



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2021 – 12:56 AM JST

PDB ID : 7DCD
Title : Nonstructural protein 7 and 8 complex of SARS-CoV-2
Authors : Zhang, C.H.; Li, L.; Su, D.
Deposited on : 2020-10-24
Resolution : 2.57 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 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 : 2.18
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) : 2.18

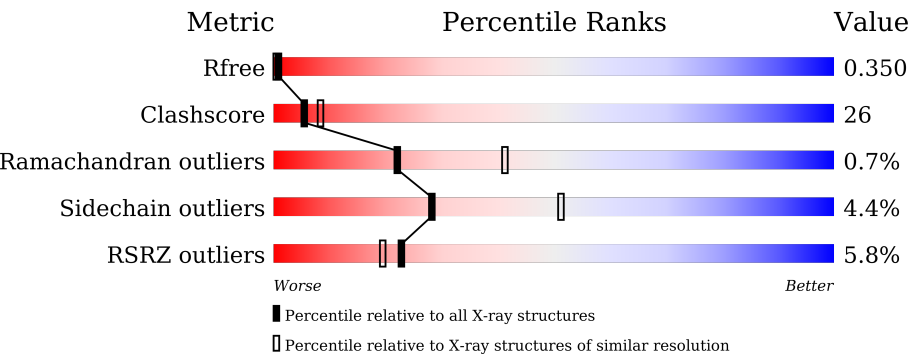
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.57 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	3676 (2.60-2.56)
Clashscore	141614	4049 (2.60-2.56)
Ramachandran outliers	138981	3979 (2.60-2.56)
Sidechain outliers	138945	3979 (2.60-2.56)
RSRZ outliers	127900	3614 (2.60-2.56)

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 $\leq 5\%$. 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	83	<div><div>2%</div><div><div></div><div>53%</div><div>34%</div><div>•</div><div>10%</div></div></div>
1	C	83	<div><div>6%</div><div><div></div><div>47%</div><div>42%</div><div>••</div><div>8%</div></div></div>
1	E	83	<div><div>6%</div><div><div></div><div>48%</div><div>41%</div><div>•</div><div>8%</div></div></div>
1	G	83	<div><div>7%</div><div><div></div><div>46%</div><div>39%</div><div>6%</div><div>10%</div></div></div>
2	B	122	<div><div>5%</div><div><div></div><div>40%</div><div>48%</div><div>7%</div><div>5%</div></div></div>
2	D	122	<div><div>7%</div><div><div></div><div>42%</div><div>52%</div><div>•</div><div>5%</div></div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	122	<div><div></div><div>7%</div><div>54%</div><div>36%</div><div>7%</div></div>
2	H	122	<div><div></div><div>3%</div><div>48%</div><div>43%</div><div>7%</div></div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 5875 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 Non-structural protein 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	75	Total	C	N	O	S	0	0	0
			562	355	92	108	7			
1	C	76	Total	C	N	O	S	0	0	0
			582	367	95	113	7			
1	E	76	Total	C	N	O	S	0	0	0
			574	359	94	114	7			
1	G	75	Total	C	N	O	S	0	0	0
			569	357	91	114	7			

- Molecule 2 is a protein called Non-structural protein 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	116	Total	C	N	O	S	0	0	0
			889	560	147	175	7			
2	D	116	Total	C	N	O	S	0	0	0
			883	555	148	173	7			
2	F	113	Total	C	N	O	S	0	0	0
			875	553	144	171	7			
2	H	114	Total	C	N	O	S	0	0	0
			866	545	143	171	7			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	8	Total	O	0	0
			8	8		
3	B	9	Total	O	0	0
			9	9		
3	C	4	Total	O	0	0
			4	4		
3	D	14	Total	O	0	0
			14	14		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	5	Total 5	O 5	0	0
3	F	11	Total 11	O 11	0	0
3	G	12	Total 12	O 12	0	0
3	H	12	Total 12	O 12	0	0

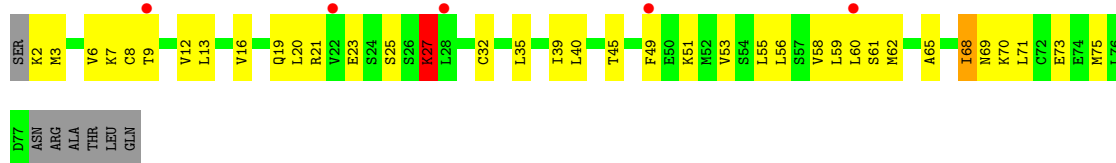
3 Residue-property plots [i](#)

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.

