Full wwPDB X-ray Structure Validation Report ⓘ

Nov 2, 2023 – 02:45 AM EDT

PDB ID	:	3S8E
Title	:	Phosphorylation regulates assembly of the caspase-6 substrate-binding groove
Authors	:	Velazquez-Delgado, E.M.; Hardy, J.A.
Deposited on	:	2011-05-27
Resolution	:	2.88 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

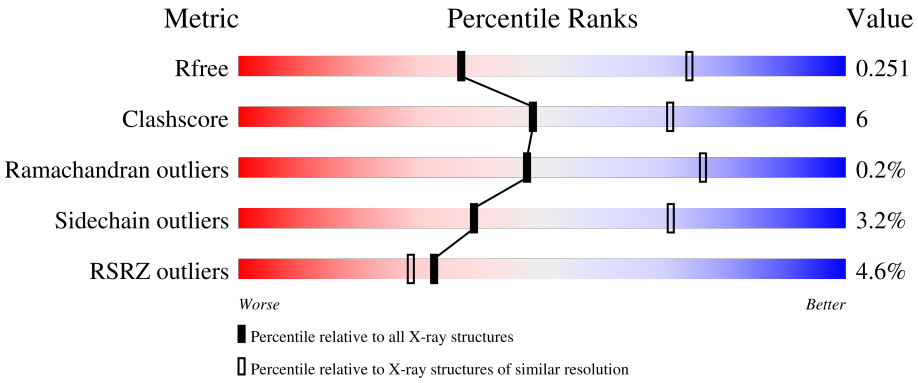
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.88 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2691 (2.90-2.86)
Clashscore	141614	2947 (2.90-2.86)
Ramachandran outliers	138981	2868 (2.90-2.86)
Sidechain outliers	138945	2871 (2.90-2.86)
RSRZ outliers	127900	2629 (2.90-2.86)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	277	4% 65% 12% • 21%
1	B	277	4% 66% 9% • 23%
1	C	277	3% 67% 10% • 21%
1	D	277	4% 67% 12% • 20%
1	E	277	4% 67% 11% • 21%

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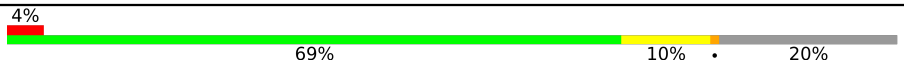
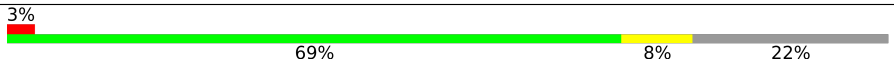
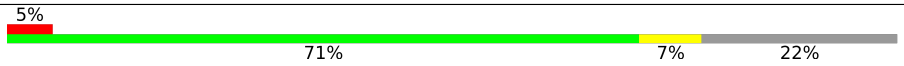
Mol	Chain	Length	Quality of chain
1	F	277	
1	G	277	
1	H	277	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 13881 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 Caspase-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	219	Total	C	N	O	S	0	0	0
			1742	1116	301	311	14			
1	B	214	Total	C	N	O	S	0	0	0
			1689	1087	289	299	14			
1	C	219	Total	C	N	O	S	0	0	0
			1726	1109	293	310	14			
1	D	221	Total	C	N	O	S	0	0	0
			1760	1127	305	314	14			
1	E	219	Total	C	N	O	S	0	0	0
			1727	1107	299	308	13			
1	F	222	Total	C	N	O	S	0	0	0
			1753	1128	300	312	13			
1	G	216	Total	C	N	O	S	0	0	0
			1714	1102	295	304	13			
1	H	217	Total	C	N	O	S	0	0	0
			1721	1106	296	306	13			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	MET	-	expression tag	UNP P55212
A	257	ASP	SER	engineered mutation	UNP P55212
A	294	HIS	-	expression tag	UNP P55212
A	295	HIS	-	expression tag	UNP P55212
A	296	HIS	-	expression tag	UNP P55212
A	297	HIS	-	expression tag	UNP P55212
A	298	HIS	-	expression tag	UNP P55212
A	299	HIS	-	expression tag	UNP P55212
B	23	MET	-	expression tag	UNP P55212
B	257	ASP	SER	engineered mutation	UNP P55212
B	294	HIS	-	expression tag	UNP P55212
B	295	HIS	-	expression tag	UNP P55212
B	296	HIS	-	expression tag	UNP P55212

