Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:27 AM GMT

PDB ID	:	2H66
Title	:	The Crystal Structure of Plasmodium Vivax 2-Cys peroxiredoxin
Authors	:	Wernimont, A.K.; Dong, A.; Zhao, Y.; Lew, J.; Melone, M.; Kozieradzki, I.; Weigelt, J.; Sundstrom, M.; Edwards, A.M.; Arrowsmith, C.H.; Bochkarev, A.; Hui, R.; Artz, J.D.; Structural Genomics Consortium (SGC)
Deposited on	:	2006-05-30
Resolution	:	2.50 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:

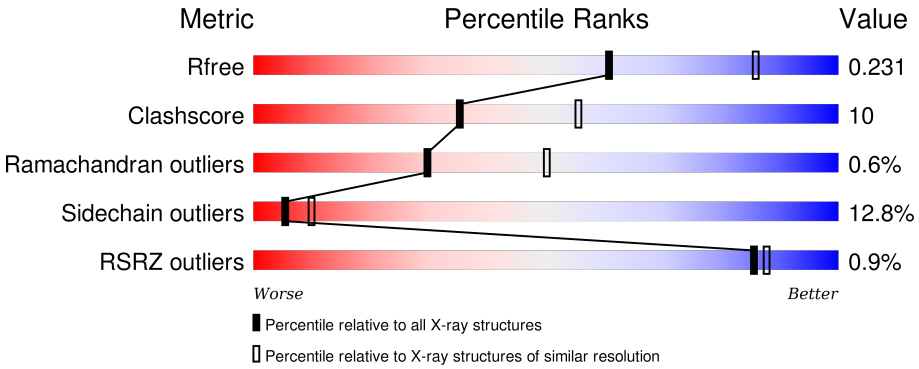
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	213	% 52% 22% 5% 22%
1	B	213	% 60% 15% 6% 20%
1	C	213	61% 15% • 20%
1	D	213	62% 15% • 21%
1	E	213	56% 15% • 24%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	213	2% 54% 20% 5% 21%
1	G	213	57% 16% 7% 20%
1	H	213	% 58% 18% 22%
1	I	213	% 63% 14% 6% 17%
1	J	213	54% 18% 23%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13448 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 PV-PF14_0368.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	167	Total	C	N	O	S	0	0	0
			1325	862	216	244	3			
1	B	171	Total	C	N	O	S	0	0	0
			1346	875	219	248	4			
1	C	170	Total	C	N	O	S	0	0	0
			1333	865	217	247	4			
1	D	169	Total	C	N	O	S	0	0	0
			1335	868	218	246	3			
1	E	161	Total	C	N	O	S	0	0	0
			1273	830	207	233	3			
1	F	168	Total	C	N	O	S	0	0	0
			1331	865	217	245	4			
1	G	171	Total	C	N	O	S	0	0	0
			1346	875	219	248	4			
1	H	167	Total	C	N	O	S	0	0	0
			1322	861	216	242	3			
1	I	177	Total	C	N	O	S	0	0	0
			1395	906	229	256	4			
1	J	163	Total	C	N	O	S	0	0	0
			1288	839	211	235	3			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	10	Total	O	0	0
			10	10		
2	B	8	Total	O	0	0
			8	8		
2	C	23	Total	O	0	0
			23	23		
2	D	14	Total	O	0	0
			14	14		

Continued on next page...

Continued from previous page...

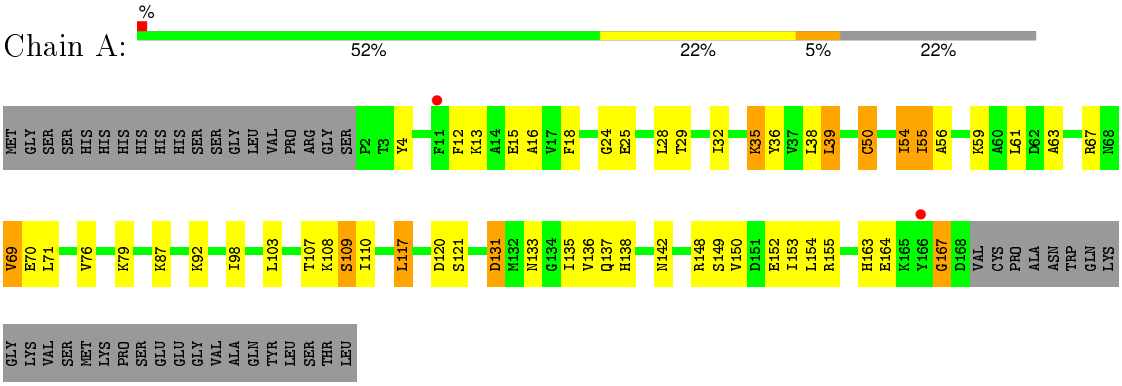
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	E	12	Total O 12 12	0	0
2	F	12	Total O 12 12	0	0
2	G	10	Total O 10 10	0	0
2	H	18	Total O 18 18	0	0
2	I	23	Total O 23 23	0	0
2	J	24	Total O 24 24	0	0

