



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 26, 2014 – 02:31 PM GMT

PDB ID : 2GAC
Title : T152C MUTANT GLYCOSYLASPARAGINASE FROM FLAVOBACTERIUM MENINGOSEPTICUM
Authors : Guo, H.-C.; Xu, Q.
Deposited on : 1998-05-29
Resolution : 2.10 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

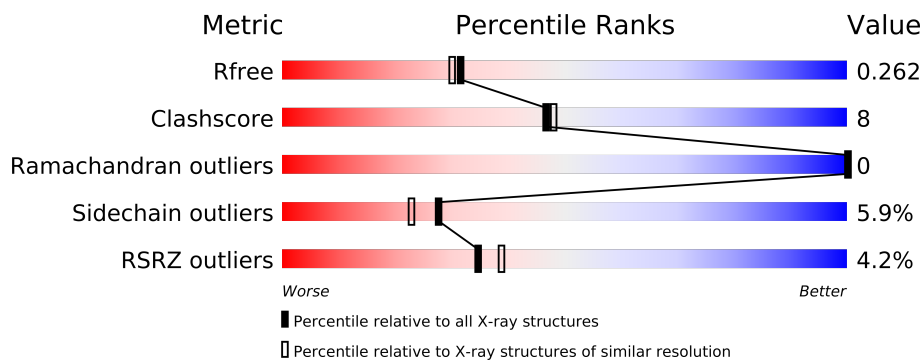
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.10 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}	66092	3012 (2.10-2.10)
Clashscore	79885	3649 (2.10-2.10)
Ramachandran outliers	78287	3610 (2.10-2.10)
Sidechain outliers	78261	3611 (2.10-2.10)
RSRZ outliers	66119	3013 (2.10-2.10)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	151	
1	C	151	
2	B	144	
2	D	144	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4432 atoms, of which 0 are hydrogen and 0 are deuterium.

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 GLYCOSYLASPARAGINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	136	Total	C	N	O	S	0	0	0
			1056	665	184	201	6			
1	C	136	Total	C	N	O	S	0	0	0
			1056	665	184	201	6			

- Molecule 2 is a protein called GLYCOSYLASPARAGINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	139	Total	C	N	O	S	0	0	0
			1037	642	191	196	8			
2	D	139	Total	C	N	O	S	0	0	0
			1037	642	191	196	8			

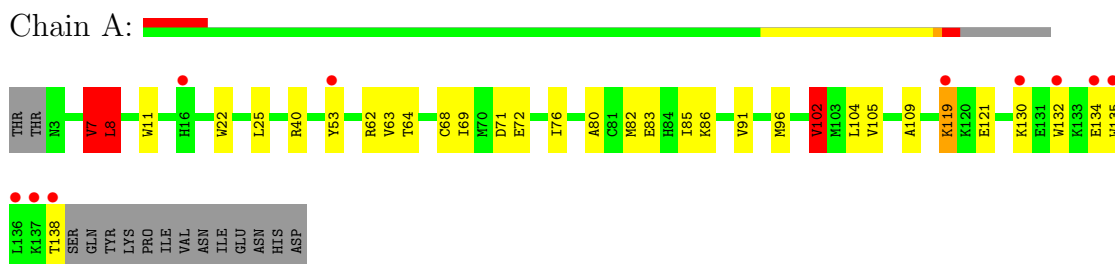
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	69	Total	O	0	0
			69	69		
3	B	52	Total	O	0	0
			52	52		
3	C	71	Total	O	0	0
			71	71		
3	D	54	Total	O	0	0
			54	54		