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Chain	Residue	Modelled	Actual	Comment	Reference
B	297	HIS	-	expression tag	UNP P55212
B	298	HIS	-	expression tag	UNP P55212
B	299	HIS	-	expression tag	UNP P55212
C	23	MET	-	expression tag	UNP P55212
C	257	ASP	SER	engineered mutation	UNP P55212
C	294	HIS	-	expression tag	UNP P55212
C	295	HIS	-	expression tag	UNP P55212
C	296	HIS	-	expression tag	UNP P55212
C	297	HIS	-	expression tag	UNP P55212
C	298	HIS	-	expression tag	UNP P55212
C	299	HIS	-	expression tag	UNP P55212
D	23	MET	-	expression tag	UNP P55212
D	257	ASP	SER	engineered mutation	UNP P55212
D	294	HIS	-	expression tag	UNP P55212
D	295	HIS	-	expression tag	UNP P55212
D	296	HIS	-	expression tag	UNP P55212
D	297	HIS	-	expression tag	UNP P55212
D	298	HIS	-	expression tag	UNP P55212
D	299	HIS	-	expression tag	UNP P55212
E	23	MET	-	expression tag	UNP P55212
E	257	ASP	SER	engineered mutation	UNP P55212
E	294	HIS	-	expression tag	UNP P55212
E	295	HIS	-	expression tag	UNP P55212
E	296	HIS	-	expression tag	UNP P55212
E	297	HIS	-	expression tag	UNP P55212
E	298	HIS	-	expression tag	UNP P55212
E	299	HIS	-	expression tag	UNP P55212
F	23	MET	-	expression tag	UNP P55212
F	257	ASP	SER	engineered mutation	UNP P55212
F	294	HIS	-	expression tag	UNP P55212
F	295	HIS	-	expression tag	UNP P55212
F	296	HIS	-	expression tag	UNP P55212
F	297	HIS	-	expression tag	UNP P55212
F	298	HIS	-	expression tag	UNP P55212
F	299	HIS	-	expression tag	UNP P55212
G	23	MET	-	expression tag	UNP P55212
G	257	ASP	SER	engineered mutation	UNP P55212
G	294	HIS	-	expression tag	UNP P55212
G	295	HIS	-	expression tag	UNP P55212
G	296	HIS	-	expression tag	UNP P55212
G	297	HIS	-	expression tag	UNP P55212
G	298	HIS	-	expression tag	UNP P55212

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Chain	Residue	Modelled	Actual	Comment	Reference
G	299	HIS	-	expression tag	UNP P55212
H	23	MET	-	expression tag	UNP P55212
H	257	ASP	SER	engineered mutation	UNP P55212
H	294	HIS	-	expression tag	UNP P55212
H	295	HIS	-	expression tag	UNP P55212
H	296	HIS	-	expression tag	UNP P55212
H	297	HIS	-	expression tag	UNP P55212
H	298	HIS	-	expression tag	UNP P55212
H	299	HIS	-	expression tag	UNP P55212

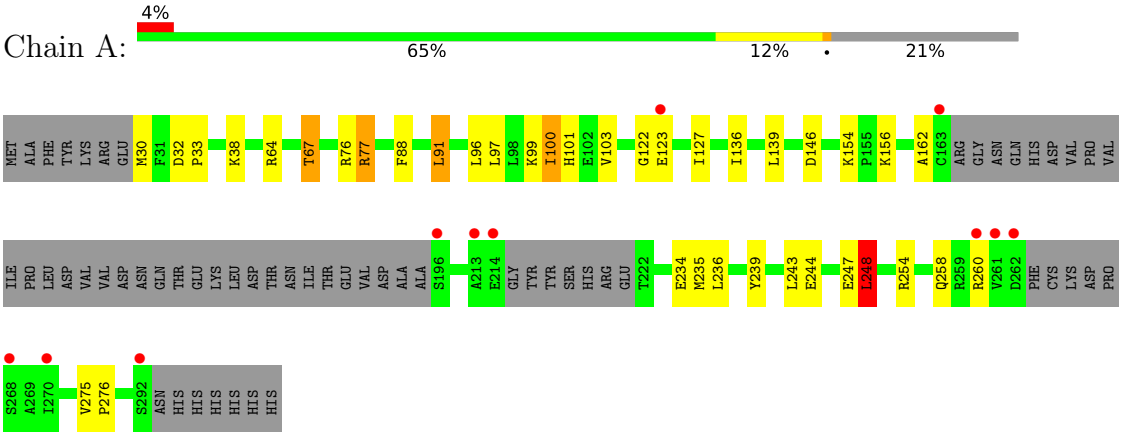
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	9	Total O 9 9	0	0
2	B	1	Total O 1 1	0	0
2	C	5	Total O 5 5	0	0
2	D	8	Total O 8 8	0	0
2	E	11	Total O 11 11	0	0
2	F	5	Total O 5 5	0	0
2	G	7	Total O 7 7	0	0
2	H	3	Total O 3 3	0	0

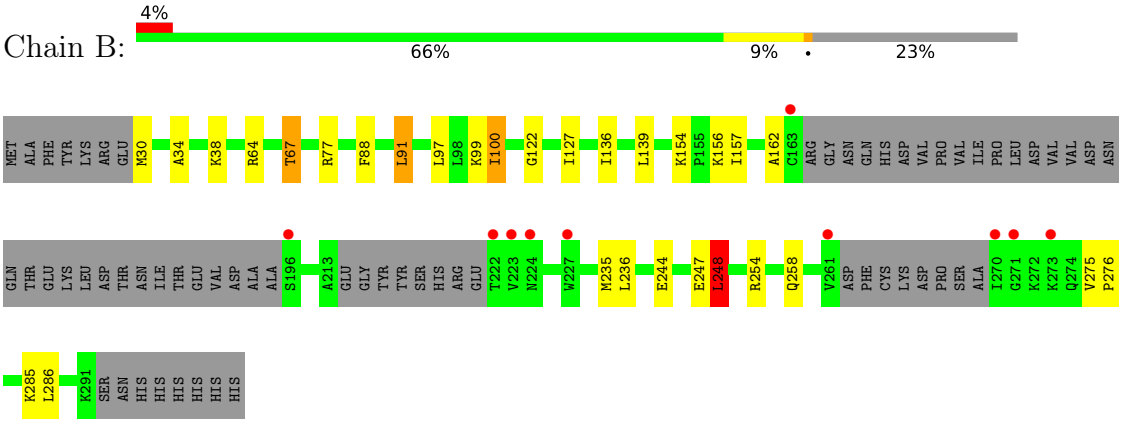
3 Residue-property plots (i)