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.

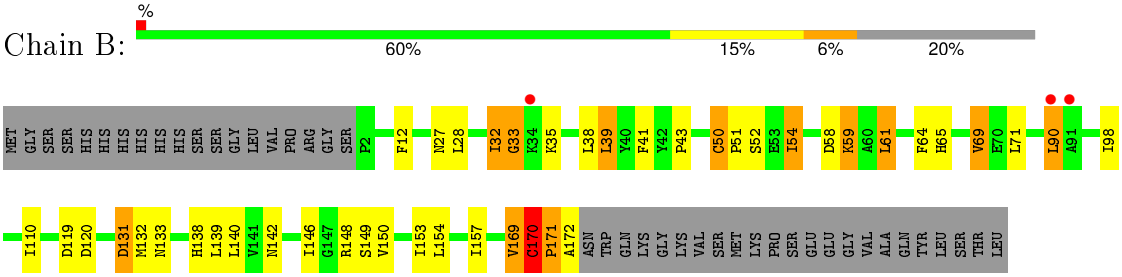
- Molecule 1: PV-PF14_0368

Chain A:



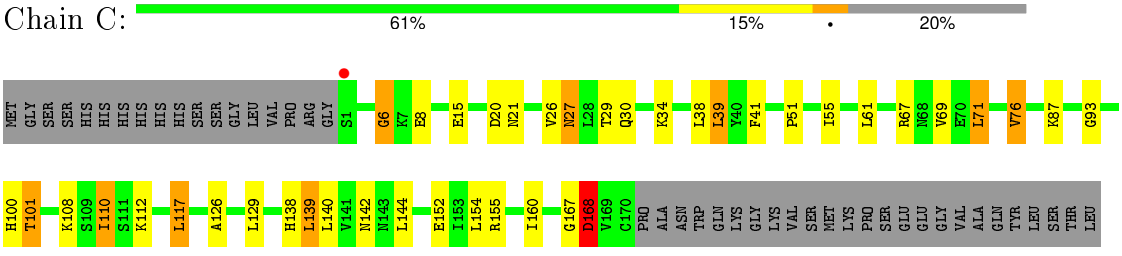
- Molecule 1: PV-PF14_0368

Chain B:



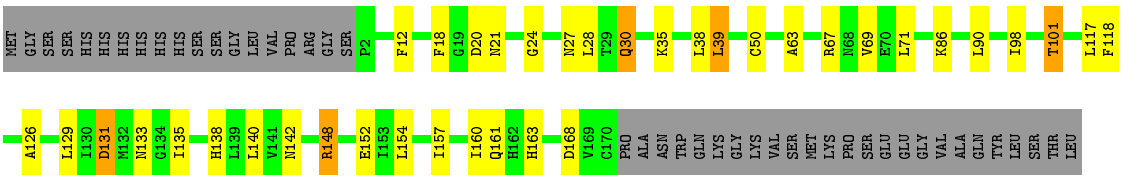
- Molecule 1: PV-PF14_0368

Chain C:



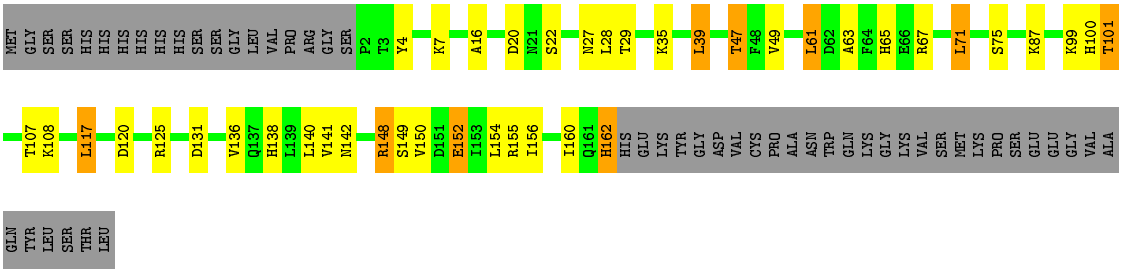
- Molecule 1: PV-PF14_0368

Chain D:



