W O R L D W I D E
wwPDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Jan 30, 2017 – 09:28 PM EST

PDB ID : 1NR1
Title : Crystal structure of the R463A mutant of human Glutamate dehydrogenase
Authors : Banerjee, S.; Schmidt, T.; Fang, J.; Stanley, C.A.; Smith, T.J.
Deposited on : 2003-01-23
Resolution : 3.30 Å(reported)

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

MolProbity : 4.02b-467
Mogul : unknown
Xtriage (Phenix) : NOT EXECUTED
EDS : NOT EXECUTED
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028442

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.30 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	Percentile Ranks	Value
Clashscore		57
Ramachandran outliers		7.4%
Sidechain outliers		13.2%

Worse   *Better*

■ Percentile relative to all X-ray structures
⧄ Percentile relative to X-ray structures of similar resolution
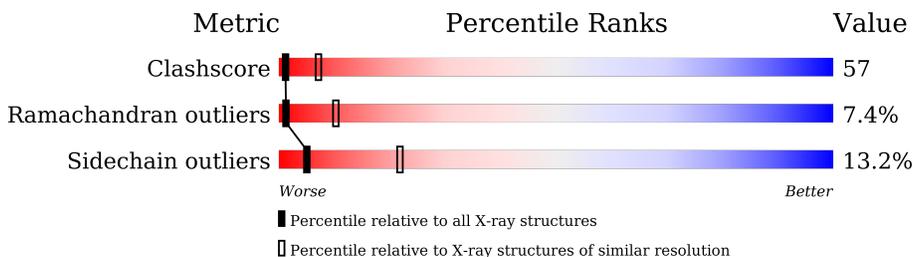
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	496	29% 55% 15%
1	B	496	33% 51% 15% •
1	C	496	37% 49% 13% •
1	D	496	28% 57% 13% •
1	E	496	37% 53% 9% •
1	F	496	31% 55% 12% •

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 23208 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 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	496	Total	C	N	O	S	0	0	0
			3868	2447	676	726	19			
1	B	496	Total	C	N	O	S	0	0	0
			3868	2447	676	726	19			
1	C	496	Total	C	N	O	S	0	0	0
			3868	2447	676	726	19			
1	D	496	Total	C	N	O	S	0	0	0
			3868	2447	676	726	19			
1	E	496	Total	C	N	O	S	0	0	0
			3868	2447	676	726	19			
1	F	496	Total	C	N	O	S	0	0	0
			3868	2447	676	726	19			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	88	GLN	HIS	CONFLICT	UNP P00367
A	89	HIS	GLN	CONFLICT	UNP P00367
A	463	ALA	ARG	ENGINEERED	UNP P00367
B	88	GLN	HIS	CONFLICT	UNP P00367
B	89	HIS	GLN	CONFLICT	UNP P00367
B	463	ALA	ARG	ENGINEERED	UNP P00367
C	88	GLN	HIS	CONFLICT	UNP P00367
C	89	HIS	GLN	CONFLICT	UNP P00367
C	463	ALA	ARG	ENGINEERED	UNP P00367
D	88	GLN	HIS	CONFLICT	UNP P00367
D	89	HIS	GLN	CONFLICT	UNP P00367
D	463	ALA	ARG	ENGINEERED	UNP P00367
E	88	GLN	HIS	CONFLICT	UNP P00367
E	89	HIS	GLN	CONFLICT	UNP P00367
E	463	ALA	ARG	ENGINEERED	UNP P00367
F	88	GLN	HIS	CONFLICT	UNP P00367
F	89	HIS	GLN	CONFLICT	UNP P00367

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| Chain	Residue	Modelled	Actual	Comment	Reference
F	463	ALA	ARG	ENGINEERED	UNP P00367

3 Residue-property plots (i)

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

Note EDS was not executed.

