



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:55 AM GMT

PDB ID : 2V9U
Title : RIM DOMAIN OF MAIN PORIN FROM MYCOBACTERIA SMEGMATIS
Authors : Grueninger, D.; Ziegler, M.O.P.; Koetter, J.W.A.; Treiber, N.; Schulze, M.-S.; Schulz, G.E.
Deposited on : 2007-08-27
Resolution : 2.59 Å(reported)

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

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

MolProbity : 4.02b-467
Mogul : 1.7 (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

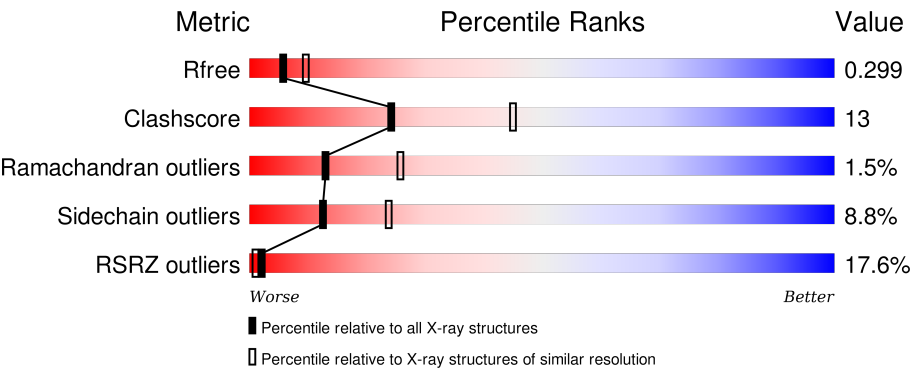
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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

Mol	Chain	Length	Quality of chain
1	A	132	<div><div>9%</div><div>67%</div><div>32%</div><div>.</div></div>
1	B	132	<div><div>6%</div><div>70%</div><div>26%</div><div>5%</div></div>
1	C	132	<div><div>15%</div><div>68%</div><div>28%</div><div>.</div></div>
1	D	132	<div><div>14%</div><div>73%</div><div>23%</div><div>5%</div></div>
1	E	132	<div><div>25%</div><div>61%</div><div>32%</div><div>8%</div></div>

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Mol	Chain	Length	Quality of chain
1	F	132	
1	G	132	
1	H	132	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7942 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 MSPA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	132	Total	C	N	O	S	0	0	0
			989	619	172	197	1			
1	B	132	Total	C	N	O	S	0	0	0
			989	619	172	197	1			
1	C	132	Total	C	N	O	S	0	0	0
			989	619	172	197	1			
1	D	132	Total	C	N	O	S	0	0	0
			989	619	172	197	1			
1	E	132	Total	C	N	O	S	0	0	0
			989	619	172	197	1			
1	F	132	Total	C	N	O	S	0	0	0
			989	619	172	197	1			
1	G	132	Total	C	N	O	S	0	0	0
			989	619	172	197	1			
1	H	132	Total	C	N	O	S	0	0	0
			989	619	172	197	1			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	6	Total	O	0	0
			6	6		
2	B	2	Total	O	0	0
			2	2		
2	C	3	Total	O	0	0
			3	3		
2	D	4	Total	O	0	0
			4	4		
2	E	3	Total	O	0	0
			3	3		
2	F	6	Total	O	0	0
			6	6		

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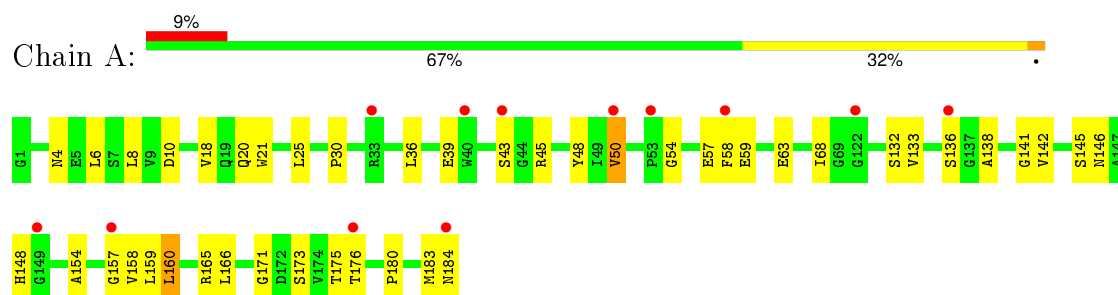
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	3	Total	O	0	0
			3	3		
2	H	3	Total	O	0	0
			3	3		

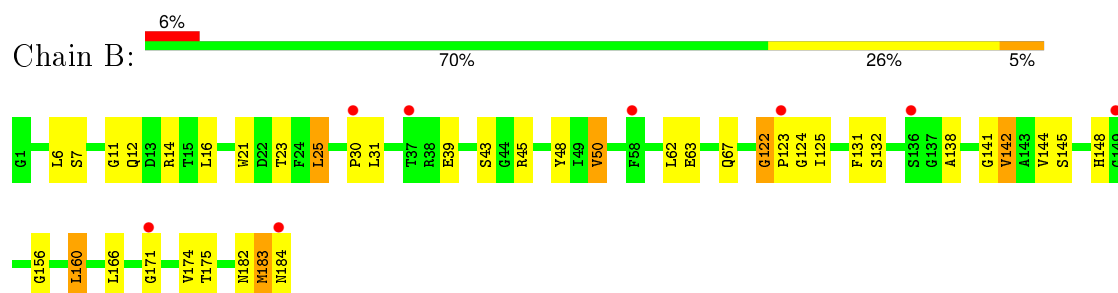
3 Residue-property plots [i](#)

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.