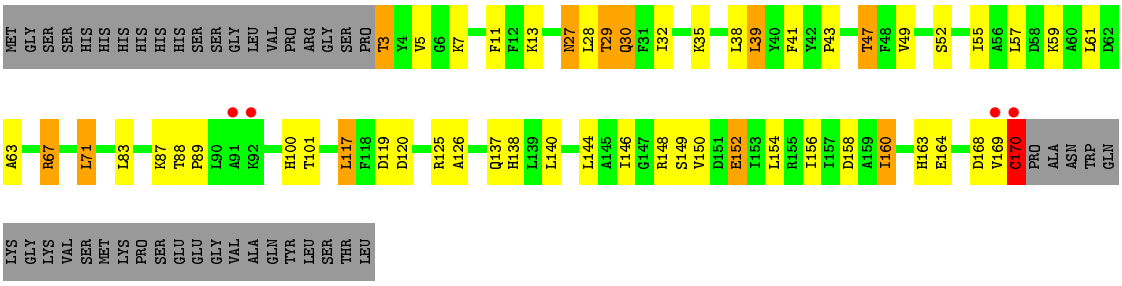
• Molecule 1: PV-PF14_0368

Chain E:



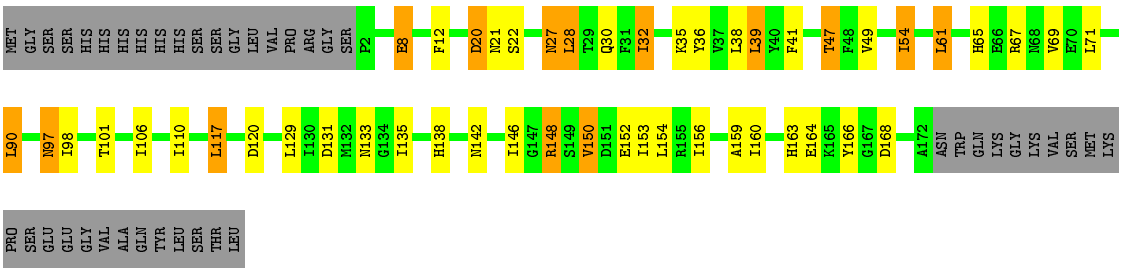
• Molecule 1: PV-PF14_0368

Chain F:



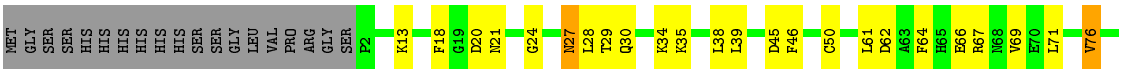
• Molecule 1: PV-PF14_0368

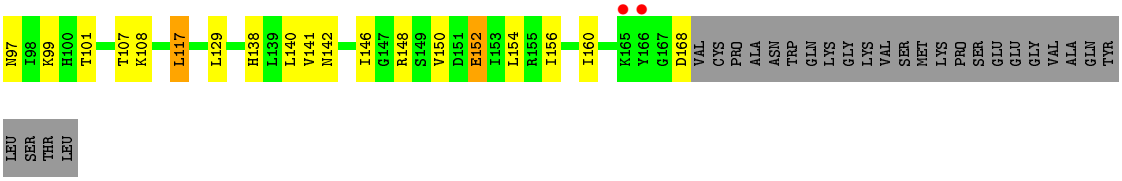
Chain G:



• Molecule 1: PV-PF14_0368

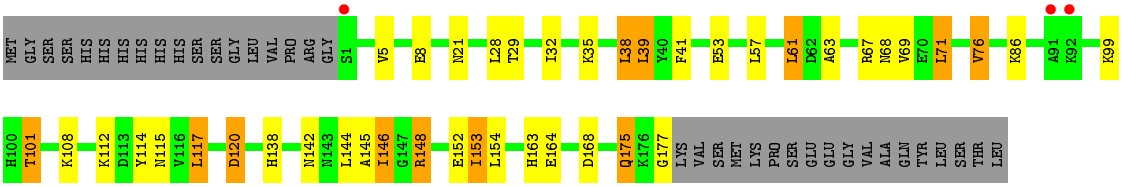
Chain H:





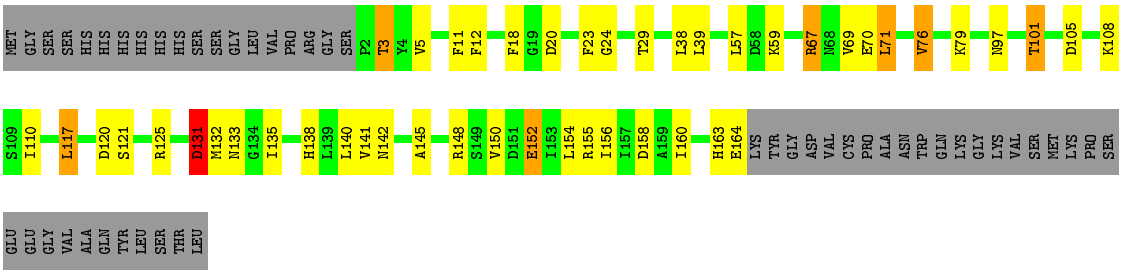
- Molecule 1: PV-PF14_0368

Chain I:



- Molecule 1: PV-PF14_0368

Chain J:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	70.55Å 149.59Å 131.91Å 90.00° 104.88° 90.00°	Depositor
Resolution (Å)	41.56 – 2.50 40.25 – 2.50	Depositor EDS
% Data completeness (in resolution range)	94.7 (41.56-2.50) 94.7 (40.25-2.50)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	1.15 (at 2.51Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.194 , 0.232 0.194 , 0.231	Depositor DCC
R_{free} test set	4302 reflections (5.24%)	DCC
Wilson B-factor (Å^2)	46.1	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 35.2	EDS
Estimated twinning fraction	0.025 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 86438 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	13448	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.69% 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	0.72	0/1355	0.78	1/1834 (0.1%)
1	B	0.75	1/1377 (0.1%)	0.82	2/1867 (0.1%)
1	C	0.82	1/1363 (0.1%)	0.87	3/1849 (0.2%)
1	D	0.72	1/1365 (0.1%)	0.76	2/1848 (0.1%)
1	E	0.78	2/1301 (0.2%)	0.81	2/1762 (0.1%)
1	F	0.84	3/1360 (0.2%)	0.80	0/1841
1	G	0.76	1/1377 (0.1%)	0.81	1/1867 (0.1%)
1	H	0.85	3/1352 (0.2%)	0.80	2/1830 (0.1%)
1	I	0.84	2/1428 (0.1%)	0.79	0/1937
1	J	0.83	1/1317 (0.1%)	0.84	1/1784 (0.1%)
All	All	0.79	15/13595 (0.1%)	0.81	14/18419 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	3
1	C	0	2
All	All	0	5

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	168	ASP	C-O	12.44	1.47	1.23
1	F	170	CYS	C-O	10.16	1.42	1.23
1	E	162	HIS	C-O	7.80	1.38	1.23
1	I	177	GLY	CA-C	7.35	1.63	1.51
1	F	152	GLU	CG-CD	7.34	1.62	1.51
1	B	50	CYS	CB-SG	-7.00	1.70	1.82
1	J	152	GLU	CG-CD	6.98	1.62	1.51
1	E	152	GLU	CG-CD	6.59	1.61	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	152	GLU	CG-CD	6.44	1.61	1.51
1	H	50	CYS	CB-SG	5.85	1.92	1.82
1	C	168	ASP	CG-OD2	5.48	1.38	1.25
1	I	152	GLU	CG-CD	5.34	1.59	1.51
1	G	152	GLU	CG-CD	5.25	1.59	1.51
1	D	50	CYS	CB-SG	-5.11	1.73	1.81
1	F	152	GLU	CB-CG	5.03	1.61	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	168	ASP	OD1-CG-OD2	-7.21	109.60	123.30
1	E	39	LEU	CA-CB-CG	6.44	130.12	115.30
1	G	28	LEU	CA-CB-CG	6.29	129.77	115.30
1	C	139	LEU	CA-CB-CG	6.01	129.13	115.30
1	B	170	CYS	C-N-CD	-5.78	107.88	120.60
1	C	168	ASP	CB-CG-OD1	5.76	123.48	118.30
1	J	131	ASP	CB-CA-C	-5.65	99.10	110.40
1	H	168	ASP	CA-C-O	-5.60	108.35	120.10
1	H	117	LEU	CB-CG-CD2	5.53	120.39	111.00
1	B	131	ASP	CB-CA-C	-5.32	99.76	110.40
1	D	131	ASP	CB-CG-OD1	-5.31	113.52	118.30
1	A	39	LEU	CA-CB-CG	5.11	127.06	115.30
1	E	131	ASP	CB-CG-OD1	5.08	122.87	118.30
1	D	39	LEU	CB-CG-CD2	5.05	119.58	111.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	169	VAL	Peptide
1	B	170	CYS	Peptide
1	B	33	GLY	Peptide
1	C	168	ASP	Sidechain
1	C	6	GLY	Peptide