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

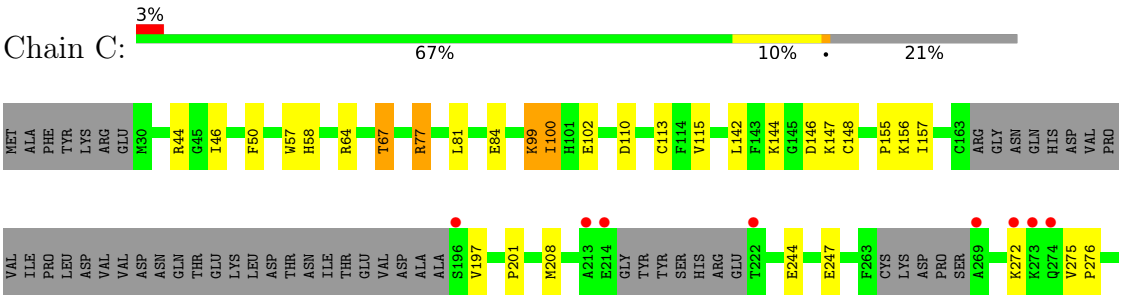
• Molecule 1: Caspase-6

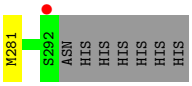


• Molecule 1: Caspase-6



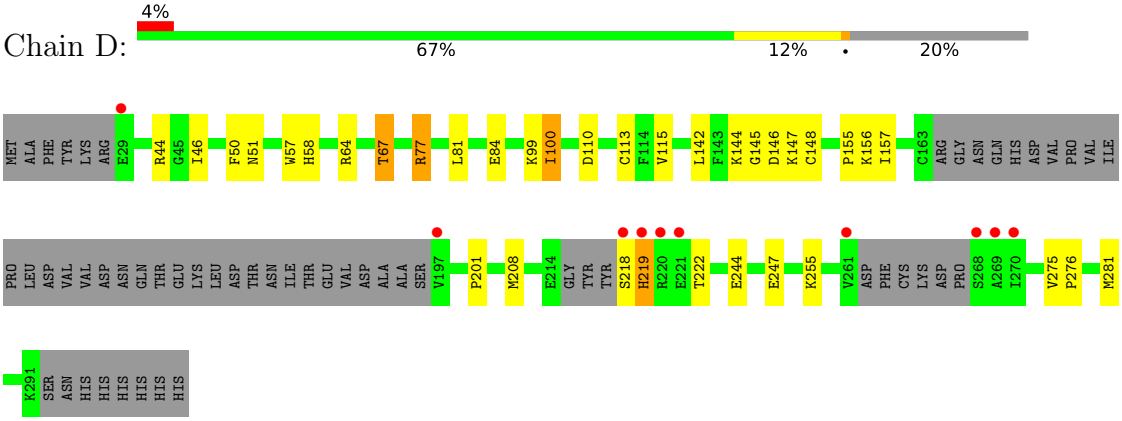
• Molecule 1: Caspase-6





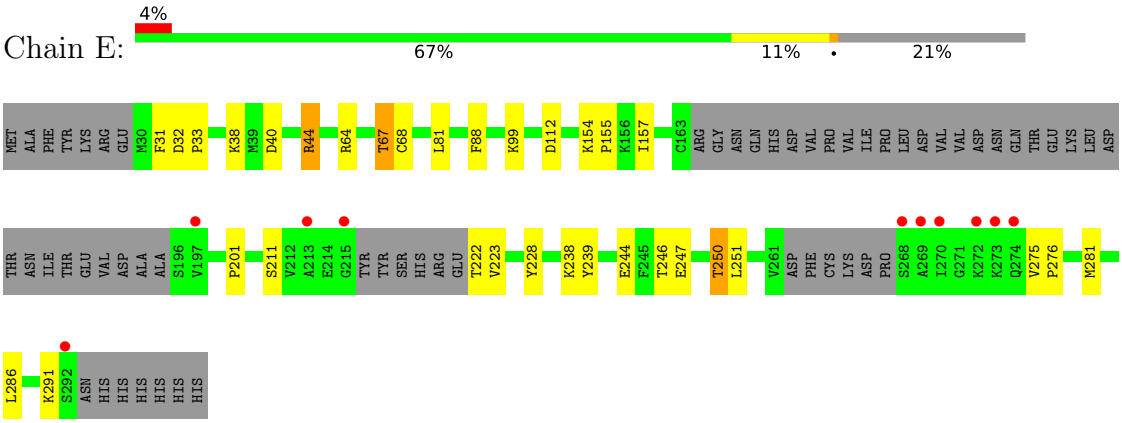
• Molecule 1: Caspase-6

Chain D:



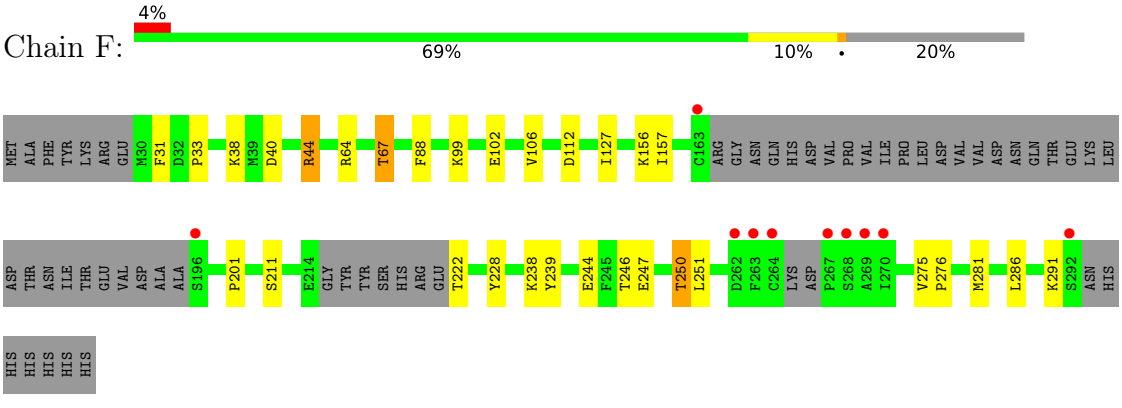
• Molecule 1: Caspase-6

Chain E:



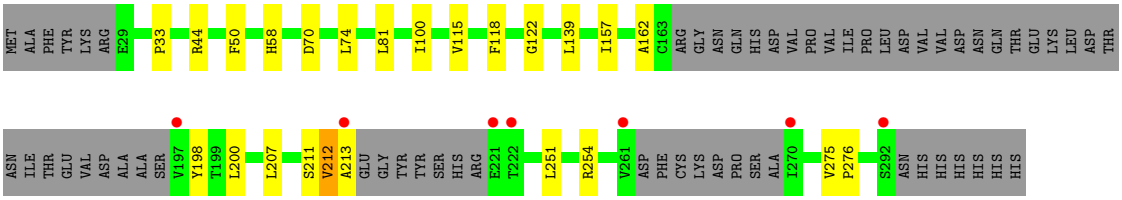
• Molecule 1: Caspase-6

Chain F:



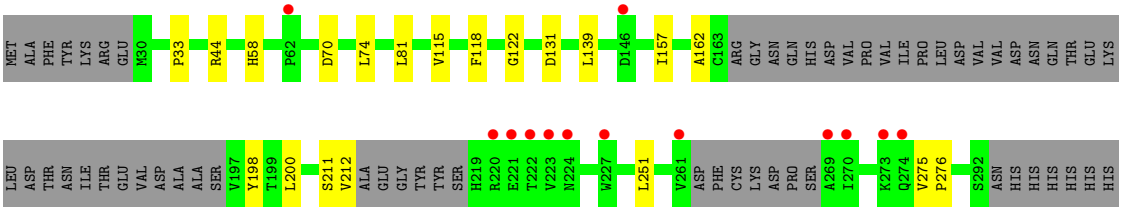
• Molecule 1: Caspase-6

Chain G:



• Molecule 1: Caspase-6

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	81.67Å 163.66Å 89.02Å 90.00° 94.17° 90.00°	Depositor
Resolution (Å)	29.59 – 2.88 29.59 – 2.88	Depositor EDS
% Data completeness (in resolution range)	90.5 (29.59-2.88) 90.5 (29.59-2.88)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) >$ [1]	1.91 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.216 , 0.256 0.211 , 0.251	Depositor DCC
R_{free} test set	2436 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	45.0	Xtriage
Anisotropy	0.122	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 25.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	13881	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.81% 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, 0.333 respectively for untwinned datasets, and 0.375, 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	0.33	0/1779	0.44	1/2393 (0.0%)
1	B	0.34	0/1726	0.44	1/2325 (0.0%)
1	C	0.33	0/1763	0.42	0/2373
1	D	0.33	0/1798	0.41	0/2419
1	E	0.33	0/1764	0.42	0/2372
1	F	0.32	0/1792	0.42	0/2411
1	G	0.32	0/1752	0.42	0/2359
1	H	0.32	0/1759	0.42	0/2368
All	All	0.33	0/14133	0.42	2/19020 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	248	LEU	CA-CB-CG	5.70	128.42	115.30
1	B	248	LEU	CA-CB-CG	5.56	128.09	115.30

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	1742	0	1713	29	0
1	B	1689	0	1654	20	0
1	C	1726	0	1683	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1760	0	1723	28	0
1	E	1727	0	1692	25	0
1	F	1753	0	1716	21	0
1	G	1714	0	1675	17	0
1	H	1721	0	1676	15	0
2	A	9	0	0	1	0
2	B	1	0	0	0	0
2	C	5	0	0	0	0
2	D	8	0	0	0	0
2	E	11	0	0	0	0
2	F	5	0	0	0	0
2	G	7	0	0	0	0
2	H	3	0	0	0	0
All	All	13881	0	13532	164	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 6.