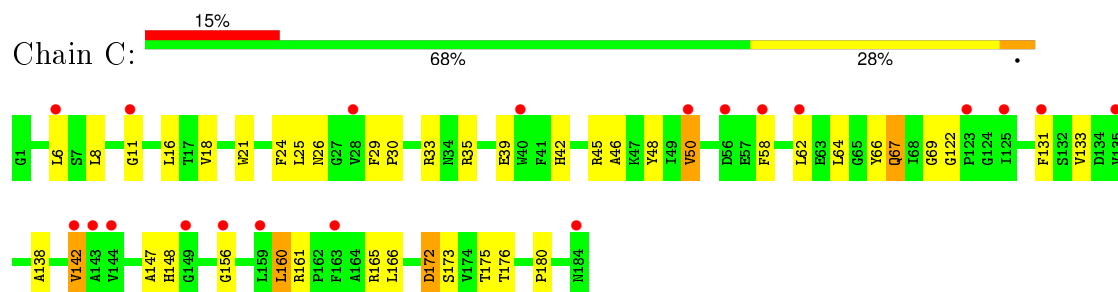
• Molecule 1: MSPA



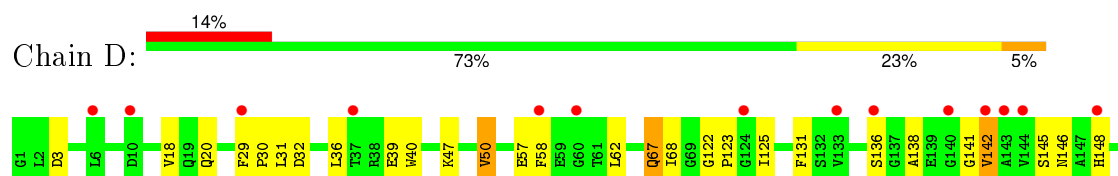
• Molecule 1: MSPA

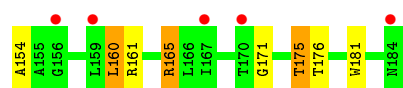


• Molecule 1: MSPA

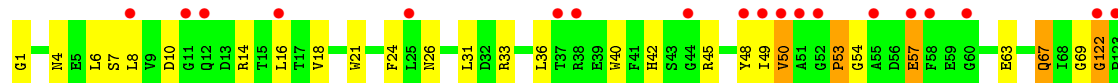


• Molecule 1: MSPA

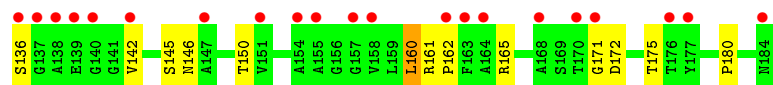
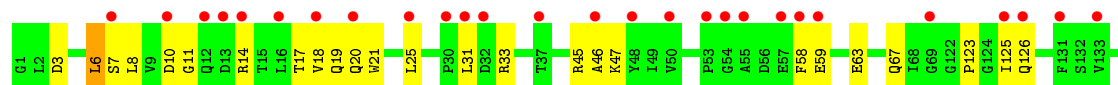




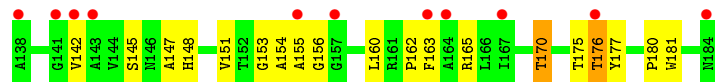
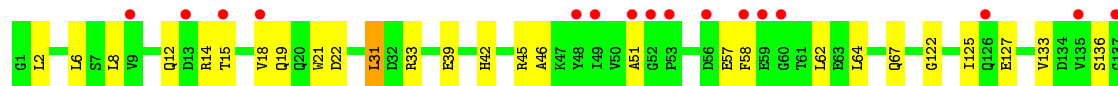
• Molecule 1: MSPA