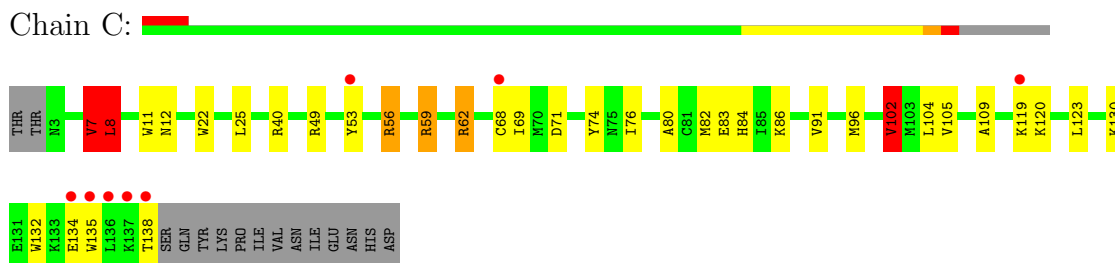
3 Residue-property plots

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

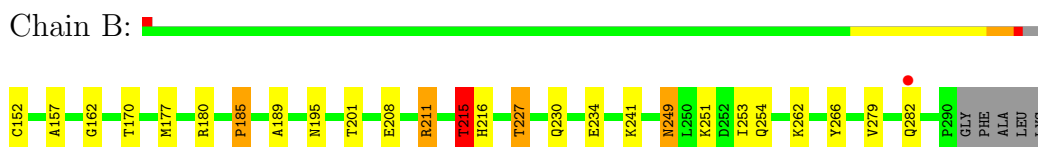
• Molecule 1: GLYCOSYLASPARAGINASE



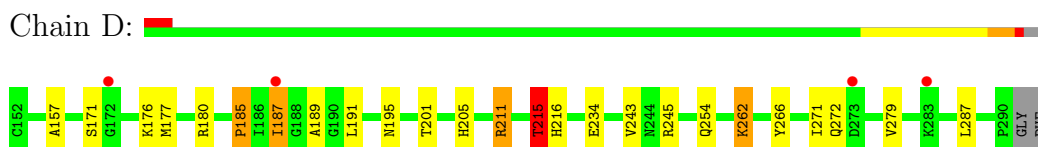
• Molecule 1: GLYCOSYLASPARAGINASE



• Molecule 2: GLYCOSYLASPARAGINASE



• Molecule 2: GLYCOSYLASPARAGINASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	46.20Å 97.30Å 61.80Å 90.00° 90.30° 90.00°	Depositor
Resolution (Å)	6.00 – 2.10 34.66 – 2.10	Depositor EDS
% Data completeness (in resolution range)	95.5 (6.00-2.10) 95.9 (34.66-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.10 (at 2.10Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.233 , 0.280 0.221 , 0.262	Depositor DCC
R_{free} test set	2893 reflections (9.92%)	DCC
Wilson B-factor (Å ²)	16.5	Xtriage
Anisotropy	0.624	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 50.8	EDS
Estimated twinning fraction	0.043 for h,-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 30512 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	4432	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 5.51% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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	0.79	0/1076	1.49	19/1453 (1.3%)
1	C	0.81	0/1076	1.61	23/1453 (1.6%)
2	B	0.67	0/1050	1.40	5/1412 (0.4%)
2	D	0.69	0/1050	1.47	11/1412 (0.8%)
All	All	0.74	0/4252	1.49	58/5730 (1.0%)

There are no bond length outliers.

