Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 12:26 AM GMT

PDB ID	:	2AFA
Title	:	Crystal Structure of putative NAG isomerase from Salmonella typhimurium
Authors	:	Kumaran, D.; Swaminathan, S.; Burley, S.K.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2005-07-25
Resolution	:	2.15 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

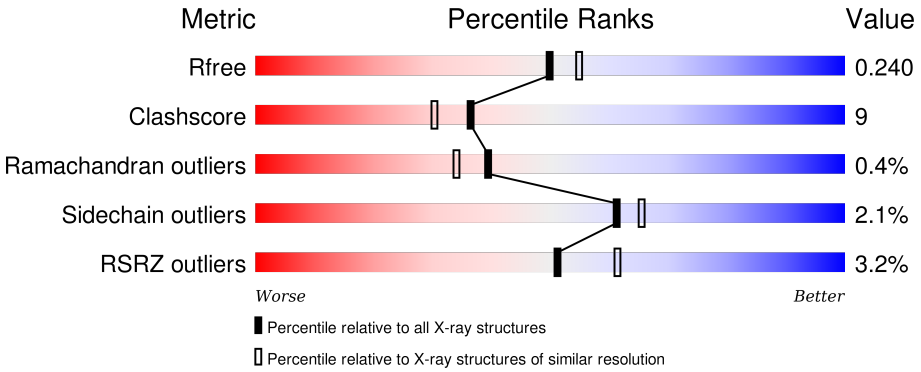
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.15 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1045 (2.16-2.16)
Clashscore	102246	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)
RSRZ outliers	91569	1050 (2.16-2.16)

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

Mol	Chain	Length	Quality of chain
1	A	425	2% 76% 20%
1	B	425	3% 72% 23%
1	C	425	4% 72% 23%
1	D	425	3% 72% 23%
1	E	425	4% 73% 22%

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Mol	Chain	Length	Quality of chain
1	F	425	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 20569 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 NAG isomerase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	408	Total	C	N	O	S	Se	0	0	0
			3318	2131	573	601	4	9			
1	B	408	Total	C	N	O	S	Se	0	0	0
			3318	2131	573	601	4	9			
1	C	408	Total	C	N	O	S	Se	0	0	0
			3318	2131	573	601	4	9			
1	D	408	Total	C	N	O	S	Se	0	0	0
			3318	2131	573	601	4	9			
1	E	408	Total	C	N	O	S	Se	0	0	0
			3318	2131	573	601	4	9			
1	F	408	Total	C	N	O	S	Se	0	0	0
			3318	2131	573	601	4	9			

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	CLONING ARTIFACT	UNP Q8ZKT7
A	2	SER	-	CLONING ARTIFACT	UNP Q8ZKT7
A	3	LEU	-	CLONING ARTIFACT	UNP Q8ZKT7
A	48	MSE	MET	MODIFIED RESIDUE	UNP Q8ZKT7
A	58	MSE	MET	MODIFIED RESIDUE	UNP Q8ZKT7
A	68	MSE	MET	MODIFIED RESIDUE	UNP Q8ZKT7
A	84	MSE	MET	MODIFIED RESIDUE	UNP Q8ZKT7
A	155	MSE	MET	MODIFIED RESIDUE	UNP Q8ZKT7
A	177	MSE	MET	MODIFIED RESIDUE	UNP Q8ZKT7
A	258	MSE	MET	MODIFIED RESIDUE	UNP Q8ZKT7
A	325	MSE	MET	MODIFIED RESIDUE	UNP Q8ZKT7
A	356	MSE	MET	MODIFIED RESIDUE	UNP Q8ZKT7
A	417	GLU	-	CLONING ARTIFACT	UNP Q8ZKT7
A	418	GLY	-	CLONING ARTIFACT	UNP Q8ZKT7
A	419	GLY	-	CLONING ARTIFACT	UNP Q8ZKT7
A	420	SER	-	CLONING ARTIFACT	UNP Q8ZKT7
A	421	HIS	-	EXPRESSION TAG	UNP Q8ZKT7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	422	HIS	-	EXPRESSION TAG	UNP Q8ZKT7
A	423	HIS	-	EXPRESSION TAG	UNP Q8ZKT7
A	424	HIS	-	EXPRESSION TAG	UNP Q8ZKT7
A	425	HIS	-	EXPRESSION TAG	UNP Q8ZKT7
A	426	HIS	-	EXPRESSION TAG	UNP Q8ZKT7
B	1	MSE	-	cloning artifact	UNP Q8ZKT7
B	2	SER	-	cloning artifact	UNP Q8ZKT7
B	3	LEU	-	cloning artifact	UNP Q8ZKT7
B	48	MSE	MET	modified residue	UNP Q8ZKT7
B	58	MSE	MET	modified residue	UNP Q8ZKT7
B	68	MSE	MET	modified residue	UNP Q8ZKT7
B	84	MSE	MET	modified residue	UNP Q8ZKT7
B	155	MSE	MET	modified residue	UNP Q8ZKT7
B	177	MSE	MET	modified residue	UNP Q8ZKT7
B	258	MSE	MET	modified residue	UNP Q8ZKT7
B	325	MSE	MET	modified residue	UNP Q8ZKT7
B	356	MSE	MET	modified residue	UNP Q8ZKT7
B	417	GLU	-	cloning artifact	UNP Q8ZKT7
B	418	GLY	-	cloning artifact	UNP Q8ZKT7
B	419	GLY	-	cloning artifact	UNP Q8ZKT7
B	420	SER	-	cloning artifact	UNP Q8ZKT7
B	421	HIS	-	EXPRESSION TAG	UNP Q8ZKT7
B	422	HIS	-	EXPRESSION TAG	UNP Q8ZKT7
B	423	HIS	-	EXPRESSION TAG	UNP Q8ZKT7
B	424	HIS	-	EXPRESSION TAG	UNP Q8ZKT7
B	425	HIS	-	EXPRESSION TAG	UNP Q8ZKT7
B	426	HIS	-	EXPRESSION TAG	UNP Q8ZKT7
C	1	MSE	-	cloning artifact	UNP Q8ZKT7
C	2	SER	-	cloning artifact	UNP Q8ZKT7
C	3	LEU	-	cloning artifact	UNP Q8ZKT7
C	48	MSE	MET	modified residue	UNP Q8ZKT7
C	58	MSE	MET	modified residue	UNP Q8ZKT7
C	68	MSE	MET	modified residue	UNP Q8ZKT7
C	84	MSE	MET	modified residue	UNP Q8ZKT7
C	155	MSE	MET	modified residue	UNP Q8ZKT7
C	177	MSE	MET	modified residue	UNP Q8ZKT7
C	258	MSE	MET	modified residue	UNP Q8ZKT7
C	325	MSE	MET	modified residue	UNP Q8ZKT7
C	356	MSE	MET	modified residue	UNP Q8ZKT7
C	417	GLU	-	cloning artifact	UNP Q8ZKT7
C	418	GLY	-	cloning artifact	UNP Q8ZKT7
C	419	GLY	-	cloning artifact	UNP Q8ZKT7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	420	SER	-	cloning artifact	UNP Q8ZKT7
C	421	HIS	-	EXPRESSION TAG	UNP Q8ZKT7
C	422	HIS	-	EXPRESSION TAG	UNP Q8ZKT7
C	423	HIS	-	EXPRESSION TAG	UNP Q8ZKT7
C	424	HIS	-	EXPRESSION TAG	UNP Q8ZKT7
C	425	HIS	-	EXPRESSION TAG	UNP Q8ZKT7
C	426	HIS	-	EXPRESSION TAG	UNP Q8ZKT7
D	1	MSE	-	cloning artifact	UNP Q8ZKT7
D	2	SER	-	cloning artifact	UNP Q8ZKT7
D	3	LEU	-	cloning artifact	UNP Q8ZKT7
D	48	MSE	MET	modified residue	UNP Q8ZKT7
D	58	MSE	MET	modified residue	UNP Q8ZKT7
D	68	MSE	MET	modified residue	UNP Q8ZKT7
D	84	MSE	MET	modified residue	UNP Q8ZKT7
D	155	MSE	MET	modified residue	UNP Q8ZKT7
D	177	MSE	MET	modified residue	UNP Q8ZKT7
D	258	MSE	MET	modified residue	UNP Q8ZKT7
D	325	MSE	MET	modified residue	UNP Q8ZKT7
D	356	MSE	MET	modified residue	UNP Q8ZKT7
D	417	GLU	-	cloning artifact	UNP Q8ZKT7
D	418	GLY	-	cloning artifact	UNP Q8ZKT7
D	419	GLY	-	cloning artifact	UNP Q8ZKT7
D	420	SER	-	cloning artifact	UNP Q8ZKT7
D	421	HIS	-	EXPRESSION TAG	UNP Q8ZKT7
D	422	HIS	-	EXPRESSION TAG	UNP Q8ZKT7
D	423	HIS	-	EXPRESSION TAG	UNP Q8ZKT7
D	424	HIS	-	EXPRESSION TAG	UNP Q8ZKT7
D	425	HIS	-	EXPRESSION TAG	UNP Q8ZKT7
D	426	HIS	-	EXPRESSION TAG	UNP Q8ZKT7
E	1	MSE	-	cloning artifact	UNP Q8ZKT7
E	2	SER	-	cloning artifact	UNP Q8ZKT7
E	3	LEU	-	cloning artifact	UNP Q8ZKT7
E	48	MSE	MET	modified residue	UNP Q8ZKT7
E	58	MSE	MET	modified residue	UNP Q8ZKT7
E	68	MSE	MET	modified residue	UNP Q8ZKT7
E	84	MSE	MET	modified residue	UNP Q8ZKT7
E	155	MSE	MET	modified residue	UNP Q8ZKT7
E	177	MSE	MET	modified residue	UNP Q8ZKT7
E	258	MSE	MET	modified residue	UNP Q8ZKT7
E	325	MSE	MET	modified residue	UNP Q8ZKT7
E	356	MSE	MET	modified residue	UNP Q8ZKT7
E	417	GLU	-	cloning artifact	UNP Q8ZKT7