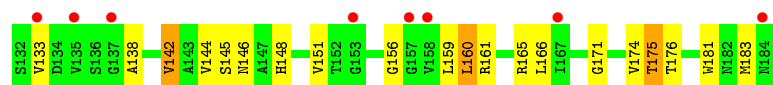
• Molecule 1: MSPA



• Molecule 1: MSPA



• Molecule 1: MSPA



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	139.38Å 105.65Å 102.96Å 90.00° 109.26° 90.00°	Depositor
Resolution (Å)	65.79 – 2.59 65.79 – 2.59	Depositor EDS
% Data completeness (in resolution range)	100.0 (65.79-2.59) 82.7 (65.79-2.59)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.48 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.273 , 0.299 0.275 , 0.299	Depositor DCC
R_{free} test set	1089 reflections (3.09%)	DCC
Wilson B-factor (Å ²)	37.2	Xtriage
Anisotropy	0.386	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 43.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	1 of 36299 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	7942	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.39% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 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	0.77	2/1010 (0.2%)	0.85	2/1374 (0.1%)
1	B	0.70	0/1010	0.77	0/1374
1	C	0.67	0/1010	0.79	0/1374
1	D	0.64	0/1010	0.76	2/1374 (0.1%)
1	E	0.69	0/1010	0.79	1/1374 (0.1%)
1	F	0.66	0/1010	0.74	0/1374
1	G	0.65	0/1010	0.75	0/1374
1	H	0.68	0/1010	0.77	0/1374
All	All	0.68	2/8080 (0.0%)	0.78	5/10992 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	30	PRO	C-N	-5.75	1.20	1.34
1	A	184	ASN	C-OXT	5.41	1.33	1.23

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	184	ASN	N-CA-CB	-8.52	95.27	110.60
1	E	165	ARG	NE-CZ-NH2	-6.31	117.14	120.30
1	D	165	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	A	165	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	D	165	ARG	NE-CZ-NH1	5.08	122.84	120.30

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	989	0	941	31	0
1	B	989	0	942	25	0
1	C	989	0	942	28	0
1	D	989	0	942	25	0
1	E	989	0	942	38	0
1	F	989	0	942	27	0
1	G	989	0	942	28	0
1	H	989	0	942	33	0
2	A	6	0	0	0	0
2	B	2	0	0	0	0
2	C	3	0	0	0	0
2	D	4	0	0	0	0
2	E	3	0	0	0	0
2	F	6	0	0	1	0
2	G	3	0	0	0	0
2	H	3	0	0	0	0
All	All	7942	0	7535	200	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 13.