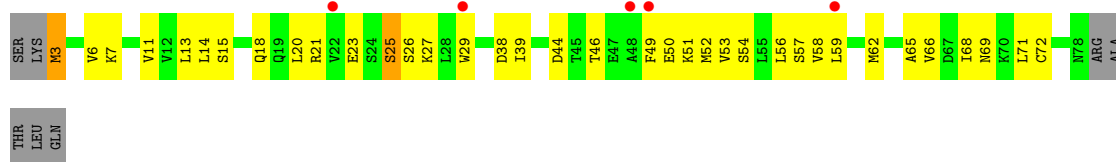
- Molecule 1: Non-structural protein 7



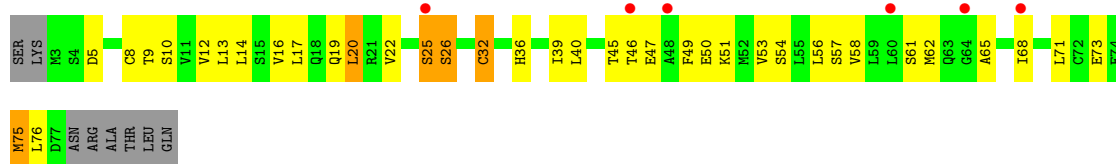
- Molecule 1: Non-structural protein 7




- Molecule 1: Non-structural protein 7

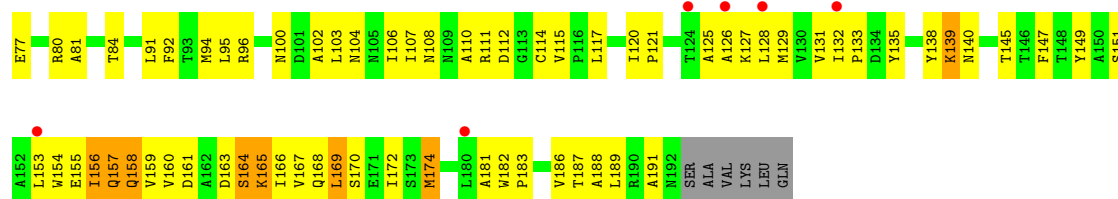


- Molecule 1: Non-structural protein 7




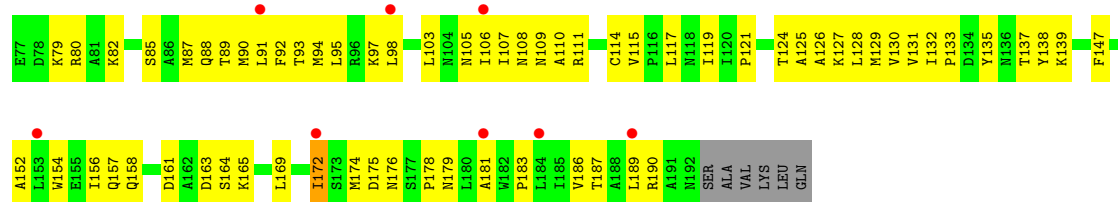
- Molecule 2: Non-structural protein 8

Chain B: 



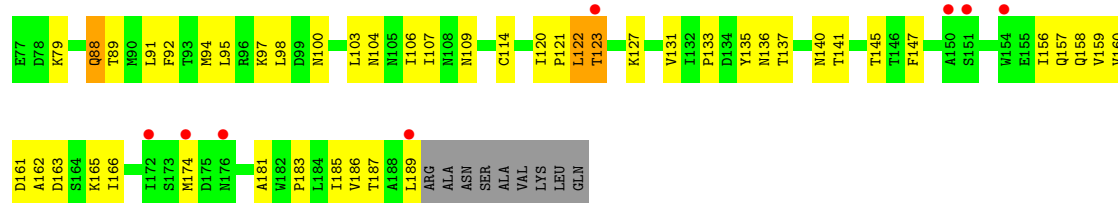
• Molecule 2: Non-structural protein 8

Chain D: 



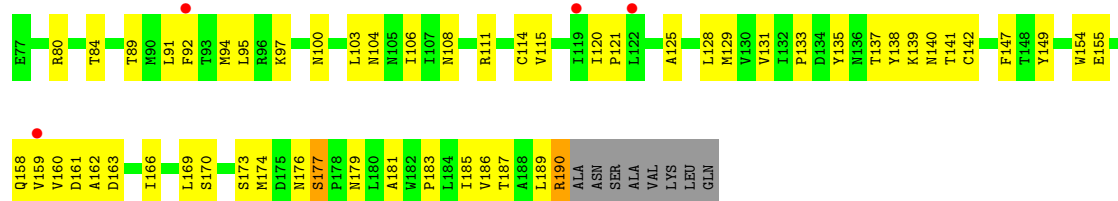
• Molecule 2: Non-structural protein 8

Chain F: 



• Molecule 2: Non-structural protein 8

Chain H: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	43.03Å 42.99Å 100.63Å 90.01° 90.03° 72.61°	Depositor
Resolution (Å)	41.06 – 2.57 41.06 – 2.57	Depositor EDS
% Data completeness (in resolution range)	93.2 (41.06-2.57) 92.9 (41.06-2.57)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.39 (at 2.58Å)	Xtriage
Refinement program	PHENIX Phenix1.18-3845	Depositor
R, R_{free}	0.254 , 0.353 0.257 , 0.350	Depositor DCC
R_{free} test set	907 reflections (4.44%)	wwPDB-VP
Wilson B-factor (Å ²)	43.6	Xtriage
Anisotropy	0.175	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 36.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.408 for -h,-k,l 0.388 for k,h,-l 0.398 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5875	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.59% 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, 0.333 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	0.56	0/565	0.76	0/764
1	C	0.58	2/585 (0.3%)	0.75	1/788 (0.1%)
1	E	0.51	0/577	0.68	0/780
1	G	0.54	1/572 (0.2%)	0.91	3/774 (0.4%)
2	B	0.50	0/902	0.77	2/1233 (0.2%)
2	D	0.51	0/896	0.78	1/1224 (0.1%)
2	F	0.47	0/888	0.85	4/1212 (0.3%)
2	H	0.44	0/879	0.75	1/1205 (0.1%)
All	All	0.51	3/5864 (0.1%)	0.78	12/7980 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	32	CYS	CB-SG	-6.12	1.71	1.82
1	G	32	CYS	CB-SG	-5.48	1.72	1.81
1	C	27	LYS	CD-CE	5.21	1.64	1.51