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Chain	Residue	Modelled	Actual	Comment	Reference
E	418	GLY	-	cloning artifact	UNP Q8ZKT7
E	419	GLY	-	cloning artifact	UNP Q8ZKT7
E	420	SER	-	cloning artifact	UNP Q8ZKT7
E	421	HIS	-	EXPRESSION TAG	UNP Q8ZKT7
E	422	HIS	-	EXPRESSION TAG	UNP Q8ZKT7
E	423	HIS	-	EXPRESSION TAG	UNP Q8ZKT7
E	424	HIS	-	EXPRESSION TAG	UNP Q8ZKT7
E	425	HIS	-	EXPRESSION TAG	UNP Q8ZKT7
E	426	HIS	-	EXPRESSION TAG	UNP Q8ZKT7
F	1	MSE	-	cloning artifact	UNP Q8ZKT7
F	2	SER	-	cloning artifact	UNP Q8ZKT7
F	3	LEU	-	cloning artifact	UNP Q8ZKT7
F	48	MSE	MET	modified residue	UNP Q8ZKT7
F	58	MSE	MET	modified residue	UNP Q8ZKT7
F	68	MSE	MET	modified residue	UNP Q8ZKT7
F	84	MSE	MET	modified residue	UNP Q8ZKT7
F	155	MSE	MET	modified residue	UNP Q8ZKT7
F	177	MSE	MET	modified residue	UNP Q8ZKT7
F	258	MSE	MET	modified residue	UNP Q8ZKT7
F	325	MSE	MET	modified residue	UNP Q8ZKT7
F	356	MSE	MET	modified residue	UNP Q8ZKT7
F	417	GLU	-	cloning artifact	UNP Q8ZKT7
F	418	GLY	-	cloning artifact	UNP Q8ZKT7
F	419	GLY	-	cloning artifact	UNP Q8ZKT7
F	420	SER	-	cloning artifact	UNP Q8ZKT7
F	421	HIS	-	EXPRESSION TAG	UNP Q8ZKT7
F	422	HIS	-	EXPRESSION TAG	UNP Q8ZKT7
F	423	HIS	-	EXPRESSION TAG	UNP Q8ZKT7
F	424	HIS	-	EXPRESSION TAG	UNP Q8ZKT7
F	425	HIS	-	EXPRESSION TAG	UNP Q8ZKT7
F	426	HIS	-	EXPRESSION TAG	UNP Q8ZKT7

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	121	Total O 121 121	0	0
2	B	98	Total O 98 98	0	0
2	C	113	Total O 113 113	0	0
2	D	115	Total O 115 115	0	0

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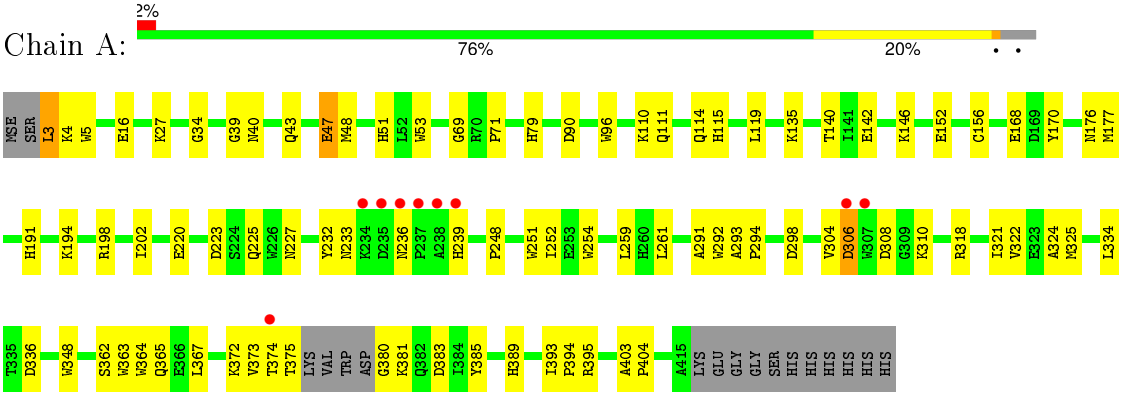
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	E	87	Total O 87 87	0	0
2	F	127	Total O 127 127	0	0

3 Residue-property plots (i)

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

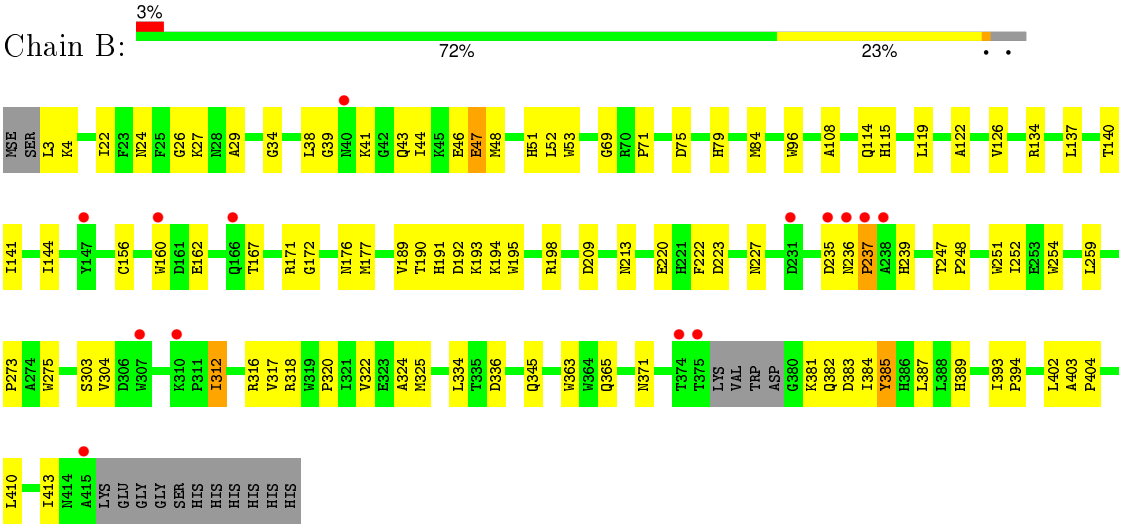
- Molecule 1: NAG isomerase

Chain A:



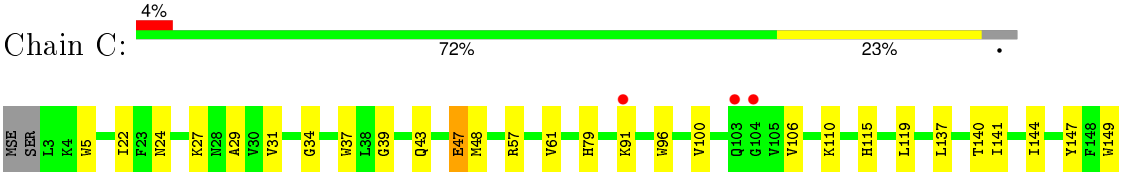
- Molecule 1: NAG isomerase

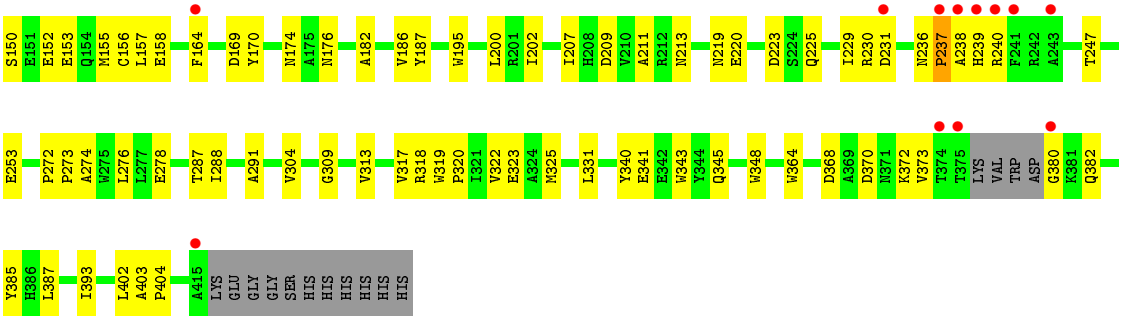
Chain B:



- Molecule 1: NAG isomerase

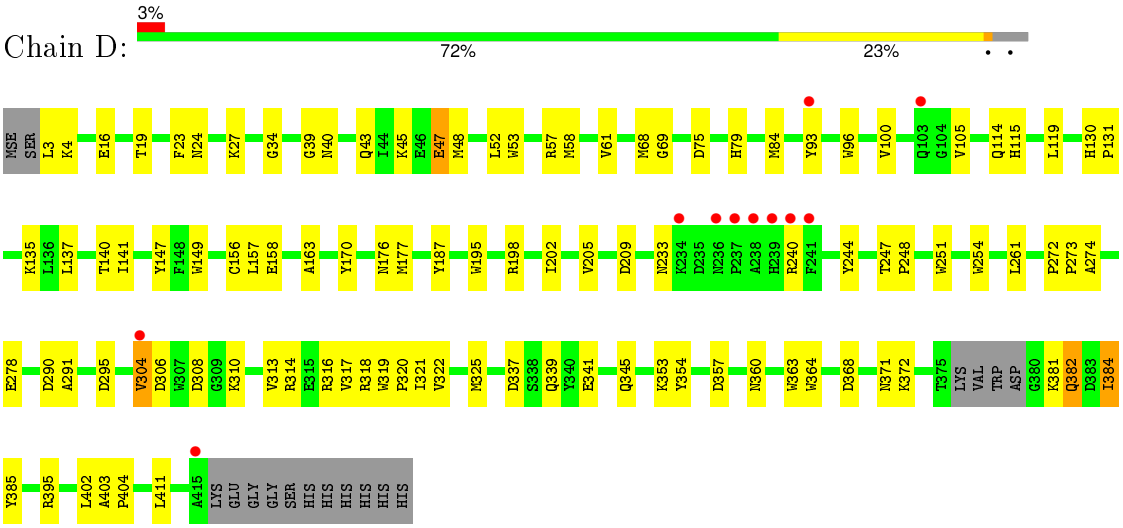
Chain C:





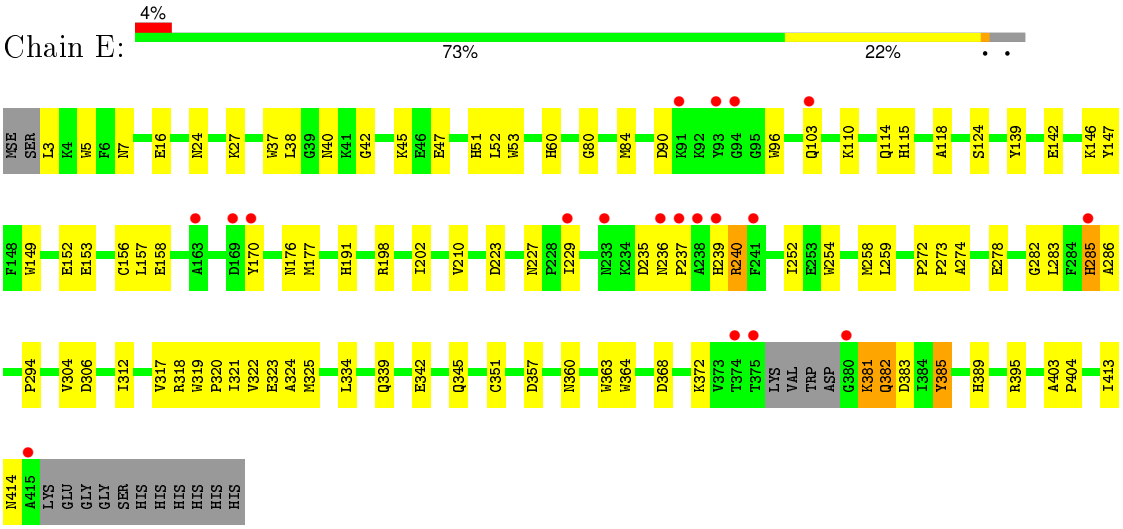
- Molecule 1: NAG isomerase

Chain D:



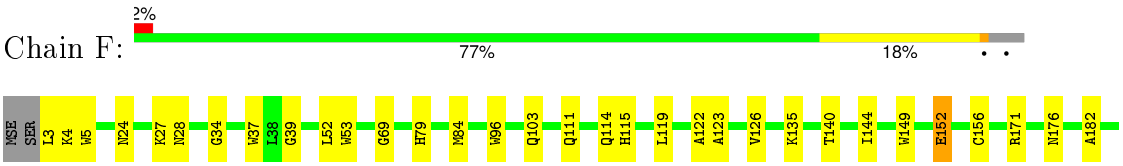
- Molecule 1: NAG isomerase

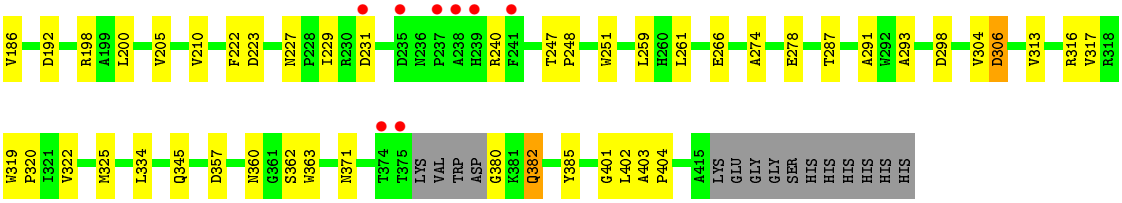
Chain E:



- Molecule 1: NAG isomerase

Chain F:




V186 D192 R198 A199 L200 V205 V210 F222 D223 N227 P228 I229 R230 D231 D235 N236 P237 A238 H239 R240 F241 T247 P248 W251 L259 H260 L261 E266 A274 E278 T287 A291 W292 A293 D298 V304 D306 V313 R316 V317 R318
W319 P320 I321 V322 M325 L334 Q345 D357 N360 G361 S362 W363 N371 T374 T375 LYS VAL TRP ASP G380 K381 Q382 Y385 G401 L402 A403 P404 A415 LYS GLU GLY GLY SER HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	88.93Å 91.14Å 95.10Å 106.81° 103.52° 111.79°	Depositor
Resolution (Å)	45.77 – 2.15 45.77 – 2.15	Depositor EDS
% Data completeness (in resolution range)	95.4 (45.77-2.15) 81.7 (45.77-2.15)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.71 (at 2.16Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.207 , 0.246 0.205 , 0.240	Depositor DCC
R_{free} test set	2517 reflections (1.98%)	DCC
Wilson B-factor (Å^2)	30.1	Xtriage
Anisotropy	0.281	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 43.2	EDS
Estimated twinning fraction	0.009 for -k,-h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 132272 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	20569	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.96% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.38	0/3414	0.60	0/4633
1	B	0.38	0/3414	0.60	0/4633
1	C	0.38	0/3414	0.59	0/4633
1	D	0.37	0/3414	0.60	0/4633
1	E	0.37	0/3414	0.59	0/4633
1	F	0.38	0/3414	0.60	0/4633
All	All	0.38	0/20484	0.59	0/27798

There are no bond length outliers.