All (164) 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:F:44:ARG:HH11	1:F:44:ARG:HG3	1.21	1.03
1:E:44:ARG:HG3	1:E:44:ARG:HH11	1.20	0.99
1:A:64:ARG:HH12	1:A:67:THR:HG21	1.27	0.98
1:B:64:ARG:HH12	1:B:67:THR:HG21	1.27	0.97
1:F:275:VAL:HB	1:F:276:PRO:HD2	1.57	0.86
1:E:275:VAL:HB	1:E:276:PRO:HD2	1.59	0.84
1:B:275:VAL:HB	1:B:276:PRO:HD2	1.61	0.83
1:E:246:THR:O	1:E:250:THR:HG22	1.81	0.81
1:A:64:ARG:NH1	1:A:67:THR:HG21	1.96	0.81
1:F:64:ARG:HH12	1:F:67:THR:HG21	1.45	0.81
1:B:64:ARG:NH1	1:B:67:THR:HG21	1.96	0.81
1:F:246:THR:O	1:F:250:THR:HG22	1.81	0.80
1:E:44:ARG:HG3	1:E:44:ARG:NH1	1.95	0.80
1:A:275:VAL:HB	1:A:276:PRO:HD2	1.64	0.79
1:D:219:HIS:CD2	1:D:222:THR:HG21	2.18	0.79
1:E:64:ARG:HH12	1:E:67:THR:HG21	1.47	0.78
1:F:44:ARG:HG3	1:F:44:ARG:NH1	1.96	0.75
1:C:113:CYS:HB3	1:C:155:PRO:HG2	1.71	0.73
1:D:219:HIS:HD2	1:D:222:THR:HG21	1.58	0.69
1:D:113:CYS:HB3	1:D:155:PRO:HG2	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:77:ARG:HH21	1:C:77:ARG:HG2	1.62	0.65
1:A:100:ILE:HD13	1:A:139:LEU:HD22	1.79	0.64
1:G:211:SER:O	1:G:212:VAL:HG22	2.00	0.61
1:B:100:ILE:HD13	1:B:139:LEU:HD22	1.83	0.60
1:D:219:HIS:CD2	1:D:222:THR:CG2	2.84	0.60
1:D:201:PRO:HA	1:D:208:MET:HE2	1.84	0.60
1:H:211:SER:O	1:H:212:VAL:HG22	2.02	0.59
1:D:44:ARG:HD2	1:D:81:LEU:O	2.02	0.59
1:C:64:ARG:HH21	1:C:67:THR:HG23	1.66	0.59
1:A:235:MET:HB3	1:A:248:LEU:HD13	1.84	0.59
1:B:235:MET:HB3	1:B:248:LEU:HD13	1.84	0.59
1:F:211:SER:HB3	1:F:228:TYR:CD2	2.38	0.59
1:A:101:HIS:CG	1:D:58:HIS:HE1	2.21	0.58
1:D:57:TRP:CZ2	1:D:58:HIS:CE1	2.91	0.58
1:D:275:VAL:HB	1:D:276:PRO:HD2	1.84	0.58
1:C:275:VAL:HB	1:C:276:PRO:HD2	1.84	0.58
1:E:64:ARG:NH1	1:E:67:THR:HG21	2.18	0.58
1:E:33:PRO:HA	1:F:251:LEU:HD11	1.85	0.57
1:F:64:ARG:HH12	1:F:67:THR:CG2	2.15	0.57
1:G:200:LEU:HG	1:H:198:TYR:HE1	1.69	0.57
1:G:200:LEU:HG	1:H:198:TYR:CE1	2.39	0.57
1:E:112:ASP:OD2	1:E:291:LYS:HE2	2.05	0.57
1:E:211:SER:HB3	1:E:228:TYR:CD2	2.40	0.57
1:H:275:VAL:HB	1:H:276:PRO:CD	2.35	0.57
1:F:64:ARG:NH1	1:F:67:THR:HG21	2.17	0.56
1:D:64:ARG:HH21	1:D:67:THR:CG2	2.18	0.56
1:H:118:PHE:CZ	1:H:139:LEU:HD13	2.41	0.56
1:C:113:CYS:CB	1:C:155:PRO:HG2	2.35	0.56
1:G:122:GLY:HA3	1:G:162:ALA:HB1	1.89	0.55
1:A:101:HIS:CG	1:D:58:HIS:CE1	2.93	0.55
1:D:64:ARG:HH21	1:D:67:THR:HG23	1.71	0.55
1:F:112:ASP:OD2	1:F:291:LYS:HE2	2.07	0.55
1:H:275:VAL:HB	1:H:276:PRO:HD2	1.89	0.55
1:C:44:ARG:HD2	1:C:81:LEU:O	2.06	0.54
1:C:201:PRO:HA	1:C:208:MET:CE	2.38	0.54
1:A:64:ARG:HH12	1:A:67:THR:CG2	2.12	0.54
1:C:275:VAL:HB	1:C:276:PRO:CD	2.38	0.54
1:G:275:VAL:HB	1:G:276:PRO:HD2	1.90	0.54