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	211	ARG	NE-CZ-NH2	-17.46	111.57	120.30
2	D	211	ARG	NE-CZ-NH2	-17.23	111.69	120.30
1	C	59	ARG	NE-CZ-NH2	-14.59	113.00	120.30
2	B	211	ARG	NE-CZ-NH1	13.98	127.29	120.30
2	D	211	ARG	NE-CZ-NH1	13.65	127.12	120.30
1	C	40	ARG	NE-CZ-NH2	-10.61	115.00	120.30
1	A	40	ARG	NE-CZ-NH2	-10.06	115.27	120.30
2	D	187	ILE	CA-C-N	9.32	134.83	116.20
2	B	215	THR	N-CA-CB	-8.76	93.66	110.30
2	D	215	THR	N-CA-CB	-8.68	93.81	110.30
1	A	22	TRP	CD1-CG-CD2	8.25	112.90	106.30
1	C	22	TRP	CD1-CG-CD2	8.06	112.75	106.30
1	C	59	ARG	CB-CG-CD	-8.01	90.79	111.60
1	C	56	ARG	NE-CZ-NH2	-7.92	116.34	120.30
1	C	135	TRP	CD1-CG-CD2	7.87	112.59	106.30
1	A	22	TRP	CE2-CD2-CG	-7.82	101.05	107.30
2	D	180	ARG	NE-CZ-NH2	-7.82	116.39	120.30
1	C	11	TRP	CD1-CG-CD2	7.75	112.50	106.30
1	A	135	TRP	CD1-CG-CD2	7.71	112.47	106.30
1	C	22	TRP	CE2-CD2-CG	-7.70	101.14	107.30
1	A	132	TRP	CD1-CG-CD2	7.69	112.45	106.30
1	C	132	TRP	CD1-CG-CD2	7.63	112.40	106.30
1	A	11	TRP	CD1-CG-CD2	7.46	112.27	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	135	TRP	CE2-CD2-CG	-7.42	101.36	107.30
1	C	11	TRP	CE2-CD2-CG	-7.42	101.36	107.30
1	A	135	TRP	CE2-CD2-CG	-7.33	101.44	107.30
1	C	62	ARG	NE-CZ-NH2	-7.14	116.73	120.30
2	D	245	ARG	NE-CZ-NH1	6.92	123.76	120.30
2	D	211	ARG	CA-CB-CG	6.85	128.47	113.40
1	A	132	TRP	CE2-CD2-CG	-6.83	101.84	107.30
2	B	211	ARG	CA-CB-CG	6.82	128.41	113.40
1	A	8	LEU	CA-CB-CG	6.81	130.97	115.30
1	C	7	VAL	CB-CA-C	-6.81	98.47	111.40
1	A	11	TRP	CE2-CD2-CG	-6.78	101.87	107.30
1	C	8	LEU	CA-CB-CG	6.76	130.85	115.30
1	A	7	VAL	CB-CA-C	-6.71	98.65	111.40
1	C	132	TRP	CE2-CD2-CG	-6.64	101.99	107.30
1	A	40	ARG	NE-CZ-NH1	6.52	123.56	120.30
2	D	187	ILE	O-C-N	-6.26	112.56	123.20
1	C	40	ARG	NE-CZ-NH1	6.25	123.43	120.30
2	B	180	ARG	NE-CZ-NH2	-6.25	117.17	120.30
1	A	62	ARG	NE-CZ-NH2	-6.05	117.27	120.30
2	D	245	ARG	CA-CB-CG	5.99	126.57	113.40
1	C	102	VAL	N-CA-CB	-5.82	98.69	111.50
1	A	53	TYR	CA-C-N	5.80	127.81	116.20
1	C	71	ASP	CB-CG-OD1	5.67	123.40	118.30
1	A	102	VAL	N-CA-CB	-5.56	99.26	111.50
1	A	71	ASP	CB-CG-OD1	5.51	123.26	118.30
1	A	22	TRP	CG-CD2-CE3	5.37	138.73	133.90
1	C	74	TYR	CB-CG-CD1	-5.37	117.78	121.00
1	C	22	TRP	CG-CD2-CE3	5.29	138.67	133.90
2	D	171	SER	N-CA-C	-5.25	96.81	111.00
1	C	11	TRP	CG-CD2-CE3	5.21	138.59	133.90
1	A	22	TRP	CG-CD1-NE1	-5.18	104.92	110.10
1	C	135	TRP	CG-CD2-CE3	5.11	138.50	133.90
1	A	135	TRP	CG-CD2-CE3	5.08	138.47	133.90
2	D	171	SER	CA-C-N	5.07	126.33	116.20
1	C	22	TRP	CG-CD1-NE1	-5.06	105.04	110.10

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1056	0	1052	24	0
1	C	1056	0	1052	22	0
2	B	1037	0	1039	21	0
2	D	1037	0	1039	20	0
3	A	69	0	0	4	0
3	B	52	0	0	4	0
3	C	71	0	0	1	0
3	D	54	0	0	3	0
All	All	4432	0	4182	68	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 8.