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	26	SER	CB-CA-C	12.52	133.90	110.10
2	F	123	THR	N-CA-CB	12.13	133.34	110.30
2	H	97	LYS	CB-CA-C	10.07	130.54	110.40
2	D	172	ILE	N-CA-C	-9.67	84.90	111.00
1	G	20	LEU	CB-CA-C	7.28	124.03	110.20
2	F	122	LEU	N-CA-C	-6.49	93.48	111.00
2	F	97	LYS	CB-CA-C	5.99	122.38	110.40
1	G	25	SER	N-CA-C	-5.97	94.87	111.00
2	B	165	LYS	N-CA-CB	5.93	121.27	110.60
1	C	68	ILE	CB-CA-C	-5.93	99.74	111.60
2	F	123	THR	N-CA-C	-5.47	96.23	111.00
2	B	164	SER	O-C-N	-5.29	114.24	122.70

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	562	0	581	29	4
1	C	582	0	611	43	1
1	E	574	0	584	31	0
1	G	569	0	580	34	0
2	B	889	0	890	55	0
2	D	883	0	879	58	5
2	F	875	0	888	43	0
2	H	866	0	851	55	0
3	A	8	0	0	0	0
3	B	9	0	0	1	0
3	C	4	0	0	0	0
3	D	14	0	0	0	0
3	E	5	0	0	0	0
3	F	11	0	0	0	0
3	G	12	0	0	0	0
3	H	12	0	0	0	0
All	All	5875	0	5864	304	5

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 26.