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	3318	0	3137	60	0
1	B	3318	0	3137	61	0
1	C	3318	0	3137	67	0
1	D	3318	0	3137	76	0
1	E	3318	0	3137	65	0
1	F	3318	0	3137	49	0
2	A	121	0	0	3	0
2	B	98	0	0	4	0
2	C	113	0	0	5	0
2	D	115	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	87	0	0	3	0
2	F	127	0	0	3	0
All	All	20569	0	18822	367	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 9.

All (367) 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:E:306:ASP:HB3	1:E:312:ILE:HD11	1.48	0.94
1:D:156:CYS:H	1:D:176:ASN:HD21	1.27	0.82
1:E:176:ASN:HD22	1:E:202:ILE:HD12	1.44	0.82
1:F:156:CYS:H	1:F:176:ASN:HD21	1.29	0.79
1:C:156:CYS:H	1:C:176:ASN:HD21	1.32	0.78
1:E:259:LEU:HD22	1:E:334:LEU:HD12	1.66	0.77
1:D:58:MSE:SE	1:D:384:ILE:HD11	2.35	0.76
1:B:189:VAL:HG23	2:B:498:HOH:O	1.86	0.75
1:A:3:LEU:HD23	1:A:4:LYS:HG3	1.67	0.74
1:E:156:CYS:H	1:E:176:ASN:HD21	1.33	0.73
1:E:40:ASN:HA	1:E:381:LYS:HE2	1.70	0.73
1:F:274:ALA:O	1:F:278:GLU:HG3	1.89	0.72
1:B:29:ALA:HA	1:B:44:ILE:HD11	1.71	0.72
1:D:48:MSE:HE2	1:D:48:MSE:HA	1.70	0.72
1:C:96:TRP:H	1:C:115:HIS:HE1	1.38	0.71
1:D:176:ASN:HD22	1:D:202:ILE:HD12	1.54	0.71
1:C:368:ASP:HB2	1:C:372:LYS:H	1.55	0.71
1:F:37:TRP:CE2	1:F:382:GLN:HG2	2.25	0.71
1:A:156:CYS:H	1:A:176:ASN:HD21	1.39	0.70
1:E:322:VAL:HA	1:E:325:MSE:HE3	1.73	0.70
1:A:39:GLY:HA3	1:A:43:GLN:NE2	2.07	0.70
1:D:306:ASP:OD2	1:D:310:LYS:HB3	1.92	0.69
1:B:259:LEU:HD22	1:B:334:LEU:HD12	1.73	0.69
1:D:39:GLY:HA3	1:D:43:GLN:NE2	2.07	0.69
1:F:135:LYS:HG3	2:F:484:HOH:O	1.92	0.69
1:B:156:CYS:H	1:B:176:ASN:HD21	1.41	0.68
1:B:137:LEU:O	1:B:141:ILE:HG12	1.93	0.68
1:F:3:LEU:HD23	1:F:4:LYS:HG3	1.74	0.68
1:C:137:LEU:O	1:C:141:ILE:HG12	1.93	0.68
1:C:237:PRO:HD2	1:C:239:HIS:NE2	2.09	0.68
1:E:3:LEU:N	2:E:490:HOH:O	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:24:ASN:O	1:C:27:LYS:HG2	1.93	0.67
1:F:317:VAL:O	1:F:320:PRO:HD2	1.95	0.67
1:B:317:VAL:O	1:B:320:PRO:HD2	1.94	0.67
1:D:322:VAL:HA	1:D:325:MSE:HE3	1.77	0.67
1:B:24:ASN:O	1:B:27:LYS:HG2	1.96	0.66
1:C:322:VAL:HA	1:C:325:MSE:HE3	1.77	0.66
1:A:318:ARG:HD3	1:A:364:TRP:O	1.97	0.65
1:D:53:TRP:HB3	1:D:114:GLN:HG2	1.78	0.65
1:D:53:TRP:HH2	1:D:382:GLN:HE21	1.44	0.65
1:D:45:LYS:HB3	1:D:47:GLU:OE2	1.97	0.65
1:A:191:HIS:HD2	1:D:187:TYR:OH	1.80	0.65
1:A:348:TRP:HB3	1:B:71:PRO:HB3	1.80	0.64
1:A:322:VAL:HA	1:A:325:MSE:HE3	1.80	0.64
1:D:240:ARG:HH11	1:D:240:ARG:HG3	1.61	0.64
1:B:190:THR:HG23	2:B:498:HOH:O	1.98	0.64
1:C:96:TRP:H	1:C:115:HIS:CE1	2.17	0.63
1:E:223:ASP:HB3	1:E:229:ILE:HD11	1.80	0.63
1:B:322:VAL:HA	1:B:325:MSE:HE3	1.79	0.63
1:C:403:ALA:HB3	1:C:404:PRO:HD3	1.82	0.61
1:F:223:ASP:OD2	1:F:227:ASN:HB2	2.00	0.61
1:C:156:CYS:H	1:C:176:ASN:ND2	1.99	0.61
1:E:223:ASP:OD2	1:E:227:ASN:HB2	2.00	0.61
1:A:53:TRP:HB3	1:A:114:GLN:HG2	1.83	0.61
1:E:317:VAL:O	1:E:320:PRO:HD2	2.01	0.60
1:A:306:ASP:HB3	1:A:310:LYS:O	2.01	0.60
1:F:152:GLU:H	1:F:152:GLU:CD	2.04	0.60
1:E:149:TRP:HZ3	1:E:202:ILE:HD11	1.67	0.60
1:C:220:GLU:HB2	2:C:518:HOH:O	2.01	0.60
1:E:318:ARG:HD3	1:E:364:TRP:O	2.01	0.60
1:C:176:ASN:HD22	1:C:202:ILE:HD12	1.66	0.59
1:D:403:ALA:HB3	1:D:404:PRO:HD3	1.84	0.59
1:D:149:TRP:HZ3	1:D:202:ILE:HD11	1.67	0.59
1:A:259:LEU:HD22	1:A:334:LEU:HD12	1.84	0.59
1:C:240:ARG:HH12	1:C:313:VAL:HG11	1.68	0.59
1:A:168:GLU:HG2	1:A:170:TYR:HB3	1.84	0.58
1:D:24:ASN:O	1:D:27:LYS:HG2	2.03	0.58
1:E:235:ASP:C	1:E:237:PRO:HD3	2.24	0.58
1:C:318:ARG:HD3	1:C:364:TRP:O	2.04	0.58
1:F:24:ASN:O	1:F:27:LYS:HG2	2.03	0.58
1:B:393:ILE:HB	1:B:394:PRO:HD3	1.86	0.58
1:D:137:LEU:O	1:D:141:ILE:HG12	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:GLU:OE1	1:A:48:MSE:HE3	2.03	0.58
1:F:3:LEU:N	2:F:517:HOH:O	2.36	0.58
1:C:152:GLU:HG2	1:C:153:GLU:N	2.20	0.57
1:D:177:MSE:HB2	1:D:254:TRP:CZ2	2.40	0.57
1:D:318:ARG:HD3	1:D:364:TRP:O	2.04	0.56
1:B:383:ASP:OD2	1:B:385:TYR:HB3	2.04	0.56
1:D:141:ILE:HD12	1:D:195:TRP:CZ2	2.40	0.56
1:D:295:ASP:HB2	1:D:314:ARG:HH11	1.69	0.56
1:C:240:ARG:HG2	1:C:240:ARG:HH11	1.70	0.56
1:B:192:ASP:OD1	1:B:194:LYS:HG2	2.04	0.56
1:B:236:ASN:HB3	1:B:239:HIS:CD2	2.41	0.56
1:F:259:LEU:HD22	1:F:334:LEU:HD12	1.86	0.56
1:F:248:PRO:HG2	1:F:291:ALA:HB2	1.88	0.56
1:F:171:ARG:HB2	1:F:222:PHE:HB2	1.88	0.56