All (200) 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:D:145:SER:HB2	1:E:8:LEU:HD13	1.54	0.90
1:E:16:LEU:HD23	1:E:50:VAL:HB	1.62	0.82
1:C:21:TRP:HB2	1:C:45:ARG:HB3	1.64	0.79
1:H:16:LEU:HD23	1:H:50:VAL:HB	1.67	0.77
1:H:46:ALA:HB2	1:H:64:LEU:HD13	1.68	0.76
1:E:42:HIS:HB3	1:E:147:ALA:HB3	1.65	0.76
1:F:145:SER:HB2	1:G:8:LEU:HD13	1.68	0.76
1:C:24:PHE:CE2	1:C:26:ASN:HB2	2.22	0.74
1:B:31:LEU:HG	1:C:69:GLY:HA3	1.70	0.73
1:B:21:TRP:HB2	1:B:45:ARG:HB2	1.71	0.71
1:A:8:LEU:HD13	1:H:145:SER:HB2	1.73	0.71
1:C:16:LEU:HD23	1:C:50:VAL:HB	1.72	0.70
1:G:58:PHE:O	1:G:136:SER:HA	1.92	0.69
1:G:133:VAL:HG11	1:H:171:GLY:HA3	1.75	0.69
1:E:54:GLY:O	1:E:57:GLU:HG2	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:48:TYR:HB2	1:C:166:LEU:HD22	1.74	0.68
1:A:141:GLY:O	1:B:11:GLY:HA3	1.94	0.68
1:B:50:VAL:HG13	1:B:138:ALA:HA	1.77	0.67
1:B:131:PHE:CZ	1:B:142:VAL:HG22	2.28	0.67
1:E:16:LEU:CD2	1:E:50:VAL:HB	2.23	0.67
1:D:31:LEU:HG	1:E:69:GLY:HA3	1.76	0.67
1:F:19:GLN:NE2	2:F:2002:HOH:O	2.28	0.66
1:G:18:VAL:HG13	1:G:176:THR:HG22	1.78	0.66
1:E:31:LEU:HB2	1:F:161:ARG:NH1	2.12	0.65
1:C:46:ALA:HB2	1:C:64:LEU:HD13	1.77	0.65
1:G:15:THR:HB	1:G:51:ALA:HB3	1.78	0.65
1:H:39:GLU:OE2	1:H:148:HIS:HE1	1.80	0.65
1:G:163:PHE:HB3	1:G:177:TYR:CD2	2.32	0.65
1:G:31:LEU:HD22	1:H:159:LEU:HB3	1.81	0.63
1:D:36:LEU:O	1:D:154:ALA:HB3	1.98	0.63
1:E:36:LEU:O	1:E:154:ALA:HB3	1.98	0.63
1:C:50:VAL:HG13	1:C:138:ALA:HA	1.81	0.62
1:C:18:VAL:HG13	1:C:176:THR:HG22	1.80	0.62
1:E:165:ARG:HD3	1:E:175:THR:HB	1.80	0.62
1:A:50:VAL:HG13	1:A:138:ALA:HA	1.81	0.62
1:G:21:TRP:HB2	1:G:45:ARG:HB2	1.81	0.62
1:G:127:GLU:CD	1:G:165:ARG:HH22	2.02	0.62
1:D:18:VAL:HG13	1:D:176:THR:HG22	1.82	0.62
1:F:21:TRP:HB2	1:F:45:ARG:HB2	1.82	0.61
1:A:48:TYR:HB2	1:A:166:LEU:HD22	1.82	0.61
1:E:18:VAL:HG13	1:E:176:THR:HG22	1.83	0.61
1:H:24:PHE:CE2	1:H:26:ASN:HB2	2.36	0.60
1:H:67:GLN:NE2	1:H:161:ARG:HH21	2.00	0.60
1:E:26:ASN:O	1:E:40:TRP:HA	2.02	0.60
1:E:183:MET:O	1:E:184:ASN:HB2	2.02	0.59
1:A:160:LEU:HD22	1:A:183:MET:HG2	1.84	0.59
1:H:67:GLN:HE21	1:H:161:ARG:HH21	1.50	0.58
1:A:133:VAL:HG11	1:B:171:GLY:HA3	1.84	0.58
1:D:146:ASN:O	1:E:175:THR:CG2	2.52	0.57
1:C:39:GLU:OE2	1:C:148:HIS:HE1	1.87	0.57
1:B:160:LEU:HD22	1:B:183:MET:HG2	1.87	0.57
1:G:2:LEU:HD11	1:G:19:GLN:HG2	1.87	0.56
1:E:145:SER:HB2	1:F:8:LEU:HD13	1.88	0.56
1:D:146:ASN:O	1:E:175:THR:HG21	2.05	0.56
1:H:18:VAL:HG13	1:H:176:THR:HG22	1.87	0.55
1:B:12:GLN:HE21	1:B:14:ARG:CZ	2.19	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:62:LEU:HD23	1:D:142:VAL:HG12	1.89	0.55
1:G:19:GLN:HB3	1:G:21:TRP:HE1	1.72	0.54
1:B:39:GLU:OE2	1:B:148:HIS:HE1	1.90	0.54
1:B:48:TYR:HB2	1:B:166:LEU:HD22	1.89	0.54
1:C:67:GLN:NE2	1:C:161:ARG:HH21	2.06	0.54
1:A:10:ASP:C	1:A:10:ASP:OD1	2.46	0.54
1:H:50:VAL:HG13	1:H:138:ALA:HA	1.88	0.54
1:A:21:TRP:HB2	1:A:45:ARG:HB2	1.89	0.54
1:B:7:SER:HA	1:B:16:LEU:O	2.07	0.53
1:D:47:LYS:HG2	1:D:141:GLY:HA3	1.90	0.53
1:F:3:ASP:HB2	1:F:20:GLN:O	2.08	0.53
1:D:39:GLU:OE2	1:D:148:HIS:HE1	1.92	0.53
1:C:160:LEU:O	1:C:180:PRO:HA	2.08	0.53