- Molecule 1: Glutamate dehydrogenase 1
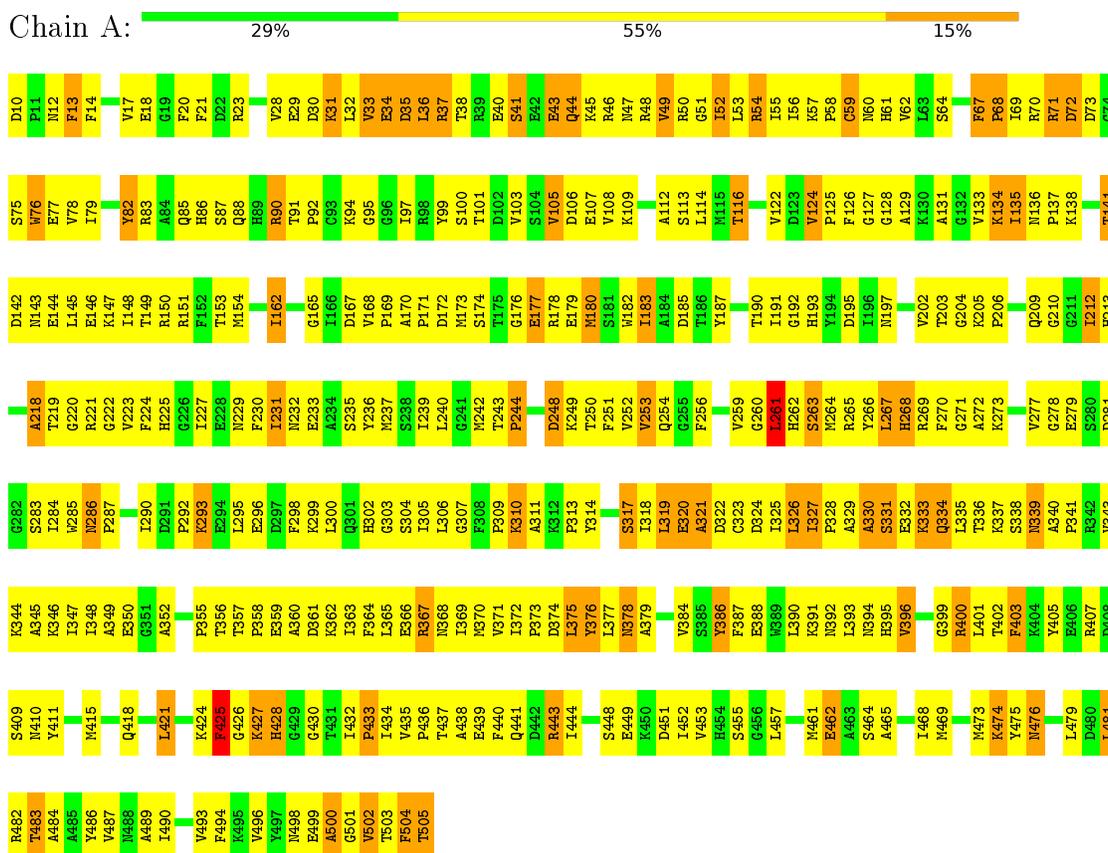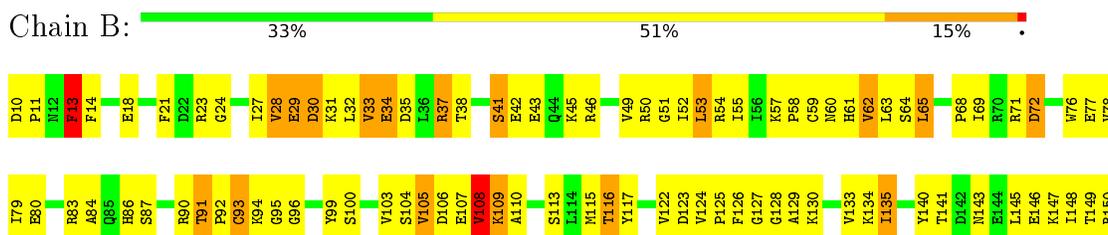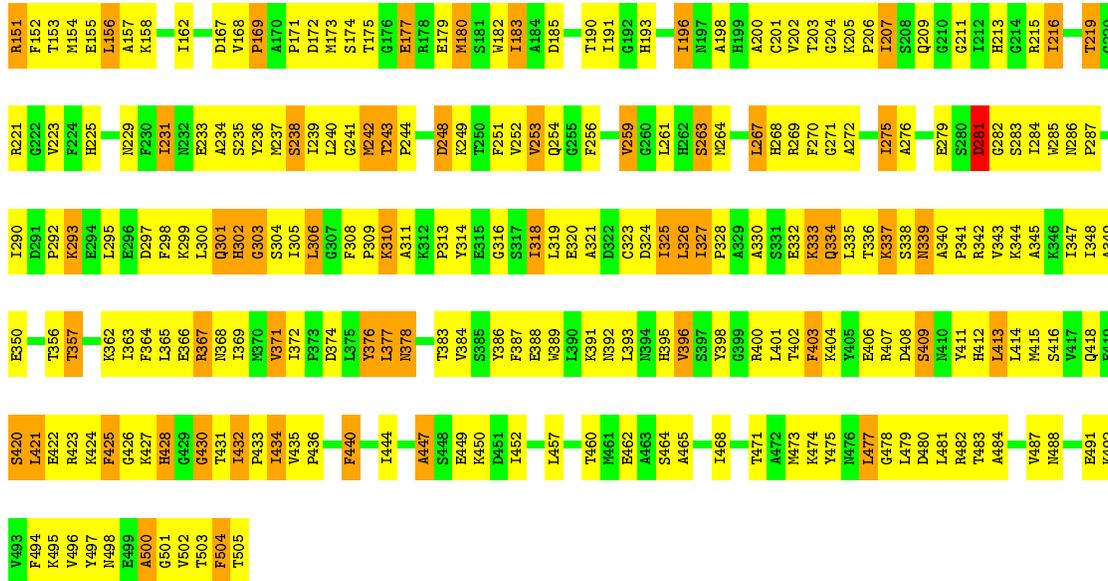
- Molecule 1: Glutamate dehydrogenase 1