5.2 Too-close contacts (i)

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	1325	0	1327	29	0
1	B	1346	0	1342	24	0
1	C	1333	0	1316	27	0
1	D	1335	0	1331	25	0
1	E	1273	0	1286	25	0
1	F	1331	0	1334	34	0
1	G	1346	0	1342	35	0
1	H	1322	0	1325	18	0
1	I	1395	0	1386	40	0
1	J	1288	0	1294	30	0
2	A	10	0	0	0	0
2	B	8	0	0	0	0
2	C	23	0	0	3	0
2	D	14	0	0	1	0
2	E	12	0	0	3	0
2	F	12	0	0	0	0
2	G	10	0	0	2	0
2	H	18	0	0	0	0
2	I	23	0	0	4	0
2	J	24	0	0	1	0
All	All	13448	0	13283	260	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 10.

All (260) 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:B:171:PRO:HB2	1:B:172:ALA:O	1.43	1.16
1:F:149:SER:HB3	1:F:152:GLU:HG3	1.30	1.08
1:E:16:ALA:HB3	2:E:203:HOH:O	1.60	1.00
1:B:32:ILE:HD13	1:B:33:GLY:H	1.31	0.95
1:I:67:ARG:CZ	2:I:204:HOH:O	2.16	0.93
1:G:47:THR:HB	2:G:197:HOH:O	1.67	0.92
1:I:138:HIS:HE1	1:I:148:ARG:NH2	1.69	0.90
1:C:6:GLY:HA3	1:D:118:PHE:HE2	1.35	0.90
1:I:101:THR:HG22	2:I:202:HOH:O	1.71	0.89
1:E:160:ILE:HG12	1:F:144:LEU:HD12	1.56	0.87
1:D:101:THR:HG22	2:D:204:HOH:O	1.76	0.84
1:J:148:ARG:NE	1:J:152:GLU:OE2	2.09	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:138:HIS:CE1	1:I:148:ARG:NH2	2.46	0.83
1:G:90:LEU:HD12	1:G:90:LEU:H	1.45	0.82
1:J:12:PHE:HB2	1:J:110:ILE:HD12	1.60	0.82
1:B:90:LEU:H	1:B:90:LEU:HD12	1.46	0.79
1:A:13:LYS:HE3	1:A:25:GLU:OE2	1.83	0.79
1:B:32:ILE:HD13	1:B:33:GLY:N	1.99	0.77
1:H:27:ASN:HB2	1:H:30:GLN:HE21	1.50	0.77
1:I:142:ASN:OD1	1:J:138:HIS:HD2	1.68	0.77
1:B:171:PRO:HB2	1:B:172:ALA:C	2.05	0.76
1:F:27:ASN:H	1:F:30:GLN:NE2	1.84	0.75
1:I:35:LYS:HE2	1:I:68:ASN:ND2	2.02	0.75
1:G:39:LEU:HD13	1:G:41:PHE:CE1	2.24	0.73
1:F:149:SER:HB3	1:F:152:GLU:CG	2.14	0.71
1:E:47:THR:HB	2:E:199:HOH:O	1.90	0.70
1:E:149:SER:HB3	1:E:152:GLU:HG3	1.74	0.69
1:C:6:GLY:HA3	1:D:118:PHE:CE2	2.26	0.68
1:D:131:ASP:HB3	1:D:133:ASN:H	1.59	0.68
1:D:90:LEU:HD12	1:D:90:LEU:H	1.59	0.67
1:I:29:THR:O	1:I:32:ILE:HG22	1.94	0.67
1:G:67:ARG:HH11	1:G:67:ARG:HG3	1.58	0.67
1:B:171:PRO:CB	1:B:172:ALA:O	2.33	0.67
1:I:144:LEU:O	1:I:146:ILE:N	2.29	0.66
1:G:117:LEU:HD13	1:G:120:ASP:HA	1.77	0.66