All (68) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:82:MET:HE3	1:C:109:ALA:HB1	1.65	0.77
2:B:216:HIS:HD2	2:D:216:HIS:HD2	1.35	0.72
2:B:208:GLU:HG3	2:B:253:ILE:HG23	1.74	0.68
1:A:76:ILE:HG13	1:A:102:VAL:HG22	1.81	0.63
2:B:152:CYS:N	2:B:170:THR:HG1	1.96	0.63
3:A:668:HOH:O	2:B:282:GLN:HG2	2.00	0.62
1:A:69:ILE:HG23	1:A:96:MET:CE	2.29	0.62
1:C:69:ILE:HG23	1:C:96:MET:HE1	1.80	0.62
1:C:69:ILE:HG23	1:C:96:MET:CE	2.30	0.61
2:B:189:ALA:O	2:B:215:THR:HB	1.99	0.61
2:D:189:ALA:O	2:D:215:THR:HB	1.99	0.61
1:A:69:ILE:HG23	1:A:96:MET:HE1	1.83	0.60
1:A:68:CYS:HB3	2:B:185:PRO:HA	1.86	0.57
1:A:104:LEU:HD21	2:D:177:MET:HE3	1.86	0.56
1:C:53:TYR:HB2	1:C:86:LYS:HG3	1.89	0.55
1:A:82:MET:HE3	1:A:109:ALA:HB1	1.88	0.55
1:A:8:LEU:HD22	2:B:279:VAL:HG13	1.89	0.54
1:C:12:ASN:HA	2:D:287:LEU:HD11	1.91	0.53
1:C:76:ILE:HG13	1:C:102:VAL:HG22	1.91	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:216:HIS:HE1	3:D:683:HOH:O	1.93	0.52
1:C:8:LEU:HD11	2:D:266:TYR:HB2	1.92	0.51
1:C:84:HIS:HB3	1:C:120:LYS:HG3	1.93	0.50
1:A:104:LEU:HD11	2:D:177:MET:HE1	1.92	0.50
1:A:63:VAL:O	1:A:83:GLU:HG2	2.12	0.50
2:B:249:ASN:HD22	2:B:251:LYS:H	1.58	0.50
1:C:8:LEU:HD22	2:D:279:VAL:HG13	1.93	0.50
2:B:211:ARG:NH2	3:B:617:HOH:O	2.43	0.49
1:A:8:LEU:HD11	2:B:266:TYR:HB2	1.94	0.48
1:A:7:VAL:HG22	1:A:25:LEU:HD12	1.95	0.48
1:A:82:MET:CE	1:A:109:ALA:HB1	2.43	0.48
1:C:7:VAL:HG22	1:C:25:LEU:HD12	1.95	0.48
1:C:62:ARG:HD3	1:C:83:GLU:OE2	2.14	0.48
2:D:195:ASN:O	2:D:262:LYS:HD3	2.14	0.47
3:B:653:HOH:O	2:D:216:HIS:HE1	1.97	0.47
1:A:102:VAL:HG13	3:A:717:HOH:O	2.14	0.47
1:A:64:THR:HG22	1:A:83:GLU:HG3	1.97	0.47
1:A:86:LYS:NZ	3:A:719:HOH:O	2.48	0.46
1:C:56:ARG:HD2	3:C:677:HOH:O	2.15	0.46
1:A:69:ILE:HG23	1:A:96:MET:HE3	1.98	0.45
2:D:211:ARG:NH2	3:D:659:HOH:O	2.44	0.45
1:C:82:MET:CE	1:C:91:VAL:HG11	2.47	0.45
1:C:68:CYS:HB3	2:D:185:PRO:HA	1.99	0.45
2:B:227:THR:HG23	3:B:722:HOH:O	2.17	0.45
2:B:177:MET:HE3	1:C:104:LEU:HD21	1.99	0.44
2:B:241:LYS:NZ	3:B:761:HOH:O	2.52	0.43
1:A:85:ILE:HG21	1:A:91:VAL:HG21	2.00	0.43
1:A:104:LEU:HD21	2:D:177:MET:CE	2.49	0.43
1:A:7:VAL:HG13	2:B:157:ALA:HB2	2.01	0.43
2:B:177:MET:HB2	2:B:177:MET:HE3	1.92	0.43
1:A:76:ILE:HG13	1:A:102:VAL:CG2	2.47	0.42
2:B:216:HIS:HD2	2:D:216:HIS:CD2	2.24	0.42
1:A:119:LYS:HB3	3:A:649:HOH:O	2.19	0.42
1:C:59:ARG:HD2	2:D:177:MET:HA	2.00	0.42
1:C:69:ILE:HG23	1:C:96:MET:HE3	2.02	0.42
1:C:7:VAL:HG13	2:D:157:ALA:HB2	2.01	0.42
2:B:227:THR:HG22	2:B:230:GLN:H	1.84	0.41
2:B:162:GLY:O	2:B:262:LYS:HE3	2.20	0.41
1:A:80:ALA:HB3	1:A:105:VAL:HG12	2.02	0.41
2:D:271:ILE:HG22	2:D:272:GLN:HG3	2.02	0.41
2:B:216:HIS:CD2	2:D:216:HIS:HD2	2.25	0.41
1:C:59:ARG:HG3	2:D:176:LYS:O	2.20	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:205:HIS:HB3	3:D:765:HOH:O	2.20	0.41
1:C:80:ALA:HB3	1:C:105:VAL:HG12	2.02	0.41
1:A:72:GLU:O	2:B:195:ASN:HB2	2.21	0.40
1:A:130:LYS:O	1:A:134:GLU:HG3	2.21	0.40
1:C:130:LYS:O	1:C:134:GLU:HG3	2.21	0.40
1:C:49:ARG:HH11	1:C:49:ARG:HD3	1.67	0.40
2:D:187:ILE:O	2:D:191:LEU:O	2.38	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	134/151 (89%)	131 (98%)	3 (2%)	0	100	100
1	C	134/151 (89%)	131 (98%)	3 (2%)	0	100	100
2	B	137/144 (95%)	133 (97%)	4 (3%)	0	100	100
2	D	137/144 (95%)	132 (96%)	5 (4%)	0	100	100
All	All	542/590 (92%)	527 (97%)	15 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	113/128 (88%)	107 (95%)	6 (5%)	32	28
1	C	113/128 (88%)	107 (95%)	6 (5%)	32	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	107/110 (97%)	100 (94%)	7 (6%)	24	20
2	D	107/110 (97%)	100 (94%)	7 (6%)	24	20
All	All	440/476 (92%)	414 (94%)	26 (6%)	28	23