All (304) 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)
2:F:122:LEU:CG	2:F:122:LEU:O	1.94	1.11
2:F:122:LEU:O	2:F:122:LEU:CD1	1.98	1.11
2:F:122:LEU:O	2:F:122:LEU:HD12	1.52	1.08
2:F:122:LEU:O	2:F:122:LEU:HG	1.58	1.02
2:H:147:PHE:HB3	2:H:154:TRP:HB2	1.48	0.92
2:D:125:ALA:HA	2:D:189:LEU:HB3	1.53	0.88
1:G:19:GLN:OE1	2:H:84:THR:OG1	1.95	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:163:ASP:HB2	2:B:165:LYS:HE2	1.58	0.84
1:E:25:SER:O	1:E:27:LYS:N	2.10	0.84
1:C:20:LEU:HD13	1:C:62:MET:CE	2.08	0.83
1:G:19:GLN:O	2:H:80:ARG:NH2	2.12	0.83
1:A:18:GLN:NE2	1:A:23:GLU:OE2	2.13	0.81
1:C:68:ILE:HG21	2:D:111:ARG:HG2	1.62	0.80
1:C:71:LEU:HD21	2:D:89:THR:HA	1.61	0.80
2:D:129:MET:HG2	2:D:187:THR:HG22	1.62	0.80
1:A:25:SER:HB3	1:A:28:LEU:HB3	1.65	0.79
1:C:71:LEU:O	1:C:71:LEU:HD23	1.83	0.77
1:C:20:LEU:HD13	1:C:62:MET:HE1	1.65	0.76
1:E:18:GLN:NE2	1:E:23:GLU:OE2	2.19	0.75
2:B:112:ASP:OD1	3:B:201:HOH:O	2.03	0.75
2:D:95:LEU:HA	2:D:98:LEU:HG	1.70	0.74
1:G:53:VAL:HA	2:H:103:LEU:HD21	1.67	0.74
2:B:104:ASN:O	2:B:108:ASN:ND2	2.21	0.74
1:G:5:ASP:O	1:G:9:THR:HG23	1.86	0.74
1:E:25:SER:HA	1:G:73:GLU:HG3	1.70	0.73
2:H:125:ALA:H	2:H:190:ARG:HB2	1.52	0.73
2:H:115:VAL:H	2:H:131:VAL:HG12	1.53	0.72
1:E:54:SER:O	1:E:57:SER:OG	2.06	0.71
1:A:18:GLN:HG2	1:A:23:GLU:HG3	1.73	0.70
2:D:133:PRO:HA	2:D:183:PRO:HB3	1.74	0.70
1:C:68:ILE:CG2	2:D:111:ARG:HG2	2.22	0.69
2:F:133:PRO:HA	2:F:183:PRO:HB3	1.74	0.69
2:B:111:ARG:NH2	1:C:21:ARG:O	2.26	0.69
2:D:156:ILE:HG23	2:D:186:VAL:HG23	1.74	0.69
1:G:46:THR:HG23	1:G:47:GLU:H	1.58	0.69
1:C:56:LEU:HD21	2:D:107:ILE:HD11	1.73	0.68
1:A:62:MET:HE2	1:A:65:ALA:HB2	1.74	0.68
2:B:133:PRO:HA	2:B:183:PRO:HB3	1.76	0.68
2:H:158:GLN:HB2	2:H:187:THR:HB	1.76	0.67
2:D:79:LYS:O	2:D:82:LYS:N	2.26	0.67
1:C:16:VAL:HG21	2:D:91:LEU:HD22	1.77	0.67
2:D:161:ASP:HB2	2:D:181:ALA:HB3	1.76	0.67
2:F:163:ASP:HB2	2:F:165:LYS:HE2	1.76	0.67
2:H:129:MET:SD	2:H:187:THR:OG1	2.54	0.66
2:B:147:PHE:HB3	2:B:156:ILE:HD11	1.76	0.66
2:H:92:PHE:HA	2:H:95:LEU:HB2	1.77	0.66
1:A:19:GLN:O	2:B:80:ARG:NH2	2.29	0.66
2:B:77:GLU:HA	2:B:80:ARG:HB3	1.77	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:125:ALA:HB1	2:D:189:LEU:HD23	1.77	0.66
2:D:147:PHE:HB3	2:D:154:TRP:HB2	1.78	0.66
2:F:79:LYS:HE2	2:H:140:ASN:O	1.97	0.65
2:H:160:VAL:HG12	2:H:166:ILE:HD13	1.76	0.65
1:G:71:LEU:HD21	2:H:89:THR:HA	1.78	0.65
1:A:17:LEU:O	1:A:22:VAL:HG22	1.97	0.65
1:A:8:CYS:O	1:A:12:VAL:HG23	1.97	0.64
2:B:169:LEU:HG	2:B:170:SER:H	1.61	0.63
2:D:103:LEU:HA	2:D:106:ILE:HG12	1.81	0.62
2:B:91:LEU:HD23	2:B:92:PHE:CE1	2.35	0.62
2:F:137:THR:O	2:F:141:THR:HG23	1.99	0.62
1:E:65:ALA:O	1:E:66:VAL:HG13	2.00	0.62
2:B:160:VAL:HA	2:B:166:ILE:HA	1.80	0.61
2:D:108:ASN:HA	2:D:111:ARG:HG3	1.83	0.61
1:E:21:ARG:CZ	2:H:108:ASN:HB3	2.30	0.61
1:C:7:LYS:HG2	1:C:40:LEU:HA	1.81	0.61
1:G:68:ILE:HG23	2:H:92:PHE:HE2	1.65	0.61
1:C:62:MET:CE	1:C:65:ALA:CB	2.79	0.60
1:E:13:LEU:HD21	1:E:56:LEU:HA	1.84	0.60
1:A:75:MET:HG3	2:B:96:ARG:HH21	1.65	0.60
1:G:17:LEU:O	1:G:22:VAL:HG22	2.02	0.60
2:H:142:CYS:HB3	2:H:147:PHE:HA	1.83	0.60
1:A:57:SER:HB3	2:B:120:ILE:HD12	1.84	0.59
2:H:125:ALA:HB1	2:H:189:LEU:HD23	1.85	0.59
2:H:176:ASN:OD1	2:H:179:ASN:ND2	2.19	0.59
1:C:62:MET:HE3	1:C:65:ALA:CB	2.32	0.59
1:A:19:GLN:NE2	2:B:84:THR:OG1	2.33	0.59
1:G:62:MET:HB2	1:G:65:ALA:HB3	1.83	0.59