1:E:282:GLY:HA2	1:E:285:HIS:CE1	2.41	0.56
1:A:90:ASP:HB2	1:A:110:LYS:NZ	2.22	0.55
1:E:3:LEU:C	1:E:345:GLN:HE22	2.09	0.55
1:D:247:THR:HG21	2:D:538:HOH:O	2.07	0.55
1:F:200:LEU:HG	1:F:261:LEU:HD21	1.89	0.55
1:B:223:ASP:OD2	1:B:227:ASN:HB2	2.06	0.55
1:D:337:ASP:OD2	1:D:339:GLN:HG2	2.07	0.55
1:A:389:HIS:HA	1:A:393:ILE:CG1	2.36	0.54
1:B:316:ARG:HG3	1:B:371:ASN:OD1	2.06	0.54
1:D:198:ARG:O	1:D:202:ILE:HG12	2.07	0.54
1:A:318:ARG:NH2	1:A:383:ASP:O	2.40	0.54
1:B:53:TRP:HB3	1:B:114:GLN:HG2	1.88	0.54
1:D:233:ASN:O	1:D:244:TYR:HB2	2.07	0.54
1:B:141:ILE:HD12	1:B:195:TRP:CZ2	2.42	0.54
1:F:322:VAL:HA	1:F:325:MSE:HE3	1.88	0.53
1:D:45:LYS:HE3	1:D:47:GLU:OE2	2.09	0.53
1:C:368:ASP:HB3	1:C:370:ASP:H	1.74	0.53
1:D:316:ARG:HG3	1:D:371:ASN:OD1	2.07	0.53
1:A:252:ILE:HD13	1:A:324:ALA:HA	1.91	0.53
1:C:152:GLU:HG2	1:C:153:GLU:H	1.73	0.53
1:E:403:ALA:HB3	1:E:404:PRO:HD3	1.89	0.53
1:C:319:TRP:CG	1:C:320:PRO:HD3	2.43	0.53
1:A:223:ASP:OD2	1:A:227:ASN:HB2	2.09	0.53
1:B:41:LYS:HB2	1:B:43:GLN:OE1	2.08	0.53
1:E:198:ARG:O	1:E:202:ILE:HG12	2.08	0.53
1:B:389:HIS:HA	1:B:393:ILE:CG1	2.39	0.53
1:D:119:LEU:HD11	1:D:141:ILE:HD13	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:ALA:HB2	1:A:298:ASP:HA	1.91	0.53
1:A:71:PRO:HB3	1:C:348:TRP:HB3	1.90	0.53
1:E:176:ASN:ND2	1:E:202:ILE:HD12	2.20	0.53
1:B:29:ALA:HB2	1:B:38:LEU:HG	1.91	0.53
1:E:318:ARG:HD2	1:E:363:TRP:HB2	1.90	0.53
1:C:147:TYR:O	1:C:157:LEU:HD12	2.09	0.52
1:D:313:VAL:HA	2:D:498:HOH:O	2.10	0.52
1:D:384:ILE:HD13	1:D:384:ILE:N	2.23	0.52
1:F:140:THR:O	1:F:144:ILE:HG12	2.09	0.52
1:A:393:ILE:HB	1:A:394:PRO:HD3	1.92	0.52
1:D:93:TYR:CG	1:D:163:ALA:HA	2.44	0.52
1:C:382:GLN:CD	1:C:382:GLN:H	2.13	0.52
1:C:100:VAL:HA	1:C:106:VAL:HG23	1.92	0.52
1:D:205:VAL:O	1:D:209:ASP:HB3	2.10	0.52
1:A:403:ALA:HB3	1:A:404:PRO:HD3	1.90	0.52
1:D:40:ASN:HA	1:D:381:LYS:HD2	1.92	0.52
1:E:236:ASN:HB3	1:E:239:HIS:ND1	2.24	0.52
1:D:295:ASP:HB2	1:D:314:ARG:NH1	2.25	0.52
1:D:57:ARG:O	1:D:61:VAL:HG23	2.10	0.52
1:C:223:ASP:OD2	1:C:225:GLN:HG2	2.10	0.52
1:B:134:ARG:NH1	2:B:498:HOH:O	2.43	0.51
1:E:323:GLU:OE2	1:E:389:HIS:HD2	1.92	0.51
1:B:22:ILE:HG12	1:B:387:LEU:HD13	1.92	0.51
1:B:171:ARG:HB2	1:B:222:PHE:HB2	1.91	0.51
1:C:47:GLU:H	1:C:47:GLU:CD	2.13	0.51
1:C:274:ALA:O	1:C:278:GLU:HG3	2.10	0.51
1:F:37:TRP:CZ2	1:F:382:GLN:HG2	2.45	0.51
1:A:304:VAL:HG12	1:A:306:ASP:O	2.11	0.51
1:D:368:ASP:OD2	1:D:372:LYS:HB2	2.10	0.51
1:B:47:GLU:CD	1:B:48:MSE:HE2	2.30	0.51
1:D:3:LEU:HD12	1:D:4:LYS:HG3	1.93	0.51
1:E:24:ASN:O	1:E:27:LYS:HG2	2.11	0.51
1:E:240:ARG:HG2	1:E:240:ARG:HH11	1.75	0.51
1:C:187:TYR:OH	1:E:191:HIS:HD2	1.94	0.51
1:E:339:GLN:HA	1:E:342:GLU:OE1	2.11	0.50
1:D:248:PRO:HG2	1:D:291:ALA:HB2	1.92	0.50
1:C:91:LYS:HD2	1:C:91:LYS:H	1.75	0.50
1:B:235:ASP:C	1:B:237:PRO:HD3	2.32	0.50
1:C:141:ILE:HD12	1:C:195:TRP:CZ2	2.46	0.50
1:D:295:ASP:OD2	1:D:314:ARG:HD2	2.12	0.50
1:D:321:ILE:HG12	1:D:325:MSE:HE2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:53:TRP:HH2	1:D:382:GLN:NE2	2.09	0.50
1:A:39:GLY:HA3	1:A:43:GLN:HE22	1.74	0.50
1:B:160:TRP:CE2	1:B:167:THR:HB	2.47	0.50
1:F:357:ASP:OD2	1:F:360:ASN:HB2	2.11	0.50
1:C:200:LEU:HD21	1:C:276:LEU:HD11	1.93	0.49
1:A:96:TRP:H	1:A:115:HIS:CE1	2.30	0.49
1:E:236:ASN:N	1:E:237:PRO:HD3	2.26	0.49
1:C:150:SER:HB3	1:C:153:GLU:HB2	1.95	0.49
1:E:252:ILE:HD13	1:E:324:ALA:HA	1.93	0.49
1:F:111:GLN:O	1:F:115:HIS:HD2	1.95	0.49
1:A:177:MSE:HB2	1:A:254:TRP:CZ2	2.48	0.49
1:D:295:ASP:CB	1:D:314:ARG:HH11	2.24	0.49
1:E:285:HIS:CD2	1:E:286:ALA:N	2.80	0.49
1:D:240:ARG:NH1	1:D:240:ARG:HG3	2.28	0.49
1:A:389:HIS:HA	1:A:393:ILE:HG13	1.95	0.49
1:B:177:MSE:HB2	1:B:254:TRP:CZ2	2.48	0.49
1:D:357:ASP:OD2	1:D:360:ASN:HB2	2.13	0.49
1:C:169:ASP:HB3	2:C:495:HOH:O	2.13	0.49
1:E:52:LEU:HB3	1:E:114:GLN:OE1	2.12	0.48
1:B:3:LEU:HD23	1:B:4:LYS:HG3	1.96	0.48
1:A:152:GLU:H	1:A:152:GLU:CD	2.17	0.48
1:B:365:GLN:HE22	1:B:382:GLN:NE2	2.11	0.48
1:A:69:GLY:HA2	1:C:5:TRP:NE1	2.29	0.48
1:B:403:ALA:HB3	1:B:404:PRO:HD3	1.94	0.48
1:B:29:ALA:HA	1:B:44:ILE:CD1	2.42	0.48
1:E:304:VAL:HG12	1:E:306:ASP:O	2.14	0.48
1:D:34:GLY:O	1:D:79:HIS:HE1	1.96	0.48
1:B:382:GLN:O	1:B:383:ASP:HB3	2.14	0.47
1:D:147:TYR:O	1:D:157:LEU:HD12	2.14	0.47