1:G:153:GLY:O	1:G:155:ALA:N	2.41	0.53
1:H:16:LEU:CD2	1:H:50:VAL:HB	2.38	0.52
1:G:14:ARG:NH2	1:G:170:THR:OG1	2.43	0.52
1:F:20:GLN:HE22	1:F:162:PRO:HB2	1.75	0.52
1:C:165:ARG:HD3	1:C:175:THR:HB	1.90	0.52
1:H:68:ILE:O	1:H:125:ILE:HA	2.10	0.52
1:E:131:PHE:CE1	1:E:142:VAL:HG22	2.45	0.52
1:A:59:GLU:OE1	1:A:136:SER:HB3	2.09	0.51
1:A:39:GLU:OE2	1:A:148:HIS:HE1	1.93	0.51
1:E:160:LEU:O	1:E:180:PRO:HA	2.11	0.51
1:C:67:GLN:NE2	1:C:161:ARG:HD2	2.26	0.51
1:B:145:SER:HB2	1:C:8:LEU:HD13	1.91	0.51
1:F:146:ASN:O	1:G:175:THR:CG2	2.59	0.51
1:H:48:TYR:HB2	1:H:166:LEU:HD22	1.93	0.50
1:A:171:GLY:CA	1:H:133:VAL:HG11	2.41	0.50
1:A:58:PHE:O	1:A:136:SER:HA	2.11	0.50
1:C:50:VAL:CG1	1:C:138:ALA:HA	2.42	0.49
1:F:10:ASP:OD1	1:F:14:ARG:HB2	2.10	0.49
1:E:24:PHE:CE2	1:E:26:ASN:HB2	2.47	0.49
1:A:145:SER:HB3	1:B:174:VAL:HG23	1.94	0.49
1:B:63:GLU:HG2	1:B:132:SER:HA	1.95	0.49
1:A:160:LEU:O	1:A:180:PRO:HA	2.12	0.49
1:B:144:VAL:HG23	1:C:173:SER:OG	2.13	0.49
1:A:18:VAL:HG13	1:A:176:THR:HG22	1.94	0.49
1:E:63:GLU:HG2	1:E:132:SER:HA	1.95	0.49
1:H:50:VAL:O	1:H:50:VAL:HG22	2.12	0.48
1:C:66:TYR:N	1:C:66:TYR:CD2	2.81	0.48
1:E:48:TYR:HB2	1:E:166:LEU:HD22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:67:GLN:NE2	1:D:161:ARG:HH21	2.12	0.48
1:E:122:GLY:C	1:E:124:GLY:H	2.17	0.48
1:G:12:GLN:NE2	1:G:170:THR:HG21	2.29	0.48
1:D:50:VAL:HG13	1:D:138:ALA:HA	1.96	0.47
1:E:133:VAL:HG11	1:F:171:GLY:CA	2.44	0.47
1:E:141:GLY:O	1:F:11:GLY:HA3	2.13	0.47
1:G:42:HIS:HB3	1:G:147:ALA:HB3	1.97	0.47
1:E:7:SER:HA	1:E:16:LEU:O	2.14	0.47
1:E:50:VAL:HG22	1:E:50:VAL:O	2.13	0.47
1:D:58:PHE:O	1:D:136:SER:HA	2.15	0.47
1:F:58:PHE:O	1:F:136:SER:HA	2.15	0.47
1:F:6:LEU:HD22	1:F:7:SER:H	1.79	0.47
1:G:145:SER:HB3	1:H:174:VAL:HG23	1.97	0.46
1:G:31:LEU:CD2	1:H:159:LEU:HB3	2.44	0.46
1:F:146:ASN:O	1:G:175:THR:HG21	2.16	0.46
1:D:165:ARG:HD3	1:D:175:THR:HB	1.97	0.46
1:G:127:GLU:OE2	1:G:165:ARG:NH2	2.44	0.46
1:A:39:GLU:OE2	1:B:125:ILE:HD13	2.16	0.46
1:A:54:GLY:HA2	1:A:57:GLU:OE1	2.16	0.46
1:C:62:LEU:HD23	1:C:142:VAL:HG13	1.97	0.46
1:F:17:THR:HG22	1:F:18:VAL:N	2.30	0.46
1:F:59:GLU:OE1	1:F:136:SER:HB3	2.16	0.46
1:H:122:GLY:C	1:H:124:GLY:H	2.19	0.46
1:G:2:LEU:CD1	1:G:19:GLN:HG2	2.45	0.46
1:F:160:LEU:O	1:F:180:PRO:HA	2.15	0.46
1:A:160:LEU:HD22	1:A:183:MET:CG	2.46	0.45
1:E:67:GLN:HB2	1:E:67:GLN:HE21	1.60	0.45
1:C:67:GLN:HE22	1:C:161:ARG:HD2	1.80	0.45
1:D:68:ILE:O	1:D:125:ILE:HA	2.16	0.45
1:A:146:ASN:HB3	1:B:175:THR:HG23	1.98	0.45
1:H:160:LEU:HD22	1:H:183:MET:CG	2.47	0.45
1:F:6:LEU:CD2	1:F:7:SER:H	2.30	0.45
1:F:25:LEU:HG	1:F:160:LEU:HD23	1.99	0.45
1:C:33:ARG:HA	1:C:33:ARG:HD2	1.72	0.45
1:C:172:ASP:N	1:C:172:ASP:OD1	2.51	0.44
1:G:22:ASP:HB2	1:G:45:ARG:HG3	2.00	0.44
1:C:24:PHE:CD2	1:C:26:ASN:HB2	2.52	0.44
1:H:37:THR:O	1:H:38:ARG:NH1	2.49	0.44
1:A:173:SER:OG	1:H:144:VAL:HG23	2.17	0.44
1:E:133:VAL:HG11	1:F:171:GLY:HA3	2.00	0.44
1:B:122:GLY:C	1:B:124:GLY:H	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:32:ASP:OD1	1:H:33:ARG:N	2.51	0.44
1:H:50:VAL:O	1:H:55:ALA:HB1	2.18	0.44