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

Mol	Chain	Res	Type
1	A	7	VAL
1	A	8	LEU
1	A	102	VAL
1	A	119	LYS
1	A	121	GLU
1	A	138	THR
2	B	185	PRO
2	B	201	THR
2	B	215	THR
2	B	227	THR
2	B	234	GLU
2	B	249	ASN
2	B	254	GLN
1	C	7	VAL
1	C	8	LEU
1	C	102	VAL
1	C	119	LYS
1	C	123	LEU
1	C	138	THR
2	D	185	PRO
2	D	201	THR
2	D	215	THR
2	D	234	GLU
2	D	243	VAL
2	D	254	GLN
2	D	262	LYS

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

Mol	Chain	Res	Type
2	B	216	HIS
2	B	244	ASN
2	B	249	ASN

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Mol	Chain	Res	Type
2	B	276	ASN
1	C	12	ASN
1	C	73	ASN
1	C	84	HIS
2	D	216	HIS
2	D	276	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

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

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	136/151 (90%)	0.46	10 (7%) 14 16	8, 14, 29, 35	0
1	C	136/151 (90%)	0.53	8 (5%) 22 24	8, 14, 29, 35	0
2	B	139/144 (96%)	0.29	1 (0%) 84 88	7, 13, 20, 22	0
2	D	139/144 (96%)	0.46	4 (2%) 49 54	7, 14, 21, 23	0
All	All	550/590 (93%)	0.43	23 (4%) 35 39	7, 14, 24, 35	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	137	LYS	5.5
1	C	138	THR	4.9
1	A	138	THR	4.7
1	A	134	GLU	4.2
1	A	137	LYS	4.1
2	D	273	ASP	3.8
1	A	135	TRP	3.2
1	C	136	LEU	3.1
2	D	283	LYS	2.8
1	A	119	LYS	2.8
2	D	172	GLY	2.7
1	A	136	LEU	2.7
1	C	134	GLU	2.7
1	A	16	HIS	2.6
1	C	68	CYS	2.6
1	A	130	LYS	2.6
1	C	119	LYS	2.4
1	A	53	TYR	2.4
1	C	53	TYR	2.3
1	A	132	TRP	2.2
2	B	282	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	135	TRP	2.1
2	D	187	ILE	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.