1:E:235:ASP:C	1:E:236:ASN:HD22	2.17	0.47
1:F:304:VAL:HG12	1:F:306:ASP:O	2.14	0.47
1:E:368:ASP:HB2	1:E:372:LYS:H	1.80	0.47
1:B:52:LEU:HD11	1:B:84:MSE:HE1	1.96	0.47
1:A:96:TRP:H	1:A:115:HIS:HE1	1.63	0.47
1:A:365:GLN:HB2	1:A:380:GLY:O	2.14	0.47
1:D:384:ILE:HD13	1:D:384:ILE:H	1.79	0.47
1:D:3:LEU:C	1:D:345:GLN:HE22	2.18	0.47
1:C:219:ASN:ND2	1:C:230:ARG:HD3	2.30	0.47
1:E:37:TRP:CE2	1:E:382:GLN:HG2	2.50	0.47
1:D:318:ARG:HD2	1:D:363:TRP:HB2	1.96	0.46
1:C:29:ALA:O	1:C:31:VAL:HG13	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:GLY:HA2	1:B:220:GLU:O	2.15	0.46
1:E:60:HIS:HD2	1:E:124:SER:OG	1.97	0.46
1:A:367:LEU:HD23	1:A:373:VAL:HA	1.98	0.46
1:E:139:TYR:O	1:E:142:GLU:HB2	2.16	0.46
1:F:34:GLY:O	1:F:79:HIS:HE1	1.98	0.46
1:C:373:VAL:O	1:C:373:VAL:HG23	2.15	0.46
1:E:383:ASP:OD1	1:E:385:TYR:HB3	2.16	0.46
1:B:259:LEU:HD22	1:B:334:LEU:CD1	2.44	0.46
1:B:96:TRP:H	1:B:115:HIS:CE1	2.34	0.46
1:F:205:VAL:O	1:F:210:VAL:HG23	2.16	0.46
1:E:146:LYS:HE3	1:E:147:TYR:OH	2.16	0.46
1:D:316:ARG:HG2	1:D:368:ASP:O	2.16	0.46
1:A:306:ASP:OD2	1:A:308:ASP:N	2.27	0.45
1:B:194:LYS:O	1:B:198:ARG:HG3	2.16	0.45
1:E:80:GLY:O	1:E:84:MSE:HG2	2.16	0.45
1:C:110:LYS:HG3	1:C:164:PHE:CZ	2.51	0.45
1:F:240:ARG:HE	1:F:313:VAL:HG11	1.81	0.45
1:F:248:PRO:HB3	1:F:287:THR:HG23	1.98	0.45
1:A:389:HIS:HA	1:A:393:ILE:HG12	1.98	0.45
1:C:223:ASP:HB3	1:C:229:ILE:HD11	1.98	0.45
1:F:52:LEU:HD11	1:F:84:MSE:HE1	1.98	0.45
1:D:100:VAL:HG12	1:D:105:VAL:HA	1.98	0.45
1:F:103:GLN:NE2	2:F:545:HOH:O	2.49	0.45
1:F:293:ALA:HB2	1:F:298:ASP:HA	1.98	0.45
1:E:381:LYS:HA	2:E:457:HOH:O	2.16	0.45
1:D:158:GLU:HG2	1:D:170:TYR:HD2	1.81	0.45
1:E:152:GLU:HG2	1:E:153:GLU:N	2.32	0.45
1:E:285:HIS:HD2	1:E:286:ALA:N	2.15	0.45
1:B:193:LYS:HD2	1:F:192:ASP:HB2	1.97	0.45
1:A:236:ASN:HB3	1:A:239:HIS:ND1	2.31	0.45
1:F:3:LEU:C	1:F:345:GLN:HE22	2.20	0.45
1:C:237:PRO:C	1:C:239:HIS:H	2.19	0.45
1:B:389:HIS:HA	1:B:393:ILE:HG12	1.98	0.45
1:B:389:HIS:HA	1:B:393:ILE:HG13	1.99	0.45
1:A:111:GLN:O	1:A:115:HIS:HD2	2.00	0.45
1:D:19:THR:HG22	1:D:23:PHE:CE2	2.52	0.45
1:A:220:GLU:HG3	2:A:485:HOH:O	2.16	0.45
1:A:34:GLY:O	1:A:79:HIS:HE1	2.00	0.45
1:C:22:ILE:HD13	1:C:387:LEU:HD13	1.99	0.44
1:F:248:PRO:HA	1:F:251:TRP:CD2	2.52	0.44
1:F:96:TRP:H	1:F:115:HIS:HE1	1.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:53:TRP:O	1:D:57:ARG:HG3	2.18	0.44
1:A:259:LEU:HD22	1:A:334:LEU:CD1	2.47	0.44
1:C:174:ASN:HA	2:C:531:HOH:O	2.17	0.44
1:B:122:ALA:O	1:B:126:VAL:HG23	2.18	0.44
1:F:259:LEU:HD22	1:F:334:LEU:CD1	2.47	0.44
1:B:209:ASP:O	1:B:213:ASN:ND2	2.51	0.44
1:C:140:THR:O	1:C:144:ILE:HG12	2.17	0.44
1:B:273:PRO:HB2	1:B:275:TRP:CD1	2.52	0.44
1:C:57:ARG:O	1:C:61:VAL:HG23	2.18	0.44
1:B:303:SER:OG	1:B:312:ILE:HB	2.17	0.44
1:D:119:LEU:HA	1:D:140:THR:HG21	1.99	0.43
1:D:130:HIS:HA	1:D:131:PRO:HD3	1.89	0.43
1:C:155:MSE:SE	1:C:202:ILE:HD13	2.67	0.43
1:D:47:GLU:H	1:D:47:GLU:HG3	1.49	0.43
1:D:52:LEU:HD11	1:D:84:MSE:HE1	2.00	0.43
1:A:321:ILE:HG12	1:A:325:MSE:HE2	2.00	0.43
1:C:272:PRO:HA	1:C:273:PRO:HD3	1.92	0.43
1:E:96:TRP:H	1:E:115:HIS:CE1	2.36	0.43
1:B:34:GLY:O	1:B:79:HIS:HE1	2.01	0.43
1:E:357:ASP:OD2	1:E:360:ASN:HB2	2.18	0.43
1:E:147:TYR:O	1:E:157:LEU:HD12	2.18	0.43
1:B:248:PRO:HA	1:B:251:TRP:CD2	2.54	0.43
1:F:401:GLY:O	1:F:404:PRO:HG2	2.17	0.43
1:B:51:HIS:HD2	2:B:471:HOH:O	2.02	0.43
1:A:135:LYS:HG3	2:A:431:HOH:O	2.17	0.43
1:F:182:ALA:O	1:F:186:VAL:HG23	2.19	0.43
1:E:254:TRP:O	1:E:258:MSE:HG3	2.18	0.43
1:C:207:ILE:HA	1:C:211:ALA:HB3	1.98	0.43
1:D:47:GLU:OE1	1:D:48:MSE:HE3	2.18	0.43
1:F:119:LEU:HA	1:F:140:THR:HG21	2.01	0.43
1:F:149:TRP:CZ2	1:F:198:ARG:HG2	2.54	0.43
1:D:274:ALA:O	1:D:278:GLU:HG3	2.19	0.43
1:E:236:ASN:HB3	1:E:239:HIS:CG	2.54	0.43
1:A:119:LEU:HA	1:A:140:THR:HG21	2.00	0.43
1:E:274:ALA:O	1:E:278:GLU:HG3	2.19	0.43
1:B:141:ILE:HD12	1:B:195:TRP:CH2	2.53	0.43
1:D:341:GLU:O	1:D:345:GLN:HG3	2.18	0.43
1:C:39:GLY:HA2	1:C:380:GLY:N	2.34	0.43
1:D:317:VAL:O	1:D:320:PRO:HD2	2.19	0.42
1:D:96:TRP:H	1:D:115:HIS:CE1	2.37	0.42
1:F:362:SER:OG	1:F:363:TRP:N	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:190:THR:O	1:B:191:HIS:HB2	2.19	0.42
1:E:319:TRP:CG	1:E:320:PRO:HD3	2.54	0.42