1:C:101:THR:HG21	2:C:210:HOH:O	1.96	0.66
1:I:175:GLN:HE21	1:I:175:GLN:H	1.44	0.66
1:I:144:LEU:HB2	1:I:146:ILE:HD13	1.79	0.65
1:C:138:HIS:HD2	1:D:142:ASN:OD1	1.80	0.64
1:H:129:LEU:HD23	1:H:160:ILE:HD13	1.78	0.64
1:E:20:ASP:OD1	1:E:22:SER:HB2	1.97	0.64
1:G:20:ASP:O	1:G:22:SER:N	2.30	0.63
1:C:101:THR:HG22	2:C:198:HOH:O	1.99	0.63
1:I:138:HIS:CE1	1:I:148:ARG:HH21	2.15	0.63
1:E:117:LEU:CD1	1:E:120:ASP:HA	2.29	0.62
1:D:148:ARG:HE	1:D:152:GLU:CD	2.03	0.62
1:C:27:ASN:HD22	1:C:27:ASN:N	1.96	0.62
1:I:138:HIS:HD2	1:J:142:ASN:OD1	1.83	0.61
1:B:54:ILE:HD11	1:B:98:ILE:HD13	1.81	0.61
1:C:142:ASN:OD1	1:D:138:HIS:HD2	1.83	0.61
1:C:144:LEU:HD13	1:D:163:HIS:CD2	2.36	0.61
1:J:3:THR:HB	1:J:5:VAL:H	1.65	0.61
1:I:138:HIS:HE1	1:I:148:ARG:HH22	1.46	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:159:ALA:HB1	1:H:146:ILE:HG13	1.83	0.60
1:J:152:GLU:O	1:J:156:ILE:HG12	2.02	0.60
1:G:138:HIS:HD2	1:H:142:ASN:OD1	1.85	0.60
1:F:169:VAL:HG12	1:F:170:CYS:H	1.66	0.60
1:E:152:GLU:O	1:E:156:ILE:HG12	2.02	0.59
1:D:157:ILE:O	1:D:161:GLN:HG3	2.03	0.59
1:A:138:HIS:CE1	1:A:148:ARG:HH22	2.21	0.59
1:J:131:ASP:HB3	1:J:133:ASN:H	1.68	0.59
1:B:32:ILE:O	1:B:132:MET:O	2.21	0.59
1:I:138:HIS:CE1	1:I:148:ARG:HH22	2.17	0.59
1:H:76:VAL:HG22	1:H:108:LYS:HG2	1.84	0.59
1:F:47:THR:HG22	1:F:49:VAL:H	1.67	0.59
1:I:144:LEU:C	1:I:146:ILE:H	2.06	0.58
1:C:152:GLU:HG2	1:C:155:ARG:NH1	2.18	0.58
1:I:117:LEU:HD13	1:I:120:ASP:HA	1.85	0.58
1:G:27:ASN:HB3	1:G:30:GLN:HE21	1.68	0.58
1:A:12:PHE:HB2	1:A:110:ILE:HD12	1.86	0.58
1:F:27:ASN:HB2	1:F:30:GLN:HE21	1.69	0.57
1:I:112:LYS:HG2	1:I:117:LEU:HD12	1.86	0.57
1:E:138:HIS:CE1	1:F:140:LEU:HD11	2.40	0.57
1:C:20:ASP:O	1:C:21:ASN:HB2	2.05	0.57
1:J:76:VAL:HG22	1:J:108:LYS:HG2	1.85	0.57
1:A:63:ALA:O	1:A:67:ARG:HG2	2.05	0.56
1:F:156:ILE:O	1:F:160:ILE:HG23	2.04	0.56
1:I:21:ASN:HD21	1:I:86:LYS:HE2	1.71	0.56
1:I:138:HIS:HE1	1:I:148:ARG:HH21	1.50	0.56
1:B:90:LEU:H	1:B:90:LEU:CD1	2.18	0.56
1:A:155:ARG:HH12	1:B:149:SER:H	1.53	0.56
1:F:11:PHE:HE1	1:F:29:THR:HG22	1.71	0.56
1:G:27:ASN:HB3	1:G:30:GLN:NE2	2.19	0.56