• Molecule 1: Glutamate dehydrogenase 1

Chain C:
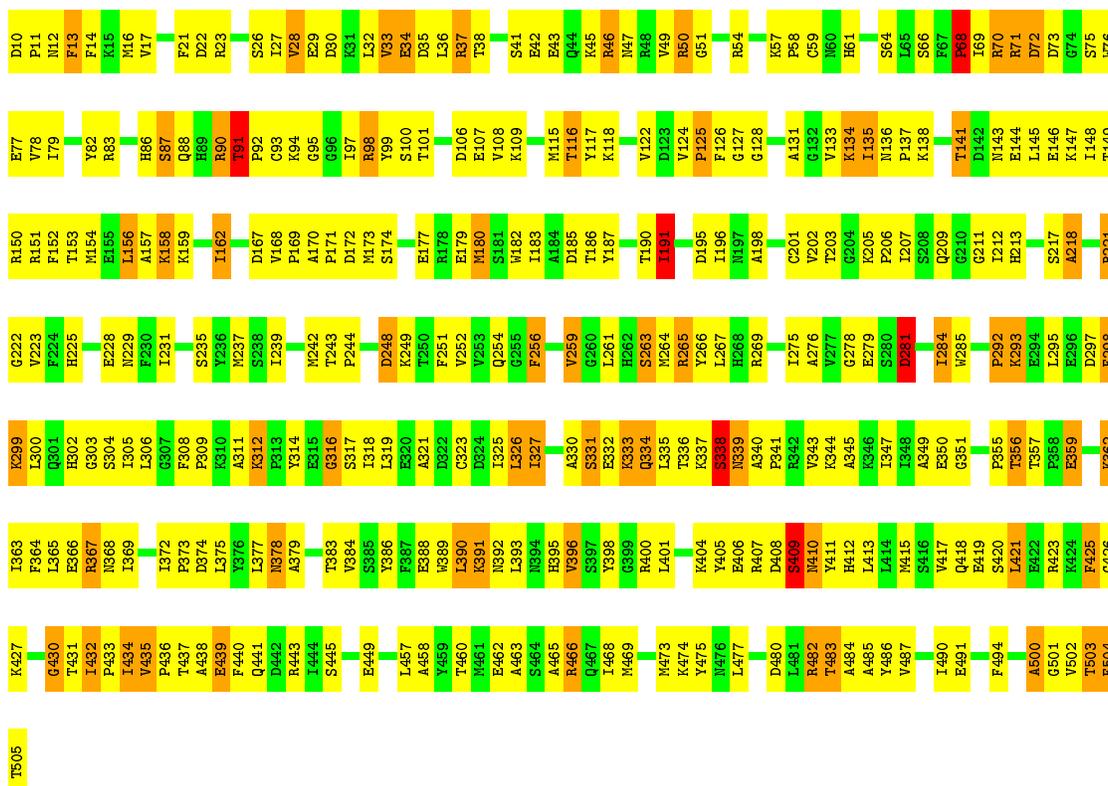
• Molecule 1: Glutamate dehydrogenase 1
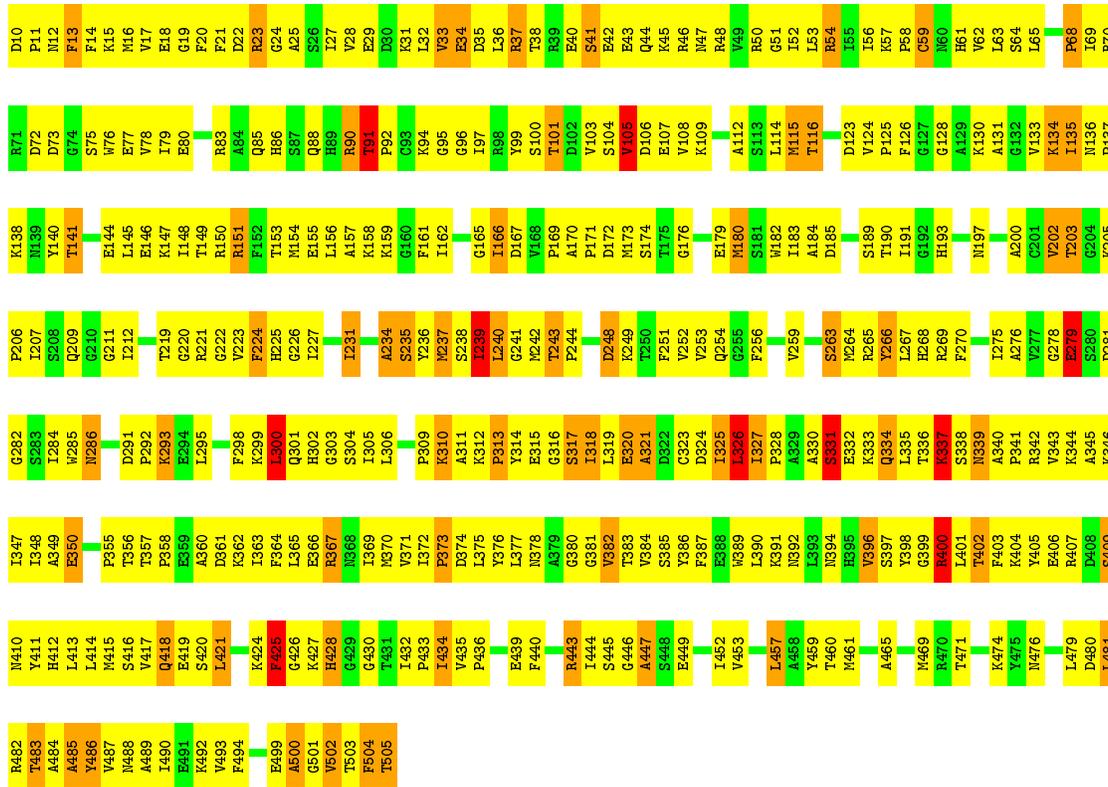
Chain D:

• Molecule 1: Glutamate dehydrogenase 1
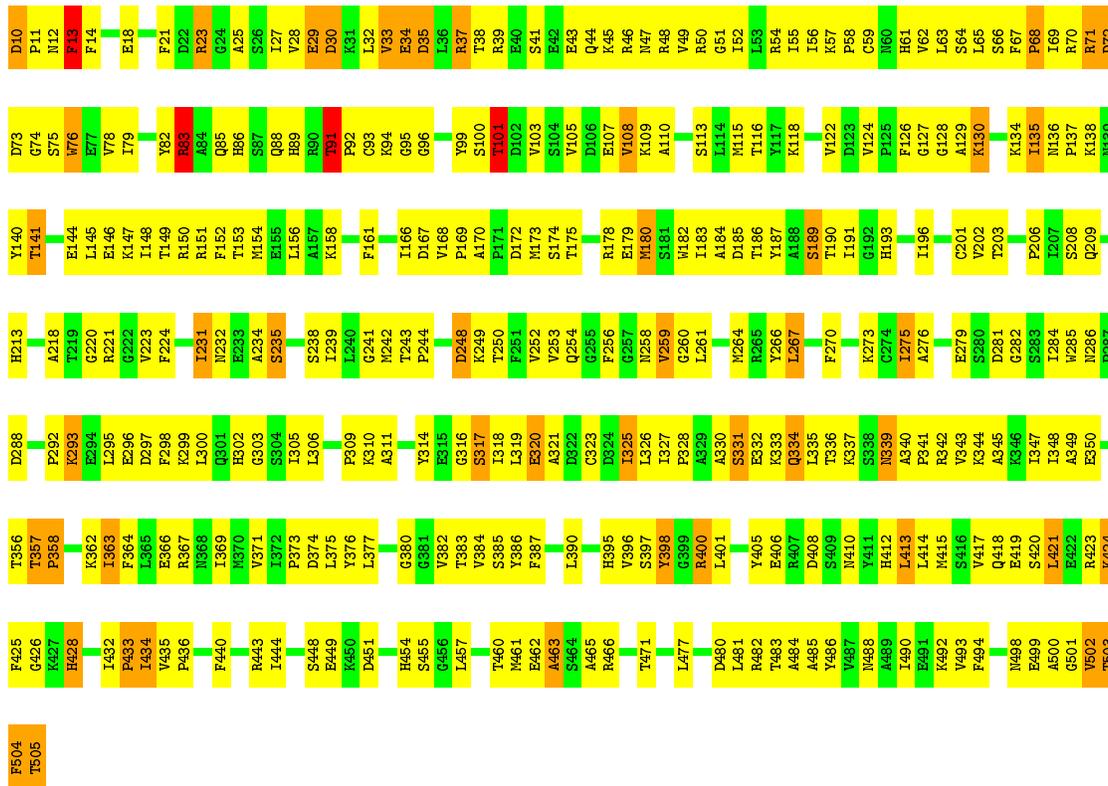
Chain E:

• Molecule 1: Glutamate dehydrogenase 1

Chain F:
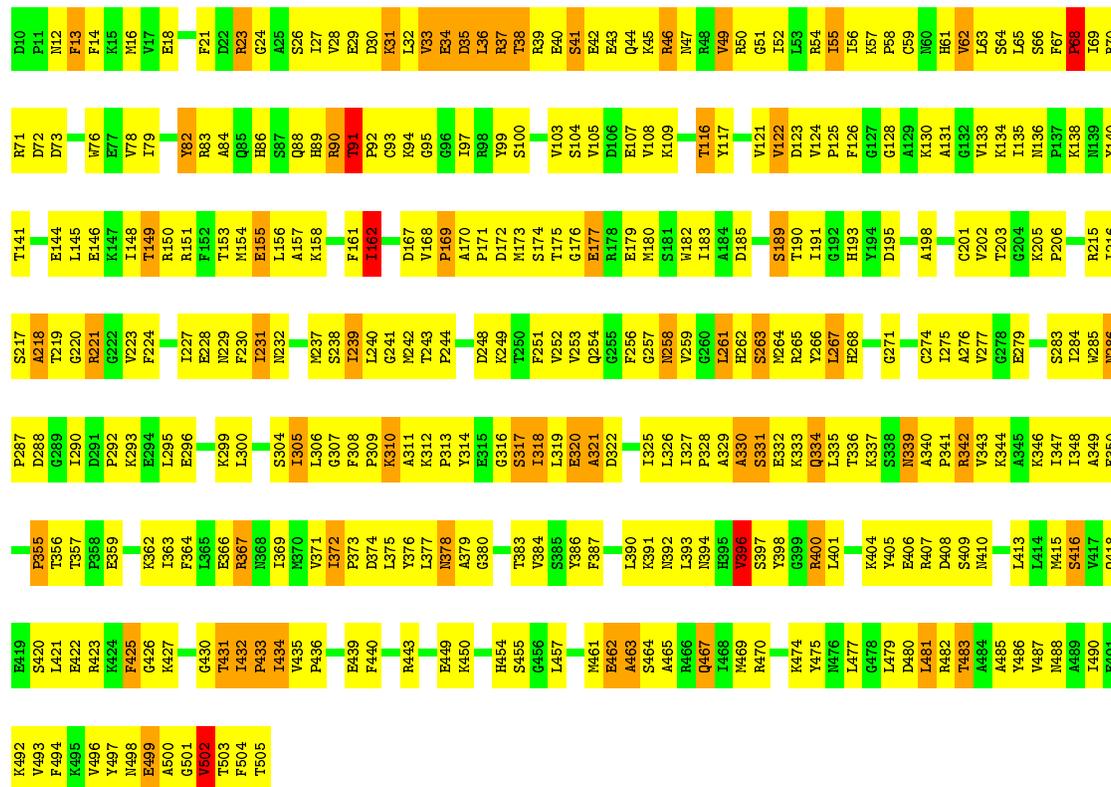
4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	96.92Å　　98.64Å　　124.26Å 86.48°　　69.69°　　60.87°	Depositor
Resolution (Å)	19.99　　–　　3.30	Depositor
% Data completeness (in resolution range)	90.9 (19.99-3.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.222　　,　　0.284	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	23208	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