1:E:37:TRP:CD1	1:E:45:LYS:HD3	2.54	0.42
1:C:182:ALA:O	1:C:186:VAL:HG23	2.19	0.42
1:E:158:GLU:HG2	1:E:170:TYR:HD2	1.83	0.42
1:A:232:TYR:O	1:A:233:ASN:HB2	2.19	0.42
1:D:52:LEU:HB3	1:D:114:GLN:OE1	2.19	0.42
1:D:353:LYS:HD3	1:D:354:TYR:CE1	2.55	0.42
1:A:372:LYS:NZ	1:A:372:LYS:HB3	2.35	0.42
1:F:223:ASP:HB3	1:F:229:ILE:HD11	2.00	0.42
1:A:142:GLU:O	1:A:146:LYS:HB2	2.18	0.42
1:D:69:GLY:HA2	1:F:5:TRP:CE2	2.54	0.42
1:C:236:ASN:HD22	1:C:236:ASN:N	2.16	0.42
1:D:3:LEU:CD1	1:D:4:LYS:HG3	2.49	0.42
1:C:341:GLU:O	1:C:345:GLN:HG3	2.19	0.42
1:F:53:TRP:HB3	1:F:114:GLN:HG2	2.01	0.42
1:F:316:ARG:HG3	1:F:371:ASN:OD1	2.19	0.42
1:F:96:TRP:H	1:F:115:HIS:CE1	2.37	0.42
1:E:321:ILE:HG12	1:E:325:MSE:HE2	2.02	0.42
1:B:3:LEU:C	1:B:345:GLN:HE22	2.23	0.42
1:C:119:LEU:HA	1:C:140:THR:HG21	2.00	0.42
1:E:177:MSE:HB2	1:E:254:TRP:CZ2	2.54	0.42
1:C:149:TRP:HZ3	1:C:202:ILE:HD11	1.84	0.42
1:D:248:PRO:HA	1:D:251:TRP:CD2	2.54	0.42
1:B:140:THR:O	1:B:144:ILE:HG12	2.19	0.42
1:E:51:HIS:HB3	1:E:53:TRP:CD1	2.55	0.42
1:B:26:GLY:HA3	1:B:384:ILE:HD13	2.02	0.42
1:E:325:MSE:HE1	1:E:351:CYS:SG	2.60	0.41
1:F:39:GLY:HA2	1:F:380:GLY:N	2.35	0.41
1:E:38:LEU:HD22	1:E:42:GLY:O	2.20	0.41
1:D:39:GLY:HA3	1:D:43:GLN:HE22	1.81	0.41
1:E:115:HIS:O	1:E:118:ALA:HB3	2.19	0.41
1:E:258:MSE:HE2	1:E:283:LEU:HD12	2.02	0.41
1:E:5:TRP:NE1	1:F:69:GLY:HA2	2.36	0.41
1:B:318:ARG:HD2	1:B:363:TRP:HB2	2.01	0.41
1:D:58:MSE:SE	1:D:384:ILE:CD1	3.11	0.41
1:F:122:ALA:O	1:F:126:VAL:HG23	2.21	0.41
1:D:68:MSE:HE3	1:D:411:LEU:HD21	2.03	0.41
1:C:304:VAL:HG22	1:C:309:GLY:C	2.41	0.41
1:A:5:TRP:NE1	1:B:69:GLY:HA2	2.35	0.41
1:A:194:LYS:O	1:A:198:ARG:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:ARG:O	1:A:202:ILE:HG13	2.21	0.41
1:D:16:GLU:HB2	1:D:395:ARG:NH1	2.35	0.41
1:D:319:TRP:CG	1:D:320:PRO:HD3	2.55	0.41
1:C:158:GLU:HG2	1:C:170:TYR:HD2	1.86	0.41
1:A:248:PRO:HA	1:A:251:TRP:CD2	2.55	0.41
1:A:51:HIS:HD2	2:A:520:HOH:O	2.04	0.41
1:E:272:PRO:HA	1:E:273:PRO:HD3	1.96	0.41
1:D:384:ILE:HD13	2:D:434:HOH:O	2.21	0.41
1:C:236:ASN:HB3	1:C:239:HIS:CE1	2.56	0.41
1:F:319:TRP:CG	1:F:320:PRO:HD3	2.56	0.41
1:C:240:ARG:HG2	1:C:240:ARG:NH1	2.33	0.41
1:F:259:LEU:HD23	1:F:259:LEU:HA	1.88	0.41
1:A:292:TRP:C	1:A:294:PRO:HD3	2.42	0.41
1:A:248:PRO:HG2	1:A:291:ALA:HB2	2.02	0.41
1:C:253:GLU:HG3	1:C:323:GLU:OE1	2.21	0.41
1:C:331:LEU:HD13	1:C:340:TYR:CE2	2.56	0.41
1:A:374:THR:HG22	1:A:375:THR:N	2.35	0.41
1:D:272:PRO:HA	1:D:273:PRO:HD3	1.98	0.41
1:C:393:ILE:HG23	2:C:464:HOH:O	2.21	0.41
1:A:90:ASP:HB2	1:A:110:LYS:HZ1	1.86	0.41
1:C:317:VAL:O	1:C:320:PRO:HD2	2.21	0.41
1:D:290:ASP:HB3	1:D:304:VAL:HG21	2.03	0.41
1:B:252:ILE:HD13	1:B:324:ALA:HA	2.02	0.41
1:A:40:ASN:HA	1:A:381:LYS:HD2	2.02	0.41
1:A:16:GLU:HB2	1:A:395:ARG:NH1	2.36	0.41
1:A:292:TRP:O	1:A:293:ALA:C	2.59	0.40
1:C:110:LYS:HA	2:C:462:HOH:O	2.20	0.40
1:B:39:GLY:O	1:B:381:LYS:HB2	2.21	0.40
1:B:410:LEU:HD22	1:B:413:ILE:HD12	2.03	0.40
1:D:156:CYS:H	1:D:176:ASN:ND2	2.05	0.40
1:B:119:LEU:HA	1:B:140:THR:HG21	2.01	0.40
1:E:51:HIS:CD2	1:E:53:TRP:HE1	2.38	0.40
1:E:7:ASN:ND2	2:E:430:HOH:O	2.49	0.40
1:A:27:LYS:HB3	1:A:27:LYS:HE2	1.90	0.40
1:B:108:ALA:HB1	1:B:162:GLU:HG3	2.03	0.40
1:E:240:ARG:HG2	1:E:240:ARG:NH1	2.35	0.40
1:A:5:TRP:CD1	1:B:69:GLY:HA2	2.55	0.40
1:C:288:ILE:HD13	1:C:343:TRP:CE2	2.55	0.40
1:E:413:ILE:HG23	1:E:414:ASN:N	2.36	0.40
1:C:209:ASP:O	1:C:213:ASN:ND2	2.55	0.40
1:F:403:ALA:N	1:F:404:PRO:HD2	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:287:THR:O	1:C:291:ALA:HB3	2.21	0.40
1:C:37:TRP:CZ2	1:C:48:MSE:HE3	2.56	0.40
1:A:69:GLY:HA2	1:C:5:TRP:CE2	2.57	0.40
1:F:123:ALA:O	1:F:126:VAL:HB	2.21	0.40
1:E:90:ASP:HB2	1:E:110:LYS:NZ	2.37	0.40
1:A:362:SER:OG	1:A:363:TRP:N	2.54	0.40
1:E:16:GLU:HB2	1:E:395:ARG:NH1	2.36	0.40
1:C:34:GLY:O	1:C:79:HIS:HE1	2.04	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	404/425 (95%)	386 (96%)	18 (4%)	0	100	100
1	B	404/425 (95%)	378 (94%)	22 (5%)	4 (1%)	19	11
1	C	404/425 (95%)	380 (94%)	21 (5%)	3 (1%)	26	18
1	D	404/425 (95%)	387 (96%)	16 (4%)	1 (0%)	52	51
1	E	404/425 (95%)	385 (95%)	18 (4%)	1 (0%)	52	51
1	F	404/425 (95%)	389 (96%)	14 (4%)	1 (0%)	52	51
All	All	2424/2550 (95%)	2305 (95%)	109 (4%)	10 (0%)	39	34