1:G:118:PHE:CZ	1:G:139:LEU:HD13	2.41	0.54
1:G:275:VAL:HB	1:G:276:PRO:CD	2.37	0.54
1:D:201:PRO:HA	1:D:208:MET:CE	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:ARG:HD2	2:A:304:HOH:O	2.08	0.53
1:F:244:GLU:O	1:F:247:GLU:HB2	2.09	0.53
1:D:113:CYS:CB	1:D:155:PRO:HG2	2.38	0.53
1:C:64:ARG:HH21	1:C:67:THR:CG2	2.22	0.53
1:E:244:GLU:O	1:E:247:GLU:HB2	2.09	0.53
1:G:198:TYR:HE1	1:H:200:LEU:HG	1.74	0.53
1:E:64:ARG:HH12	1:E:67:THR:CG2	2.18	0.53
1:G:198:TYR:CE1	1:H:200:LEU:HG	2.45	0.52
1:B:64:ARG:HH12	1:B:67:THR:CG2	2.13	0.52
1:D:275:VAL:HB	1:D:276:PRO:CD	2.39	0.52
1:A:122:GLY:HA3	1:A:162:ALA:HB1	1.92	0.52
1:C:99:LYS:HE3	1:C:102:GLU:OE2	2.09	0.51
1:A:248:LEU:C	1:A:248:LEU:HD12	2.31	0.51
1:F:201:PRO:HB2	1:F:281:MET:SD	2.51	0.51
1:H:122:GLY:HA3	1:H:162:ALA:HB1	1.90	0.51
1:A:244:GLU:O	1:A:247:GLU:HB2	2.10	0.51
1:C:57:TRP:CZ2	1:C:58:HIS:CE1	2.99	0.51
1:D:201:PRO:HB2	1:D:281:MET:SD	2.51	0.51
1:B:122:GLY:HA3	1:B:162:ALA:HB1	1.92	0.51
1:A:154:LYS:O	1:A:156:LYS:HE2	2.11	0.50
1:B:248:LEU:C	1:B:248:LEU:HD12	2.31	0.50
1:E:88:PHE:CZ	1:E:99:LYS:HD2	2.46	0.50
1:C:272:LYS:HA	1:D:145:GLY:HA3	1.94	0.50
1:A:123:GLU:HG3	1:A:123:GLU:O	2.11	0.49
1:B:154:LYS:O	1:B:156:LYS:HE2	2.11	0.49
1:G:70:ASP:O	1:G:74:LEU:HB2	2.13	0.49
1:B:88:PHE:CZ	1:B:99:LYS:HD2	2.47	0.48
1:H:70:ASP:O	1:H:74:LEU:HB2	2.13	0.48
1:B:34:ALA:HA	1:B:285:LYS:HE2	1.95	0.48
1:F:88:PHE:CZ	1:F:99:LYS:HD2	2.49	0.47
1:C:201:PRO:HB2	1:C:281:MET:SD	2.54	0.47
1:C:201:PRO:HA	1:C:208:MET:HE2	1.96	0.47
1:E:275:VAL:HB	1:E:276:PRO:CD	2.38	0.47
1:E:201:PRO:HB2	1:E:281:MET:SD	2.54	0.47
1:C:115:VAL:HG22	1:C:157:ILE:HB	1.96	0.47
1:A:76:ARG:HD3	1:E:68:CYS:HB2	1.96	0.47
1:B:236:LEU:HD12	1:B:248:LEU:HD21	1.96	0.47
1:B:244:GLU:O	1:B:247:GLU:HB2	2.15	0.46
1:C:64:ARG:NH2	1:C:67:THR:HG23	2.29	0.46
1:D:144:LYS:O	1:D:147:LYS:O	2.33	0.46
1:A:236:LEU:HD12	1:A:248:LEU:HD21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:38:LYS:NZ	1:E:40:ASP:OD1	2.49	0.46
1:F:44:ARG:HB2	1:F:291:LYS:HD2	1.99	0.45
1:D:115:VAL:HG22	1:D:157:ILE:HB	1.97	0.45
1:D:77:ARG:HD2	1:D:77:ARG:HA	1.75	0.45
1:D:64:ARG:NH2	1:D:67:THR:HG23	2.31	0.45
1:F:38:LYS:NZ	1:F:40:ASP:OD1	2.48	0.45
1:E:44:ARG:HB2	1:E:291:LYS:HD2	1.98	0.45
1:G:251:LEU:HD21	1:H:33:PRO:HB3	1.98	0.45
1:A:97:LEU:HD23	1:A:100:ILE:HD11	1.99	0.45
1:E:44:ARG:NE	1:E:81:LEU:O	2.48	0.45
1:G:33:PRO:HB3	1:H:251:LEU:HD21	1.98	0.45
1:G:115:VAL:HG22	1:G:157:ILE:HB	1.99	0.44
1:D:46:ILE:HD13	1:D:84:GLU:HB3	1.99	0.44
1:E:32:ASP:HA	1:E:33:PRO:HD3	1.87	0.44
1:B:97:LEU:HD23	1:B:100:ILE:HD11	1.99	0.44