2:H:133:PRO:HA	2:H:183:PRO:HB3	1.85	0.59
2:H:137:THR:O	2:H:141:THR:HG23	2.02	0.59
2:B:169:LEU:HD23	2:B:169:LEU:H	1.68	0.58
1:G:13:LEU:HD21	1:G:56:LEU:HA	1.85	0.58
1:C:69:ASN:O	1:C:73:GLU:HG2	2.04	0.58
2:B:102:ALA:HB2	2:B:151:SER:HB2	1.86	0.58
1:C:58:VAL:HG22	2:D:119:ILE:HG22	1.84	0.58
2:F:103:LEU:O	2:F:106:ILE:HG12	2.03	0.58
2:B:159:VAL:HG13	2:B:186:VAL:HG12	1.85	0.58
2:D:163:ASP:HB2	2:D:165:LYS:HE2	1.83	0.58
1:G:54:SER:OG	2:H:120:ILE:O	2.22	0.58
1:C:62:MET:HE3	1:C:65:ALA:HB1	1.85	0.57
2:B:145:THR:O	2:B:156:ILE:HG12	2.03	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:95:LEU:HD22	2:D:103:LEU:HD13	1.86	0.57
2:F:135:TYR:CE2	2:F:174:MET:HG2	2.39	0.57
1:C:20:LEU:CD1	1:C:62:MET:HE1	2.32	0.57
2:F:135:TYR:HE2	2:F:174:MET:HG2	1.68	0.57
1:C:13:LEU:HD23	1:C:55:LEU:HG	1.86	0.57
2:B:132:ILE:HG22	2:B:182:TRP:HZ3	1.70	0.57
1:C:27:LYS:HD2	1:C:27:LYS:N	2.04	0.57
2:H:147:PHE:HB3	2:H:154:TRP:CB	2.28	0.57
1:G:58:VAL:O	1:G:61:SER:OG	2.08	0.57
2:B:167:VAL:HG12	2:B:168:GLN:H	1.69	0.57
2:F:145:THR:C	2:F:156:ILE:HD12	2.25	0.56
1:C:9:THR:HG22	2:D:94:MET:HB3	1.87	0.56
1:C:13:LEU:HD13	2:D:91:LEU:HD21	1.87	0.56
1:G:75:MET:HB3	1:G:76:LEU:HD12	1.87	0.56
2:H:176:ASN:O	2:H:177:SER:C	2.44	0.56
2:D:85:SER:O	2:D:89:THR:OG1	2.12	0.56
2:B:77:GLU:O	2:B:81:ALA:N	2.37	0.56
1:G:45:THR:O	1:G:49:PHE:HB2	2.05	0.56
2:B:92:PHE:HB3	2:B:96:ARG:NH1	2.21	0.56
2:F:158:GLN:HB3	2:F:187:THR:HB	1.87	0.55
2:B:169:LEU:HG	2:B:170:SER:N	2.21	0.55
2:H:155:GLU:N	2:H:189:LEU:O	2.28	0.55
1:E:25:SER:C	1:E:27:LYS:H	2.05	0.55
2:F:103:LEU:O	2:F:107:ILE:HG12	2.07	0.55
2:D:117:LEU:HB2	2:D:129:MET:HB3	1.88	0.55
2:F:141:THR:HG1	2:F:147:PHE:HE1	1.55	0.55
1:A:46:THR:HG23	1:A:47:GLU:H	1.72	0.55
2:D:90:MET:SD	2:D:94:MET:HG2	2.47	0.55
1:A:9:THR:HG22	2:B:94:MET:HB3	1.90	0.54
1:G:36:HIS:O	1:G:40:LEU:HG	2.07	0.54
1:C:62:MET:CE	1:C:65:ALA:HB1	2.38	0.54
2:D:189:LEU:N	2:D:189:LEU:HD12	2.22	0.54
2:B:96:ARG:HG3	2:B:96:ARG:HH11	1.73	0.54
2:B:100:ASN:O	2:B:104:ASN:HB2	2.06	0.54
1:E:23:GLU:HG2	1:E:29:TRP:CE2	2.42	0.54
2:F:163:ASP:HB2	2:F:165:LYS:CE	2.38	0.54
1:C:62:MET:HB3	1:C:65:ALA:HB3	1.88	0.54
2:D:128:LEU:O	2:D:187:THR:HA	2.07	0.54
2:H:159:VAL:HA	2:H:185:ILE:O	2.08	0.54
1:A:57:SER:HB3	2:B:120:ILE:CD1	2.38	0.54
2:H:161:ASP:HB2	2:H:181:ALA:O	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:159:VAL:HG22	2:F:186:VAL:HG22	1.89	0.54
2:F:161:ASP:HB2	2:F:181:ALA:HB3	1.89	0.53
1:E:71:LEU:HD11	2:F:89:THR:OG1	2.08	0.53
2:B:117:LEU:HB2	2:B:129:MET:HB2	1.90	0.53
1:A:58:VAL:O	1:A:62:MET:HG3	2.09	0.53
1:G:16:VAL:HG21	2:H:91:LEU:HD22	1.89	0.53
2:F:162:ALA:HB3	2:F:181:ALA:HB1	1.91	0.53
2:B:128:LEU:HD23	2:B:188:ALA:HB3	1.90	0.52
2:D:163:ASP:CB	2:D:165:LYS:HE2	2.38	0.52
1:G:25:SER:O	1:G:26:SER:C	2.46	0.52
1:E:54:SER:OG	2:F:120:ILE:O	2.28	0.52
2:F:163:ASP:O	2:F:165:LYS:HG3	2.09	0.52
2:H:100:ASN:OD1	2:H:103:LEU:HD12	2.10	0.52
1:G:68:ILE:HG22	2:H:111:ARG:HD3	1.92	0.52
1:E:3:MET:HA	1:E:6:VAL:HG12	1.92	0.52
2:B:135:TYR:CZ	2:B:139:LYS:HB3	2.45	0.52
2:B:140:ASN:HD21	2:D:80:ARG:HB2	1.75	0.52
1:C:39:ILE:HG12	1:C:51:LYS:HB2	1.92	0.51
1:C:71:LEU:HD23	1:C:71:LEU:C	2.30	0.51
2:F:131:VAL:HG12	2:F:185:ILE:HG12	1.91	0.51
2:B:161:ASP:HB2	2:B:181:ALA:HB3	1.93	0.51
1:C:62:MET:HE2	1:C:65:ALA:CB	2.41	0.51
2:D:156:ILE:CG2	2:D:186:VAL:HG23	2.40	0.51
1:G:68:ILE:HG23	2:H:92:PHE:CE2	2.45	0.51