1:G:39:GLU:OE2	1:G:148:HIS:HE1	2.01	0.43
1:G:160:LEU:O	1:G:180:PRO:HA	2.17	0.43
1:G:46:ALA:HB2	1:G:64:LEU:HD13	2.00	0.43
1:E:49:ILE:HG22	1:E:50:VAL:N	2.33	0.43
1:E:1:GLY:O	1:E:21:TRP:HA	2.17	0.43
1:B:62:LEU:CD2	1:B:141:GLY:HA2	2.48	0.43
1:A:39:GLU:CD	1:B:125:ILE:HD13	2.39	0.43
1:B:182:ASN:C	1:B:184:ASN:H	2.20	0.43
1:A:36:LEU:O	1:A:154:ALA:HB3	2.17	0.43
1:A:157:GLY:O	1:A:158:VAL:HG23	2.17	0.43
1:E:10:ASP:C	1:E:10:ASP:OD2	2.57	0.43
1:A:171:GLY:HA3	1:H:133:VAL:HG11	2.00	0.43
1:D:40:TRP:CD1	1:D:40:TRP:C	2.92	0.43
1:E:36:LEU:O	1:E:154:ALA:CB	2.66	0.43
1:A:63:GLU:HG2	1:A:132:SER:CB	2.49	0.43
1:E:40:TRP:NE1	1:E:149:GLY:HA3	2.33	0.43
1:A:159:LEU:HB3	1:H:31:LEU:HD11	2.01	0.43
1:A:175:THR:CG2	1:H:146:ASN:O	2.66	0.43
1:B:25:LEU:HG	1:B:160:LEU:HD23	2.00	0.42
1:F:150:THR:CG2	1:F:150:THR:O	2.67	0.42
1:E:131:PHE:CZ	1:E:142:VAL:HG22	2.54	0.42
1:A:68:ILE:HA	1:A:160:LEU:HD12	2.01	0.42
1:E:181:TRP:CD1	1:E:181:TRP:N	2.88	0.42
1:F:63:GLU:N	1:F:165:ARG:O	2.47	0.42
1:F:14:ARG:NH1	1:F:58:PHE:HD1	2.17	0.42
1:C:131:PHE:CZ	1:C:142:VAL:HG22	2.55	0.42
1:D:68:ILE:HA	1:D:160:LEU:HD12	2.02	0.42
1:A:59:GLU:OE1	1:A:136:SER:CB	2.68	0.42
1:C:29:PHE:HA	1:C:30:PRO:HD3	1.82	0.42
1:D:181:TRP:N	1:D:181:TRP:CD1	2.88	0.42
1:D:3:ASP:HB2	1:D:20:GLN:O	2.19	0.42
1:B:131:PHE:CE1	1:B:142:VAL:HG22	2.53	0.42
1:D:146:ASN:HB3	1:E:175:THR:HG23	2.01	0.42
1:F:10:ASP:OD2	1:F:10:ASP:C	2.58	0.42
1:G:181:TRP:N	1:G:181:TRP:CD1	2.86	0.42
1:F:20:GLN:NE2	1:F:162:PRO:HB2	2.34	0.42
1:H:131:PHE:CZ	1:H:142:VAL:HG22	2.55	0.42
1:H:48:TYR:C	1:H:49:ILE:HG13	2.39	0.41
1:E:67:GLN:NE2	1:E:161:ARG:HH21	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:21:TRP:HB2	1:H:45:ARG:HB2	2.02	0.41
1:C:133:VAL:HG11	1:D:171:GLY:HA3	2.02	0.41
1:C:42:HIS:N	1:C:147:ALA:O	2.38	0.41
1:A:4:ASN:OD1	1:A:20:GLN:HB3	2.19	0.41
1:E:151:VAL:HG22	1:E:152:THR:N	2.35	0.41
1:A:6:LEU:HA	1:A:6:LEU:HD12	1.67	0.41
1:B:141:GLY:O	1:C:11:GLY:HA3	2.21	0.41
1:F:31:LEU:HB3	1:G:125:ILE:HD12	2.02	0.41
1:D:131:PHE:CZ	1:D:142:VAL:HG13	2.56	0.41
1:H:165:ARG:HG3	1:H:175:THR:HB	2.01	0.41
1:D:131:PHE:CD2	1:D:131:PHE:C	2.94	0.41
1:D:67:GLN:HE21	1:D:161:ARG:HH21	1.68	0.41
1:G:160:LEU:O	1:G:162:PRO:HD3	2.20	0.41
1:E:10:ASP:OD1	1:E:14:ARG:HB2	2.21	0.41
1:H:181:TRP:N	1:H:181:TRP:CD1	2.89	0.41
1:F:46:ALA:O	1:F:47:LYS:HG3	2.21	0.41
1:H:12:GLN:HE21	1:H:14:ARG:CZ	2.33	0.41
1:B:183:MET:HA	1:B:183:MET:CE	2.51	0.40
1:D:29:PHE:HA	1:D:30:PRO:HD3	1.95	0.40
1:C:58:PHE:CZ	1:C:166:LEU:HD11	2.56	0.40
1:D:32:ASP:C	1:D:32:ASP:OD1	2.60	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	130/132 (98%)	122 (94%)	8 (6%)	0	100	100
1	B	130/132 (98%)	124 (95%)	3 (2%)	3 (2%)	8	14
1	C	130/132 (98%)	123 (95%)	5 (4%)	2 (2%)	13	26
1	D	130/132 (98%)	122 (94%)	6 (5%)	2 (2%)	13	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	130/132 (98%)	116 (89%)	11 (8%)	3 (2%)	8	14
1	F	130/132 (98%)	124 (95%)	5 (4%)	1 (1%)	24	46
1	G	130/132 (98%)	123 (95%)	4 (3%)	3 (2%)	8	14
1	H	130/132 (98%)	124 (95%)	4 (3%)	2 (2%)	13	26
All	All	1040/1056 (98%)	978 (94%)	46 (4%)	16 (2%)	13	26