1:D:218:SER:HA	1:D:219:HIS:HA	1.63	0.44
1:A:127:ILE:HB	1:A:136:ILE:HD11	1.98	0.44
1:A:88:PHE:HB3	1:A:91:LEU:HD22	1.98	0.44
1:A:275:VAL:HB	1:A:276:PRO:CD	2.43	0.44
1:B:127:ILE:HB	1:B:136:ILE:HD11	1.99	0.44
1:C:46:ILE:HD13	1:C:84:GLU:HB3	2.00	0.43
1:B:254:ARG:O	1:B:258:GLN:HG2	2.18	0.43
1:G:44:ARG:HD2	1:G:81:LEU:O	2.18	0.43
1:A:77:ARG:HD2	1:A:77:ARG:HA	1.77	0.43
1:F:44:ARG:NH1	1:F:44:ARG:CG	2.73	0.43
1:F:157:ILE:HD11	1:F:286:LEU:HD21	2.00	0.43
1:A:88:PHE:CZ	1:A:99:LYS:HD2	2.54	0.42
1:A:239:TYR:HB3	1:A:243:LEU:HD22	2.01	0.42
1:D:244:GLU:O	1:D:247:GLU:HB3	2.19	0.42
1:C:244:GLU:O	1:C:247:GLU:HB3	2.19	0.42
1:A:32:ASP:HA	1:A:33:PRO:HD3	1.92	0.42
1:A:254:ARG:O	1:A:258:GLN:HG2	2.19	0.42
1:A:77:ARG:HB3	1:A:236:LEU:HD23	2.01	0.42
1:E:157:ILE:HD11	1:E:286:LEU:HD21	2.01	0.42
1:F:238:LYS:HE3	1:F:239:TYR:OH	2.20	0.42
1:C:100:ILE:CG2	1:C:142:LEU:HD12	2.50	0.42
1:C:144:LYS:O	1:C:147:LYS:O	2.37	0.42
1:C:50:PHE:CZ	1:C:100:ILE:HG12	2.54	0.42
1:E:238:LYS:HE3	1:E:239:TYR:OH	2.20	0.42
1:E:44:ARG:NH1	1:E:44:ARG:CG	2.72	0.41
1:D:50:PHE:CZ	1:D:100:ILE:HG12	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:251:LEU:HD11	1:F:33:PRO:HA	2.01	0.41
1:H:44:ARG:HD2	1:H:81:LEU:O	2.21	0.41
1:D:100:ILE:CG2	1:D:142:LEU:HD12	2.50	0.41
1:G:50:PHE:CZ	1:G:100:ILE:HG12	2.55	0.41
1:H:115:VAL:HG22	1:H:157:ILE:HB	2.02	0.41
1:G:211:SER:C	1:G:213:ALA:H	2.24	0.41
1:A:96:LEU:O	1:A:100:ILE:HG12	2.21	0.41
1:D:219:HIS:CD2	1:D:219:HIS:H	2.37	0.41
1:H:131:ASP:OD1	1:H:131:ASP:N	2.54	0.41
1:A:99:LYS:O	1:A:103:VAL:HG23	2.20	0.41
1:C:77:ARG:HH21	1:C:77:ARG:CG	2.31	0.41
1:D:51:ASN:OD1	1:D:67:THR:HB	2.21	0.41
1:F:102:GLU:O	1:F:106:VAL:HG23	2.21	0.41
1:F:275:VAL:HB	1:F:276:PRO:CD	2.37	0.41
1:B:64:ARG:NH1	1:B:67:THR:CG2	2.77	0.40
1:B:157:ILE:HD11	1:B:286:LEU:HD21	2.03	0.40
1:G:157:ILE:HG23	1:G:207:LEU:HD23	2.02	0.40
1:E:154:LYS:HA	1:E:155:PRO:HD3	1.97	0.40
1:A:234:GLU:HG3	1:E:223:VAL:HG21	2.02	0.40
1:B:88:PHE:HB3	1:B:91:LEU:HD22	2.03	0.40
1:B:127:ILE:HB	1:B:136:ILE:CD1	2.52	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	211/277 (76%)	202 (96%)	9 (4%)	0	100	100
1	B	206/277 (74%)	198 (96%)	8 (4%)	0	100	100
1	C	211/277 (76%)	197 (93%)	12 (6%)	2 (1%)	17	45
1	D	213/277 (77%)	201 (94%)	11 (5%)	1 (0%)	29	59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	211/277 (76%)	201 (95%)	10 (5%)	0	100	100
1	F	214/277 (77%)	205 (96%)	9 (4%)	0	100	100
1	G	208/277 (75%)	195 (94%)	12 (6%)	1 (0%)	29	59
1	H	209/277 (76%)	198 (95%)	11 (5%)	0	100	100
All	All	1683/2216 (76%)	1597 (95%)	82 (5%)	4 (0%)	47	76