1:A:107:THR:OG1	1:A:109:SER:HB2	2.06	0.56
1:F:39:LEU:HD13	1:F:41:PHE:CE1	2.41	0.56
1:A:35:LYS:HD2	1:A:70:GLU:HB2	1.87	0.55
1:F:43:PRO:HD3	1:F:125:ARG:HG3	1.87	0.55
1:E:61:LEU:HD13	1:E:65:HIS:CE1	2.41	0.55
1:I:21:ASN:HD21	1:I:86:LYS:CE	2.20	0.55
1:C:152:GLU:HG2	1:C:155:ARG:HH12	1.72	0.55
1:I:142:ASN:OD1	1:J:138:HIS:CD2	2.56	0.54
1:G:129:LEU:HD23	1:G:160:ILE:HD13	1.90	0.54
1:D:90:LEU:N	1:D:90:LEU:HD12	2.21	0.54
1:A:108:LYS:HE3	1:A:121:SER:O	2.08	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:ILE:HG22	1:A:137:GLN:NE2	2.23	0.54
1:G:117:LEU:CD1	1:G:120:ASP:HA	2.37	0.53
1:G:131:ASP:HB3	1:G:133:ASN:H	1.73	0.53
1:F:71:LEU:HD13	1:F:100:HIS:CD2	2.43	0.53
1:A:142:ASN:OD1	1:B:138:HIS:HD2	1.90	0.53
1:A:117:LEU:CD1	1:A:120:ASP:HA	2.38	0.53
1:D:126:ALA:HA	1:D:140:LEU:O	2.08	0.53
1:F:57:LEU:HD23	1:F:150:VAL:HG23	1.91	0.52
1:C:26:VAL:C	1:C:27:ASN:HD22	2.13	0.52
1:G:32:ILE:HG12	2:G:202:HOH:O	2.09	0.52
1:G:61:LEU:HD13	1:G:65:HIS:CE1	2.45	0.52
1:C:39:LEU:HD13	1:C:41:PHE:CE1	2.45	0.52
1:E:117:LEU:HD11	1:E:120:ASP:HA	1.91	0.52
1:I:115:ASN:O	1:J:3:THR:HG23	2.10	0.51
1:C:112:LYS:HG3	1:C:117:LEU:HD12	1.92	0.51
1:C:110:ILE:N	1:C:110:ILE:HD13	2.26	0.51
1:G:67:ARG:NH1	1:G:67:ARG:HG3	2.25	0.51
1:F:47:THR:CG2	1:F:49:VAL:H	2.23	0.51
1:B:90:LEU:N	1:B:90:LEU:HD12	2.22	0.51
1:F:137:GLN:HG3	1:F:160:ILE:HD13	1.92	0.51
1:J:11:PHE:HE1	1:J:29:THR:HG23	1.76	0.51
1:A:15:GLU:OE2	1:A:79:LYS:HE2	2.11	0.50
1:I:67:ARG:NH2	2:I:204:HOH:O	2.35	0.50
1:F:117:LEU:HD13	1:F:120:ASP:HA	1.92	0.50
1:A:54:ILE:HD11	1:A:98:ILE:HD13	1.93	0.50
1:H:152:GLU:O	1:H:156:ILE:HG12	2.11	0.50
1:J:131:ASP:HB2	1:J:135:ILE:H	1.76	0.50
1:C:144:LEU:HD13	1:D:163:HIS:CG	2.46	0.50
1:A:138:HIS:HE1	1:A:148:ARG:HH22	1.59	0.50
1:G:160:ILE:O	1:G:164:GLU:HG3	2.11	0.50
1:B:50:CYS:C	1:B:52:SER:H	2.14	0.50
1:I:63:ALA:O	1:I:67:ARG:HG3	2.11	0.50
1:H:18:PHE:HE1	1:H:24:GLY:HA3	1.76	0.50
1:I:163:HIS:HD2	2:I:206:HOH:O	1.95	0.50
1:C:27:ASN:H	1:C:30:GLN:NE2	2.10	0.49
1:B:64:PHE:HB3	1:B:69:VAL:HG22	1.95	0.49
1:J:163:HIS:O	1:J:164:GLU:CB	2.61	0.49
1:B:131:ASP:HB3	1:B:133:ASN:H	1.77	0.49
