRO	2.2
1	A	9	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	283	ILE	2.1
1	D	338	GLY	2.1
1	B	274	GLY	2.1
1	C	313	LYS	2.1
1	D	329	GLU	2.1
1	A	6	GLN	2.1
1	E	41	LYS	2.1
1	B	254	GLU	2.1
1	B	356	GLU	2.0
1	B	84	PHE	2.0
1	F	286	VAL	2.0
1	B	315	ASP	2.0
1	C	362	ASP	2.0
1	F	238	VAL	2.0
1	C	334	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å ²)	Q<0.9
2	2IT	A	501	10/10	0.90	0.14	1.91	16,19,23,24	0
2	2IT	F	501	10/10	0.92	0.13	1.04	17,21,24,25	0
4	K	E	501	1/1	1.00	0.07	0.38	13,13,13,13	0
5	CIT	E	502	13/13	0.90	0.10	0.05	24,26,28,28	0
3	NDP	C	502	48/48	0.94	0.10	-0.10	17,21,32,34	0
2	2IT	B	501	10/10	0.92	0.10	-0.10	25,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	NDP	B	502	48/48	0.93	0.12	-0.11	21,27,36,38	0
3	NDP	A	502	48/48	0.96	0.09	-0.27	12,15,29,31	0
3	NDP	F	502	48/48	0.94	0.10	-0.52	15,19,31,34	0
3	NDP	D	502	48/48	0.89	0.11	-0.63	24,35,41,43	0
2	2IT	C	501	10/10	0.95	0.08	-0.77	18,22,26,27	0
4	K	C	503	1/1	0.99	0.06	-0.77	23,23,23,23	0
4	K	D	501	1/1	0.99	0.07	-1.01	18,18,18,18	0
3	NDP	E	503	48/48	0.98	0.06	-1.27	16,22,29,32	0
4	K	E	506	1/1	0.95	0.05	-1.56	31,31,31,31	0
4	K	A	503	1/1	0.98	0.03	-1.57	30,30,30,30	0
4	K	F	504	1/1	0.91	0.08	-1.71	38,38,38,38	0
4	K	D	503	1/1	1.00	0.03	-2.66	22,22,22,22	0
4	K	F	503	1/1	1.00	0.03	-2.78	23,23,23,23	0
4	K	E	505	1/1	1.00	0.04	-3.11	19,19,19,19	0
4	K	B	503	1/1	1.00	0.04	-	25,25,25,25	0
4	K	C	504	1/1	0.93	0.13	-	43,43,43,43	0
4	K	A	505	1/1	0.96	0.05	-	32,32,32,32	0
4	K	A	504	1/1	0.99	0.03	-	21,21,21,21	0
4	K	E	504	1/1	0.98	0.05	-	28,28,28,28	0

6.5 Other polymers

There are no such residues in this entry.