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	156	GLY
1	C	156	GLY
1	E	156	GLY
1	H	156	GLY
1	B	123	PRO
1	D	122	GLY
1	G	122	GLY
1	G	154	ALA
1	E	53	PRO
1	B	122	GLY
1	C	122	GLY
1	E	122	GLY
1	F	123	PRO
1	H	122	GLY
1	D	123	PRO
1	G	156	GLY

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	101/101 (100%)	96 (95%)	5 (5%)	30	56
1	B	101/101 (100%)	91 (90%)	10 (10%)	10	18
1	C	101/101 (100%)	93 (92%)	8 (8%)	15	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	101/101 (100%)	95 (94%)	6 (6%)	24	47
1	E	101/101 (100%)	88 (87%)	13 (13%)	5	9
1	F	101/101 (100%)	92 (91%)	9 (9%)	12	23
1	G	101/101 (100%)	91 (90%)	10 (10%)	10	18
1	H	101/101 (100%)	91 (90%)	10 (10%)	10	18
All	All	808/808 (100%)	737 (91%)	71 (9%)	12	24

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	LEU
1	A	43	SER
1	A	50	VAL
1	A	142	VAL
1	A	160	LEU
1	B	6	LEU
1	B	23	THR
1	B	25	LEU
1	B	30	PRO
1	B	43	SER
1	B	50	VAL
1	B	67	GLN
1	B	142	VAL
1	B	160	LEU
1	B	183	MET
1	C	6	LEU
1	C	25	LEU
1	C	35	ARG
1	C	50	VAL
1	C	67	GLN
1	C	142	VAL
1	C	160	LEU
1	C	172	ASP
1	D	50	VAL
1	D	57	GLU
1	D	67	GLN
1	D	142	VAL
1	D	160	LEU
1	D	175	THR
1	E	4	ASN

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Mol	Chain	Res	Type
1	E	6	LEU
1	E	33	ARG
1	E	45	ARG
1	E	50	VAL
1	E	53	PRO
1	E	57	GLU
1	E	67	GLN
1	E	142	VAL
1	E	160	LEU
1	E	172	ASP
1	E	175	THR
1	E	176	THR
1	F	6	LEU
1	F	33	ARG
1	F	67	GLN
1	F	125	ILE
1	F	126	GLN
1	F	142	VAL
1	F	160	LEU
1	F	172	ASP
1	F	175	THR
1	G	6	LEU
1	G	31	LEU
1	G	33	ARG
1	G	57	GLU
1	G	62	LEU
1	G	67	GLN
1	G	142	VAL
1	G	151	VAL
1	G	170	THR
1	G	176	THR
1	H	8	LEU
1	H	33	ARG
1	H	35	ARG
1	H	50	VAL
1	H	57	GLU
1	H	67	GLN
1	H	142	VAL
1	H	151	VAL
1	H	160	LEU
1	H	175	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	148	HIS
1	B	12	GLN
1	B	148	HIS
1	C	67	GLN
1	C	148	HIS
1	D	12	GLN
1	D	67	GLN
1	D	148	HIS
1	E	67	GLN
1	F	20	GLN
1	F	67	GLN
1	F	126	GLN
1	F	148	HIS
1	G	67	GLN
1	G	148	HIS
1	H	4	ASN
1	H	12	GLN
1	H	20	GLN
1	H	67	GLN
1	H	148	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	132/132 (100%)	1.14	12 (9%) 11 7	31, 42, 55, 58	0
1	B	132/132 (100%)	0.96	8 (6%) 25 18	35, 43, 53, 59	0
1	C	132/132 (100%)	1.23	20 (15%) 3 1	37, 48, 60, 65	0
1	D	132/132 (100%)	1.34	19 (14%) 3 2	45, 54, 63, 67	0
1	E	132/132 (100%)	1.54	33 (25%) 1 0	38, 53, 68, 71	0
1	F	132/132 (100%)	1.81	48 (36%) 0 0	45, 55, 69, 73	0
1	G	132/132 (100%)	1.51	27 (20%) 1 1	39, 54, 69, 71	0
1	H	132/132 (100%)	1.32	19 (14%) 3 2	37, 50, 62, 65	0
All	All	1056/1056 (100%)	1.36	186 (17%) 2 1	31, 50, 65, 73	0