1:A:47:GLU:O	1:A:51:LYS:HG2	2.10	0.51
1:A:62:MET:HB2	1:A:65:ALA:HB2	1.92	0.51
1:E:71:LEU:HD21	2:F:88:GLN:O	2.11	0.50
1:E:38:ASP:HB3	1:E:51:LYS:HD2	1.93	0.50
2:D:176:ASN:OD1	2:D:179:ASN:ND2	2.27	0.50
2:F:114:CYS:HA	2:F:131:VAL:O	2.10	0.50
1:A:13:LEU:HD21	1:A:56:LEU:HA	1.93	0.50
1:C:56:LEU:HD12	1:C:59:LEU:HD23	1.94	0.50
2:D:130:VAL:HG12	2:D:131:VAL:H	1.77	0.50
2:H:103:LEU:HA	2:H:106:ILE:HG12	1.94	0.49
2:B:153:LEU:HB3	2:B:191:ALA:HB3	1.95	0.49
1:E:21:ARG:NH1	2:H:108:ASN:HB3	2.27	0.49
2:B:163:ASP:O	2:B:164:SER:C	2.50	0.49
2:D:93:THR:O	2:D:97:LYS:HG2	2.12	0.49
2:H:103:LEU:HD23	2:H:106:ILE:HD11	1.94	0.49
1:C:62:MET:HE2	1:C:65:ALA:HB3	1.93	0.49
2:D:154:TRP:HE3	2:D:189:LEU:O	1.96	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:115:VAL:H	2:H:131:VAL:CG1	2.21	0.49
2:F:160:VAL:HA	2:F:166:ILE:HA	1.95	0.49
1:A:39:ILE:HG13	1:A:51:LYS:HB2	1.94	0.49
2:D:161:ASP:O	2:D:164:SER:N	2.44	0.49
2:D:135:TYR:CE2	2:D:174:MET:HG3	2.48	0.49
2:D:124:THR:O	2:D:126:ALA:N	2.45	0.49
1:E:58:VAL:O	1:E:62:MET:HG3	2.13	0.49
1:C:3:MET:HE1	1:C:7:LYS:HE3	1.93	0.48
1:A:25:SER:O	1:A:27:LYS:N	2.47	0.48
2:B:125:ALA:O	2:B:189:LEU:HD22	2.13	0.48
1:G:12:VAL:O	1:G:16:VAL:HG23	2.14	0.48
1:A:54:SER:O	1:A:57:SER:OG	2.19	0.48
1:E:69:ASN:O	1:E:72:CYS:HB3	2.14	0.47
2:H:159:VAL:HG22	2:H:186:VAL:HG22	1.96	0.47
2:D:152:ALA:HB1	2:D:190:ARG:HH12	1.80	0.47
1:E:7:LYS:O	1:E:11:VAL:HG23	2.14	0.47
2:D:105:ASN:OD1	2:D:109:ASN:OD1	2.32	0.47
1:C:61:SER:O	1:C:61:SER:OG	2.32	0.47
1:G:20:LEU:HD13	1:G:65:ALA:HB1	1.96	0.47
1:C:49:PHE:O	1:C:53:VAL:HG23	2.15	0.46
1:E:49:PHE:O	1:E:52:MET:N	2.48	0.46
2:H:135:TYR:HE2	2:H:174:MET:HG3	1.79	0.46
2:B:147:PHE:O	2:B:154:TRP:HB2	2.14	0.46
2:B:95:LEU:HD22	2:B:107:ILE:HD11	1.98	0.46
2:B:121:PRO:HB2	2:B:126:ALA:HB3	1.96	0.46
1:C:70:LYS:O	1:C:73:GLU:HB2	2.15	0.46
1:E:20:LEU:HD13	1:E:65:ALA:HB1	1.98	0.46
2:F:157:GLN:HG3	2:F:189:LEU:HG	1.98	0.46
1:E:15:SER:HA	1:E:18:GLN:HB2	1.96	0.46
2:H:121:PRO:CD	2:H:128:LEU:HB2	2.45	0.46
1:G:9:THR:HG22	2:H:94:MET:HE2	1.98	0.46
1:E:62:MET:HB2	1:E:65:ALA:CB	2.45	0.46
1:G:75:MET:HE2	1:G:75:MET:HB2	1.85	0.46
2:D:129:MET:CG	2:D:187:THR:HG22	2.40	0.46
2:H:149:TYR:HB3	2:H:154:TRP:HE1	1.81	0.46
1:E:56:LEU:HD23	1:E:56:LEU:O	2.15	0.45
2:H:169:LEU:HG	2:H:170:SER:N	2.30	0.45
1:E:49:PHE:O	1:E:53:VAL:HG23	2.16	0.45
1:G:14:LEU:CD1	1:G:32:CYS:HB3	2.46	0.45
2:H:128:LEU:O	2:H:187:THR:HA	2.15	0.45
2:B:121:PRO:HG3	2:B:127:LYS:O	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:121:PRO:HG3	2:F:127:LYS:O	2.17	0.45
1:C:16:VAL:HG22	2:D:87:MET:HG2	1.98	0.45
2:H:91:LEU:O	2:H:95:LEU:N	2.47	0.45
2:H:104:ASN:O	2:H:108:ASN:ND2	2.50	0.45
2:D:92:PHE:N	2:D:92:PHE:CD1	2.84	0.45
2:F:136:ASN:O	2:F:140:ASN:HB2	2.16	0.45
2:H:115:VAL:N	2:H:131:VAL:HG12	2.28	0.45
2:H:149:TYR:HB3	2:H:154:TRP:NE1	2.31	0.45
1:A:39:ILE:HD11	1:A:52:MET:N	2.32	0.44
2:B:127:LYS:HE3	2:B:127:LYS:HB3	1.89	0.44
2:D:92:PHE:HA	2:D:95:LEU:HB2	1.98	0.44
1:A:70:LYS:HD2	1:A:70:LYS:HA	1.62	0.44
1:C:2:LYS:O	1:C:6:VAL:HG23	2.17	0.44
2:D:169:LEU:HD13	2:D:169:LEU:HA	1.86	0.44
2:H:125:ALA:N	2:H:190:ARG:HB2	2.28	0.44
2:D:114:CYS:HA	2:D:131:VAL:O	2.17	0.44
1:E:14:LEU:O	1:E:18:GLN:HB2	2.17	0.44
1:A:75:MET:HG3	2:B:96:ARG:NH2	2.32	0.44
2:F:94:MET:O	2:F:98:LEU:HG	2.17	0.44
2:F:133:PRO:HA	2:F:183:PRO:CB	2.44	0.44