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	0.68	1/3952 (0.0%)	0.85	1/5333 (0.0%)
1	B	0.65	1/3952 (0.0%)	0.86	5/5333 (0.1%)
1	C	0.66	2/3952 (0.1%)	0.86	6/5333 (0.1%)
1	D	0.66	1/3952 (0.0%)	0.87	5/5333 (0.1%)
1	E	0.63	0/3952	0.85	4/5333 (0.1%)
1	F	0.64	0/3952	0.85	3/5333 (0.1%)
All	All	0.65	5/23712 (0.0%)	0.86	24/31998 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	2
1	E	0	2
All	All	0	4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	59	CYS	CB-SG	9.46	1.98	1.82
1	C	59	CYS	CB-SG	8.70	1.97	1.82
1	D	59	CYS	CB-SG	7.67	1.95	1.82
1	C	93	CYS	CB-SG	-6.07	1.72	1.82
1	B	93	CYS	CB-SG	-5.53	1.72	1.81

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	240	LEU	CA-CB-CG	6.75	130.84	115.30
1	D	326	LEU	CA-CB-CG	6.73	130.78	115.30
1	C	316	GLY	N-CA-C	-6.33	97.27	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	504	PHE	N-CA-C	-6.12	94.47	111.00
1	C	503	THR	N-CA-C	-6.04	94.68	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	266	TYR	Sidechain
1	D	459	TYR	Sidechain
1	E	187	TYR	Sidechain
1	E	398	TYR	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3868	0	3833	532	0
1	B	3868	0	3833	437	0
1	C	3868	0	3833	430	0
1	D	3868	0	3833	506	0
1	E	3868	0	3833	415	0
1	F	3868	0	3833	487	0
All	All	23208	0	22998	2635	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 57.

The worst 5 of 2635 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:C:337:LYS:HE3	1:C:359:GLU:HG3	1.26	1.16
1:E:190:THR:HG22	1:E:191:ILE:H	1.09	1.15
1:A:251:PHE:HB3	1:A:325:ILE:HG13	1.29	1.14
1:A:71:ARG:HH11	1:A:71:ARG:HB3	1.07	1.13
1:D:86:HIS:CD2	1:D:116:THR:HG21	1.83	1.11

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	494/496 (100%)	350 (71%)	105 (21%)	39 (8%)	1	8
1	B	494/496 (100%)	366 (74%)	86 (17%)	42 (8%)	1	7
1	C	494/496 (100%)	386 (78%)	76 (15%)	32 (6%)	1	13
1	D	494/496 (100%)	374 (76%)	76 (15%)	44 (9%)	1	6
1	E	494/496 (100%)	382 (77%)	87 (18%)	25 (5%)	2	19
1	F	494/496 (100%)	358 (72%)	100 (20%)	36 (7%)	1	10
All	All	2964/2976 (100%)	2216 (75%)	530 (18%)	218 (7%)	1	10

5 of 218 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	34	GLU
1	A	35	ASP
1	A	134	LYS
1	A	173	MET
1	A	248	ASP

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	412/412 (100%)	356 (86%)	56 (14%)	5	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
1	B	412/412 (100%)	354 (86%)	58 (14%)		4	20
1	C	412/412 (100%)	355 (86%)	57 (14%)		4	20
1	D	412/412 (100%)	357 (87%)	55 (13%)		5	21
1	E	412/412 (100%)	364 (88%)	48 (12%)		7	28
1	F	412/412 (100%)	360 (87%)	52 (13%)		5	24
All	All	2472/2472 (100%)	2146 (87%)	326 (13%)		5	22

5 of 326 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	312	LYS
1	D	115	MET
1	F	288	ASP
1	C	338	SER
1	C	443	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 84 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	262	HIS
1	D	86	HIS
1	F	232	ASN
1	C	339	ASN
1	C	395	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.