All (186) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	55	ALA	7.4
1	F	50	VAL	6.0
1	E	52	GLY	5.3
1	G	58	PHE	5.2
1	G	15	THR	5.1
1	G	51	ALA	4.8
1	G	48	TYR	4.8
1	E	55	ALA	4.7
1	G	137	GLY	4.6
1	G	18	VAL	4.5
1	F	184	ASN	4.2
1	F	18	VAL	4.1
1	F	57	GLU	4.1
1	B	136	SER	4.1
1	F	12	GLN	4.0
1	F	58	PHE	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	156	GLY	3.8
1	C	184	ASN	3.8
1	E	50	VAL	3.7
1	A	122	GLY	3.7
1	G	49	ILE	3.7
1	A	58	PHE	3.6
1	G	164	ALA	3.6
1	E	181	TRP	3.6
1	F	138	ALA	3.6
1	H	51	ALA	3.6
1	E	142	VAL	3.6
1	F	10	ASP	3.6
1	F	125	ILE	3.6
1	E	58	PHE	3.4
1	E	122	GLY	3.4
1	G	126	GLN	3.4
1	A	184	ASN	3.4
1	E	176	THR	3.4
1	F	170	THR	3.4
1	H	153	GLY	3.3
1	C	143	ALA	3.3
1	E	25	LEU	3.2
1	F	147	ALA	3.2
1	H	135	VAL	3.2
1	F	163	PHE	3.2
1	G	141	GLY	3.1
1	C	58	PHE	3.1
1	F	48	TYR	3.1
1	G	142	VAL	3.1
1	E	11	GLY	3.1
1	G	138	ALA	3.0
1	G	52	GLY	3.0
1	F	59	GLU	3.0
1	E	44	GLY	2.9
1	D	167	ILE	2.9
1	E	12	GLN	2.9
1	C	142	VAL	2.8
1	D	124	GLY	2.8
1	F	168	ALA	2.8
1	D	143	ALA	2.8
1	E	51	ALA	2.8
1	D	144	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	G	157	GLY	2.8
1	F	136	SER	2.8
1	E	167	ILE	2.8
1	F	140	GLY	2.8
1	F	37	THR	2.8
1	H	56	ASP	2.8
1	D	60	GLY	2.7
1	E	48	TYR	2.7
1	A	53	PRO	2.7
1	D	37	THR	2.7
1	E	131	PHE	2.7
1	E	171	GLY	2.7
1	D	136	SER	2.7
1	B	58	PHE	2.7
1	H	133	VAL	2.7
1	F	177	TYR	2.7
1	F	14	ARG	2.6
1	E	16	LEU	2.6
1	E	123	PRO	2.6
1	E	37	THR	2.6
1	G	184	ASN	2.6
1	G	56	ASP	2.6
1	E	57	GLU	2.6
1	F	142	VAL	2.6
1	C	56	ASP	2.6
1	H	167	ILE	2.6
1	H	131	PHE	2.6
1	F	171	GLY	2.5
1	E	175	THR	2.5
1	F	46	ALA	2.5
1	A	149	GLY	2.5
1	C	50	VAL	2.5
1	H	64	LEU	2.5
1	G	155	ALA	2.5
1	H	29	PHE	2.5
1	G	135	VAL	2.5
1	G	13	ASP	2.5
1	H	61	THR	2.5
1	C	149	GLY	2.5
1	H	58	PHE	2.4
1	F	13	ASP	2.4
1	F	164	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	16	LEU	2.4
1	A	157	GLY	2.4
1	H	184	ASN	2.4
1	G	176	THR	2.4
1	G	167	ILE	2.4
1	F	31	LEU	2.4
1	A	176	THR	2.4
1	G	59	GLU	2.4
1	H	53	PRO	2.4
1	D	184	ASN	2.4
1	C	131	PHE	2.4
1	F	158	VAL	2.4
1	C	123	PRO	2.4
1	E	140	GLY	2.4
1	A	33	ARG	2.3
1	C	135	VAL	2.3
1	G	9	VAL	2.3
1	F	176	THR	2.3
1	F	69	GLY	2.3
1	D	58	PHE	2.3
1	B	123	PRO	2.3
1	F	131	PHE	2.3
1	H	33	ARG	2.3
1	F	20	GLN	2.3
1	E	147	ALA	2.3
1	F	30	PRO	2.3
1	D	148	HIS	2.3
1	E	135	VAL	2.3
1	F	139	GLU	2.3
1	F	155	ALA	2.3
1	C	144	VAL	2.3
1	H	1	GLY	2.3
1	C	125	ILE	2.3
1	A	43	SER	2.3
1	A	136	SER	2.3
1	H	157	GLY	2.3
1	D	140	GLY	2.2
1	H	10	ASP	2.2
1	E	137	GLY	2.2
1	A	50	VAL	2.2
1	F	126	GLN	2.2
1	C	156	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	6	LEU	2.2
1	F	53	PRO	2.2
1	C	40	TRP	2.2
1	G	163	PHE	2.2
1	D	159	LEU	2.2
1	F	154	ALA	2.2
1	G	143	ALA	2.2
1	E	136	SER	2.2
1	C	11	GLY	2.2
1	D	170	THR	2.2
1	G	53	PRO	2.2
1	D	133	VAL	2.2
1	F	151	VAL	2.2
1	E	60	GLY	2.2
1	C	159	LEU	2.2
1	H	158	VAL	2.1
1	D	10	ASP	2.1
1	F	25	LEU	2.1
1	E	134	ASP	2.1
1	F	32	ASP	2.1
1	C	62	LEU	2.1
1	B	37	THR	2.1
1	E	38	ARG	2.1
1	F	54	GLY	2.1
1	F	137	GLY	2.1
1	B	171	GLY	2.1
1	C	163	PHE	2.1
1	F	133	VAL	2.1
1	E	148	HIS	2.1
1	F	157	GLY	2.1
1	G	60	GLY	2.1
1	B	30	PRO	2.1
1	D	29	PHE	2.1
1	B	184	ASN	2.0
1	D	142	VAL	2.0
1	H	137	GLY	2.0
1	C	6	LEU	2.0
1	E	8	LEU	2.0
1	F	162	PRO	2.0
1	F	7	SER	2.0
1	B	149	GLY	2.0
1	C	28	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	49	ILE	2.0
1	A	40	TRP	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.