2:F:145:THR:O	2:F:156:ILE:HB	2.18	0.44
1:E:7:LYS:HE2	1:E:39:ILE:O	2.18	0.44
2:F:100:ASN:O	2:F:104:ASN:ND2	2.50	0.44
2:F:109:ASN:O	2:F:114:CYS:N	2.47	0.44
1:A:22:VAL:O	1:A:25:SER:HB2	2.18	0.43
1:G:57:SER:HB3	2:H:120:ILE:CD1	2.48	0.43
2:H:142:CYS:SG	2:H:147:PHE:HD1	2.41	0.43
2:B:161:ASP:OD1	2:B:165:LYS:N	2.47	0.43
2:D:95:LEU:HD23	2:D:98:LEU:HD12	2.01	0.43
2:B:163:ASP:O	2:B:165:LYS:HG3	2.19	0.43
1:C:8:CYS:O	1:C:12:VAL:HG23	2.18	0.43
1:A:34:GLN:HA	1:A:37:ASN:HB2	1.99	0.43
1:A:72:CYS:HA	1:A:75:MET:HG2	2.00	0.43
2:B:135:TYR:CE2	2:B:174:MET:HG2	2.53	0.43
1:G:14:LEU:HD22	1:G:36:HIS:CG	2.52	0.43
2:F:145:THR:O	2:F:145:THR:OG1	2.34	0.43
2:B:114:CYS:HA	2:B:131:VAL:O	2.19	0.43
1:C:27:LYS:HD2	1:C:27:LYS:HA	1.36	0.43
1:E:62:MET:HE2	1:E:65:ALA:HB2	2.01	0.43
1:E:44:ASP:OD1	1:E:44:ASP:N	2.52	0.42
1:G:56:LEU:HD23	2:H:106:ILE:HD11	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:VAL:HB	1:A:28:LEU:HD22	2.01	0.42
2:B:158:GLN:HB3	2:B:187:THR:HB	2.02	0.42
2:D:176:ASN:C	2:D:178:PRO:HD2	2.39	0.42
1:E:46:THR:O	1:E:50:GLU:HG3	2.18	0.42
2:F:79:LYS:CE	2:H:140:ASN:O	2.67	0.42
2:B:110:ALA:HB1	2:B:115:VAL:HG12	2.02	0.42
1:C:20:LEU:HD13	1:C:62:MET:HE3	1.95	0.42
2:F:92:PHE:HE1	2:F:107:ILE:HD12	1.85	0.42
2:F:122:LEU:HD12	2:F:122:LEU:C	2.31	0.42
1:G:9:THR:HG22	2:H:94:MET:CE	2.49	0.42
1:C:75:MET:HE1	2:D:92:PHE:HB2	2.01	0.42
2:D:90:MET:O	2:D:93:THR:N	2.53	0.42
2:D:110:ALA:HA	2:D:115:VAL:HG12	2.02	0.42
2:F:92:PHE:HA	2:F:95:LEU:HB2	2.02	0.42
2:B:149:TYR:O	2:B:154:TRP:NE1	2.47	0.42
1:C:60:LEU:HD11	2:D:107:ILE:HD13	2.01	0.42
1:C:62:MET:CB	1:C:65:ALA:HB3	2.49	0.42
1:C:71:LEU:HD11	2:D:88:GLN:HB3	2.02	0.42
1:A:13:LEU:HD21	1:A:56:LEU:CA	2.50	0.41
1:C:13:LEU:CD2	1:C:55:LEU:HG	2.49	0.41
2:B:92:PHE:HA	2:B:95:LEU:HB2	2.01	0.41
2:F:163:ASP:HB2	2:F:165:LYS:NZ	2.35	0.41
2:B:165:LYS:HE3	2:B:165:LYS:HB2	1.76	0.41
2:D:121:PRO:HG3	2:D:127:LYS:O	2.20	0.41
2:F:160:VAL:HG22	2:F:185:ILE:HB	2.03	0.41
1:G:46:THR:O	1:G:50:GLU:HB2	2.20	0.41
1:G:49:PHE:O	1:G:53:VAL:HG23	2.20	0.41
2:B:106:ILE:HG13	2:B:107:ILE:N	2.34	0.41
1:C:23:GLU:C	1:C:25:SER:H	2.24	0.41
2:D:107:ILE:HD13	2:D:107:ILE:HA	1.72	0.41
2:D:138:TYR:CE2	2:D:172:ILE:HG21	2.56	0.41
2:B:156:ILE:HG12	2:B:156:ILE:H	1.64	0.41
2:B:103:LEU:HD23	2:B:103:LEU:HA	1.78	0.41
1:G:39:ILE:HD11	1:G:51:LYS:O	2.21	0.41
2:H:154:TRP:HA	2:H:189:LEU:O	2.21	0.41
2:D:92:PHE:N	2:D:92:PHE:HD1	2.19	0.41
2:D:133:PRO:HD2	2:D:137:THR:HG21	2.03	0.41
2:F:88:GLN:HA	2:F:91:LEU:HB2	2.02	0.41
1:G:20:LEU:HD23	1:G:20:LEU:HA	1.88	0.41
1:G:32:CYS:O	1:G:36:HIS:N	2.49	0.41
2:H:135:TYR:O	2:H:138:TYR:N	2.52	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:138:TYR:HA	2:H:141:THR:OG1	2.21	0.41
1:E:68:ILE:HD12	1:E:68:ILE:H	1.85	0.41
2:H:162:ALA:HB2	2:H:183:PRO:HD2	2.03	0.41
1:A:72:CYS:SG	2:B:96:ARG:NH2	2.92	0.40
1:C:35:LEU:O	1:C:39:ILE:HG13	2.21	0.40
2:D:157:GLN:HG3	2:D:189:LEU:HD11	2.03	0.40
2:B:135:TYR:O	2:B:138:TYR:HB3	2.21	0.40
2:D:132:ILE:H	2:D:132:ILE:HD12	1.86	0.40
1:E:57:SER:HB3	2:F:120:ILE:HD12	2.02	0.40
2:H:115:VAL:HG22	2:H:131:VAL:HG11	2.03	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:LYS:NZ	2:D:90:MET:CG[1_655]	1.76	0.44
1:A:7:LYS:NZ	2:D:90:MET:CE[1_655]	1.96	0.24
1:A:7:LYS:NZ	2:D:90:MET:CB[1_655]	2.02	0.18
1:C:45:THR:OG1	2:D:163:ASP:O[1_455]	2.12	0.08
1:A:7:LYS:NZ	2:D:90:MET:SD[1_655]	2.19	0.01