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	210	VAL
1	C	238	ALA
1	B	46	GLU
1	B	402	LEU

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Mol	Chain	Res	Type
1	C	237	PRO
1	C	402	LEU
1	F	402	LEU
1	B	237	PRO
1	D	402	LEU
1	B	312	ILE

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	334/339 (98%)	327 (98%)	7 (2%)	61	65
1	B	334/339 (98%)	328 (98%)	6 (2%)	66	71
1	C	334/339 (98%)	329 (98%)	5 (2%)	72	78
1	D	334/339 (98%)	325 (97%)	9 (3%)	52	53
1	E	334/339 (98%)	326 (98%)	8 (2%)	57	60
1	F	334/339 (98%)	326 (98%)	8 (2%)	57	60
All	All	2004/2034 (98%)	1961 (98%)	43 (2%)	61	65

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	47	GLU
1	A	225	GLN
1	A	261	LEU
1	A	306	ASP
1	A	336	ASP
1	A	385	TYR
1	B	47	GLU
1	B	75	ASP
1	B	247	THR
1	B	304	VAL
1	B	336	ASP

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Mol	Chain	Res	Type
1	B	385	TYR
1	C	43	GLN
1	C	47	GLU
1	C	231	ASP
1	C	247	THR
1	C	385	TYR
1	D	47	GLU
1	D	75	ASP
1	D	135	LYS
1	D	261	LEU
1	D	304	VAL
1	D	308	ASP
1	D	382	GLN
1	D	384	ILE
1	D	385	TYR
1	E	47	GLU
1	E	103	GLN
1	E	240	ARG
1	E	285	HIS
1	E	294	PRO
1	E	381	LYS
1	E	382	GLN
1	E	385	TYR
1	F	28	ASN
1	F	152	GLU
1	F	231	ASP
1	F	247	THR
1	F	266	GLU
1	F	306	ASP
1	F	382	GLN
1	F	385	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (80) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	40	ASN
1	A	51	HIS
1	A	85	ASN
1	A	115	HIS
1	A	154	GLN
1	A	176	ASN

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Mol	Chain	Res	Type
1	A	191	HIS
1	A	219	ASN
1	A	233	ASN
1	B	51	HIS
1	B	79	HIS
1	B	85	ASN
1	B	103	GLN
1	B	115	HIS
1	B	176	ASN
1	B	219	ASN
1	B	225	GLN
1	B	236	ASN
1	B	239	HIS
1	B	250	HIS
1	B	345	GLN
1	B	365	GLN
1	C	40	ASN
1	C	51	HIS
1	C	79	HIS
1	C	85	ASN
1	C	115	HIS
1	C	154	GLN
1	C	176	ASN
1	C	219	ASN
1	C	225	GLN
1	C	236	ASN
1	C	345	GLN
1	C	382	GLN
1	D	7	ASN
1	D	51	HIS
1	D	79	HIS
1	D	85	ASN
1	D	115	HIS
1	D	174	ASN
1	D	176	ASN
1	D	219	ASN
1	D	236	ASN
1	D	250	HIS
1	D	345	GLN
1	D	365	GLN
1	E	7	ASN
1	E	28	ASN

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Mol	Chain	Res	Type
1	E	40	ASN
1	E	51	HIS
1	E	60	HIS
1	E	111	GLN
1	E	115	HIS
1	E	176	ASN
1	E	191	HIS
1	E	219	ASN
1	E	225	GLN
1	E	227	ASN
1	E	233	ASN
1	E	236	ASN
1	E	262	HIS
1	E	285	HIS
1	E	345	GLN
1	E	382	GLN
1	E	389	HIS
1	F	51	HIS
1	F	79	HIS
1	F	103	GLN
1	F	115	HIS
1	F	154	GLN
1	F	176	ASN
1	F	219	ASN
1	F	227	ASN
1	F	236	ASN
1	F	239	HIS
1	F	250	HIS
1	F	339	GLN
1	F	345	GLN
1	F	382	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	399/425 (93%)	0.06	9 (2%) 64 72	15, 32, 46, 55	0
1	B	399/425 (93%)	0.13	14 (3%) 48 58	19, 35, 48, 56	0
1	C	399/425 (93%)	0.21	15 (3%) 44 54	18, 35, 49, 55	0
1	D	399/425 (93%)	0.10	11 (2%) 56 66	18, 34, 46, 55	0
1	E	399/425 (93%)	0.25	19 (4%) 34 45	19, 36, 50, 57	0
1	F	399/425 (93%)	-0.02	8 (2%) 68 75	16, 32, 46, 56	0
All	All	2394/2550 (93%)	0.12	76 (3%) 51 61	15, 34, 48, 57	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	375	THR	9.0
1	C	238	ALA	6.7
1	E	375	THR	6.4
1	D	239	HIS	5.4
1	A	237	PRO	4.9
1	B	238	ALA	4.9
1	D	237	PRO	4.9
1	C	241	PHE	4.7
1	E	380	GLY	4.5
1	C	374	THR	4.5
1	C	243	ALA	4.5
1	A	238	ALA	4.3
1	A	239	HIS	4.2
1	E	239	HIS	4.2
1	D	238	ALA	3.9
1	F	239	HIS	3.9
1	F	374	THR	3.7
1	C	237	PRO	3.7
1	E	236	ASN	3.7

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Mol	Chain	Res	Type	RSRZ
1	F	241	PHE	3.6
1	F	237	PRO	3.5
1	E	237	PRO	3.4
1	A	236	ASN	3.3
1	B	160	TRP	3.3
1	E	285	HIS	3.3
1	E	241	PHE	3.2
1	B	375	THR	3.2
1	C	415	ALA	3.1
1	E	163	ALA	3.1
1	B	231	ASP	3.0
1	C	164	PHE	3.0
1	B	415	ALA	2.9
1	E	103	GLN	2.9
1	B	374	THR	2.9
1	E	91	LYS	2.9
1	D	415	ALA	2.9
1	C	375	THR	2.8
1	E	374	THR	2.7
1	B	237	PRO	2.7
1	C	103	GLN	2.7
1	C	91	LYS	2.7
1	D	103	GLN	2.6
1	C	239	HIS	2.6
1	A	306	ASP	2.6
1	E	94	GLY	2.5
1	B	166	GLN	2.5
1	E	415	ALA	2.4
1	A	234	LYS	2.4
1	E	233	ASN	2.4
1	C	231	ASP	2.4
1	D	240	ARG	2.4
1	A	235	ASP	2.3
1	B	310	LYS	2.3
1	B	236	ASN	2.3
1	C	240	ARG	2.3
1	E	238	ALA	2.3
1	F	238	ALA	2.3
1	A	374	THR	2.3
1	A	307	TRP	2.3
1	D	234	LYS	2.3
1	C	380	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	40	ASN	2.2
1	E	229	ILE	2.2
1	F	235	ASP	2.2
1	D	93	TYR	2.2
1	D	241	PHE	2.1
1	E	93	TYR	2.1
1	E	170	TYR	2.1
1	D	304	VAL	2.1
1	E	169	ASP	2.1
1	B	307	TRP	2.1
1	B	235	ASP	2.1
1	C	104	GLY	2.1
1	D	236	ASN	2.1
1	B	147	TYR	2.0
1	F	231	ASP	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.