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	212	VAL
1	C	148	CYS
1	D	148	CYS
1	C	197	VAL

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	187/245 (76%)	178 (95%)	9 (5%)	25	56
1	B	180/245 (74%)	173 (96%)	7 (4%)	32	64
1	C	183/245 (75%)	176 (96%)	7 (4%)	33	65
1	D	188/245 (77%)	179 (95%)	9 (5%)	25	56
1	E	183/245 (75%)	178 (97%)	5 (3%)	44	75
1	F	186/245 (76%)	179 (96%)	7 (4%)	33	65
1	G	182/245 (74%)	180 (99%)	2 (1%)	73	90
1	H	182/245 (74%)	181 (100%)	1 (0%)	88	96
All	All	1471/1960 (75%)	1424 (97%)	47 (3%)	39	71

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	MET
1	A	38	LYS
1	A	67	THR
1	A	77	ARG
1	A	91	LEU
1	A	100	ILE
1	A	146	ASP
1	A	248	LEU
1	A	260	ARG
1	B	30	MET
1	B	38	LYS
1	B	67	THR
1	B	77	ARG
1	B	91	LEU
1	B	100	ILE
1	B	248	LEU
1	C	67	THR
1	C	77	ARG
1	C	99	LYS
1	C	100	ILE
1	C	110	ASP
1	C	146	ASP
1	C	156	LYS
1	D	67	THR
1	D	77	ARG
1	D	99	LYS
1	D	100	ILE
1	D	110	ASP
1	D	146	ASP
1	D	156	LYS
1	D	219	HIS
1	D	255	LYS
1	E	31	PHE
1	E	44	ARG
1	E	67	THR
1	E	222	THR
1	E	250	THR
1	F	31	PHE
1	F	44	ARG
1	F	67	THR
1	F	127	ILE
1	F	156	LYS
1	F	222	THR

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Mol	Chain	Res	Type
1	F	250	THR
1	G	58	HIS
1	G	254	ARG
1	H	58	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	HIS
1	B	224	ASN
1	B	287	HIS
1	C	58	HIS
1	D	58	HIS
1	D	101	HIS
1	D	219	HIS
1	F	125	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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, 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	219/277 (79%)	-0.20	11 (5%)	28	25	17, 35, 92, 129	0
1	B	214/277 (77%)	-0.12	10 (4%)	31	27	24, 43, 96, 143	0
1	C	219/277 (79%)	-0.07	9 (4%)	37	32	25, 52, 102, 128	0
1	D	221/277 (79%)	-0.15	10 (4%)	33	29	16, 38, 107, 143	0
1	E	219/277 (79%)	-0.20	10 (4%)	32	28	18, 37, 94, 142	0
1	F	222/277 (80%)	-0.05	10 (4%)	33	29	24, 46, 107, 144	0
1	G	216/277 (77%)	-0.24	7 (3%)	47	43	17, 37, 91, 131	0
1	H	217/277 (78%)	-0.05	13 (5%)	21	17	25, 51, 113, 136	0
All	All	1747/2216 (78%)	-0.13	80 (4%)	32	28	16, 43, 104, 144	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	222	THR	7.9
1	B	270	ILE	6.0
1	F	267	PRO	5.8
1	C	292	SER	5.6
1	E	272	LYS	5.2
1	F	264	CYS	4.3
1	D	221	GLU	4.3
1	E	270	ILE	4.3
1	D	270	ILE	4.3
1	D	218	SER	4.1
1	E	292	SER	4.1
1	E	268	SER	4.0
1	H	221	GLU	3.9
1	A	214	GLU	3.9
1	F	268	SER	3.8
1	F	269	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	269	ALA	3.7
1	H	269	ALA	3.5
1	B	223	VAL	3.5
1	D	219	HIS	3.5
1	F	263	PHE	3.4
1	B	222	THR	3.4
1	A	196	SER	3.4
1	E	213	ALA	3.3
1	H	274	GLN	3.3
1	A	213	ALA	3.2
1	A	262	ASP	3.2
1	C	214	GLU	3.2
1	G	270	ILE	3.1
1	B	224	ASN	3.1
1	A	292	SER	3.1
1	E	273	LYS	2.9
1	E	274	GLN	2.8
1	F	292	SER	2.8
1	F	262	ASP	2.8
1	B	163	CYS	2.8
1	B	273	LYS	2.8
1	B	196	SER	2.8
1	H	270	ILE	2.7
1	H	261	VAL	2.7
1	H	220	ARG	2.7
1	A	270	ILE	2.7
1	F	196	SER	2.6
1	C	222	THR	2.6
1	D	261	VAL	2.6
1	G	292	SER	2.6
1	C	213	ALA	2.6
1	H	146	ASP	2.5
1	E	215	GLY	2.5
1	H	273	LYS	2.5
1	E	269	ALA	2.5
1	D	268	SER	2.5
1	C	274	GLN	2.5
1	H	62	PRO	2.5
1	B	227	TRP	2.5
1	H	224	ASN	2.4
1	F	270	ILE	2.4
1	B	271	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	197	VAL	2.4
1	A	163	CYS	2.4
1	H	223	VAL	2.3
1	G	222	THR	2.3
1	C	273	LYS	2.3
1	C	272	LYS	2.2
1	A	260	ARG	2.2
1	G	221	GLU	2.2
1	G	261	VAL	2.2
1	D	220	ARG	2.2
1	D	29	GLU	2.2
1	C	269	ALA	2.2
1	G	213	ALA	2.2
1	F	163	CYS	2.1
1	E	197	VAL	2.1
1	G	197	VAL	2.1
1	H	227	TRP	2.1
1	A	123	GLU	2.0
1	A	268	SER	2.0
1	A	261	VAL	2.0
1	C	196	SER	2.0
1	B	261	VAL	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 monosaccharides 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.