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	73/83 (88%)	69 (94%)	3 (4%)	1 (1%)	11	21
1	C	74/83 (89%)	62 (84%)	12 (16%)	0	100	100
1	E	74/83 (89%)	65 (88%)	8 (11%)	1 (1%)	11	21
1	G	73/83 (88%)	66 (90%)	7 (10%)	0	100	100
2	B	114/122 (93%)	100 (88%)	13 (11%)	1 (1%)	17	34

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	114/122 (93%)	100 (88%)	14 (12%)	0	100	100
2	F	111/122 (91%)	97 (87%)	14 (13%)	0	100	100
2	H	112/122 (92%)	96 (86%)	14 (12%)	2 (2%)	8	16
All	All	745/820 (91%)	655 (88%)	85 (11%)	5 (1%)	22	41

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	157	GLN
1	E	26	SER
1	A	26	SER
2	H	163	ASP
2	H	177	SER

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	66/77 (86%)	62 (94%)	4 (6%)	18	36
1	C	70/77 (91%)	68 (97%)	2 (3%)	42	66
1	E	68/77 (88%)	65 (96%)	3 (4%)	28	51
1	G	68/77 (88%)	65 (96%)	3 (4%)	28	51
2	B	100/107 (94%)	92 (92%)	8 (8%)	12	22
2	D	98/107 (92%)	95 (97%)	3 (3%)	40	64
2	F	100/107 (94%)	98 (98%)	2 (2%)	55	76
2	H	96/107 (90%)	92 (96%)	4 (4%)	30	53
All	All	666/736 (90%)	637 (96%)	29 (4%)	28	51

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	34	GLN
1	A	35	LEU
1	A	54	SER
2	B	139	LYS
2	B	155	GLU
2	B	156	ILE
2	B	157	GLN
2	B	158	GLN
2	B	169	LEU
2	B	172	ILE
2	B	174	MET
1	C	19	GLN
1	C	27	LYS
2	D	139	LYS
2	D	158	GLN
2	D	175	ASP
1	E	3	MET
1	E	25	SER
1	E	59	LEU
2	F	88	GLN
2	F	123	THR
1	G	8	CYS
1	G	10	SER
1	G	75	MET
2	H	114	CYS
2	H	139	LYS
2	H	173	SER
2	H	190	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 [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, 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	75/83 (90%)	0.43	2 (2%) 54 51	26, 41, 61, 65	0
1	C	76/83 (91%)	0.46	5 (6%) 18 15	25, 41, 58, 74	0
1	E	76/83 (91%)	0.54	5 (6%) 18 15	28, 43, 60, 67	0
1	G	75/83 (90%)	0.49	6 (8%) 12 10	29, 43, 65, 70	0
2	B	116/122 (95%)	0.35	6 (5%) 27 23	29, 45, 60, 74	0
2	D	116/122 (95%)	0.42	8 (6%) 16 14	32, 46, 58, 64	0
2	F	113/122 (92%)	0.47	8 (7%) 16 13	29, 44, 60, 65	0
2	H	114/122 (93%)	0.47	4 (3%) 44 39	32, 47, 60, 66	0
All	All	761/820 (92%)	0.45	44 (5%) 23 19	25, 45, 60, 74	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	122	LEU	4.2
1	E	49	PHE	4.1
2	B	153	LEU	3.8
1	G	48	ALA	3.3
2	F	151	SER	3.2
1	E	48	ALA	3.2
2	F	176	ASN	3.1
2	F	150	ALA	3.1
1	G	25	SER	3.0
2	D	106	ILE	2.9
2	D	189	LEU	2.9
2	H	92	PHE	2.9
1	G	64	GLY	2.7
1	C	9	THR	2.7
2	F	174	MET	2.6
2	H	159	VAL	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	49	PHE	2.5
1	E	59	LEU	2.5
2	F	123	THR	2.5
1	C	22	VAL	2.5
1	C	60	LEU	2.4
1	E	22	VAL	2.4
2	B	180	LEU	2.4
2	D	172	ILE	2.3
2	H	119	ILE	2.3
1	A	22	VAL	2.3
2	D	184	LEU	2.3
2	B	126	ALA	2.2
1	G	60	LEU	2.2
2	D	181	ALA	2.2
2	B	124	THR	2.2
2	D	98	LEU	2.2
2	D	153	LEU	2.2
2	B	128	LEU	2.2
2	D	91	LEU	2.2
1	G	46	THR	2.1
2	F	154	TRP	2.1
1	C	28	LEU	2.1
1	G	68	ILE	2.1
2	F	189	LEU	2.1
2	B	132	ILE	2.1
2	F	172	ILE	2.1
1	E	29	TRP	2.1
1	A	3	MET	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.