1:D:27:ASN:HB3	1:D:30:GLN:HE21	1.77	0.49
1:G:54:ILE:HD11	1:G:98:ILE:HG21	1.94	0.49
1:C:93:GLY:O	2:C:202:HOH:O	2.19	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:20:ASP:O	1:H:21:ASN:HB2	2.12	0.49
1:G:97:ASN:HD22	1:G:97:ASN:C	2.16	0.49
1:A:55:ILE:HD13	1:A:56:ALA:N	2.26	0.49
1:G:54:ILE:CD1	1:G:98:ILE:HD13	2.42	0.49
1:A:15:GLU:OE2	1:A:79:LYS:CE	2.61	0.48
1:I:163:HIS:HE1	1:I:168:ASP:OD1	1.96	0.48
1:E:27:ASN:HD22	1:E:29:THR:H	1.62	0.48
1:F:3:THR:O	1:F:7:LYS:HE2	2.13	0.48
1:J:117:LEU:HD13	1:J:120:ASP:HA	1.94	0.48
1:F:163:HIS:CE1	1:F:168:ASP:HB3	2.49	0.48
1:J:70:GLU:OE2	1:J:70:GLU:HA	2.13	0.48
1:A:131:ASP:HB3	1:A:133:ASN:H	1.77	0.48
1:C:27:ASN:H	1:C:30:GLN:HE21	1.62	0.48
1:I:38:LEU:HD11	1:I:153:ILE:CD1	2.44	0.48
1:D:90:LEU:CD1	1:D:90:LEU:H	2.26	0.47
1:C:168:ASP:OD1	1:C:168:ASP:C	2.52	0.47
1:I:39:LEU:HD13	1:I:41:PHE:CE1	2.49	0.47
1:G:39:LEU:CD1	1:G:41:PHE:CE1	2.97	0.47
1:C:27:ASN:ND2	1:C:27:ASN:N	2.62	0.47
1:F:160:ILE:O	1:F:164:GLU:HB2	2.14	0.47
1:E:160:ILE:HG12	1:F:144:LEU:CD1	2.38	0.47
1:A:110:ILE:HD13	1:A:110:ILE:N	2.30	0.47
1:E:152:GLU:HG2	1:F:152:GLU:HG2	1.97	0.47
1:E:138:HIS:CE1	1:F:140:LEU:CD1	2.97	0.47
1:I:21:ASN:ND2	1:I:86:LYS:NZ	2.62	0.47
1:D:63:ALA:O	1:D:67:ARG:HG2	2.15	0.47
1:E:141:VAL:HG12	1:F:5:VAL:HG11	1.97	0.47
1:H:140:LEU:C	1:H:140:LEU:HD23	2.35	0.47
1:I:144:LEU:C	1:I:146:ILE:N	2.68	0.47
1:D:12:PHE:CE1	1:D:28:LEU:HD12	2.49	0.47
1:F:13:LYS:HG3	1:F:27:ASN:ND2	2.30	0.47
1:G:61:LEU:CD1	1:G:65:HIS:CE1	2.98	0.46
1:D:86:LYS:HE3	1:D:98:ILE:HG13	1.96	0.46
1:D:163:HIS:CE1	1:D:168:ASP:OD1	2.68	0.46
1:A:117:LEU:HD13	1:A:120:ASP:HA	1.96	0.46
1:E:138:HIS:HE1	1:F:140:LEU:HD11	1.78	0.46
1:J:20:ASP:C	1:J:20:ASP:OD1	2.54	0.46
1:J:140:LEU:HD23	1:J:141:VAL:N	2.30	0.46
1:H:64:PHE:HB3	1:H:69:VAL:HG22	1.98	0.46
1:C:126:ALA:HA	1:C:140:LEU:O	2.15	0.46
1:F:13:LYS:HG3	1:F:27:ASN:HD21	1.79	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:SER:HB2	1:A:152:GLU:HG3	1.98	0.46
1:A:163:HIS:O	1:A:167:GLY:HA2	2.15	0.46
1:F:67:ARG:NH1	1:F:158:ASP:OD2	2.48	0.46
1:G:163:HIS:O	1:G:166:TYR:O	2.34	0.46
1:A:138:HIS:HD2	1:B:142:ASN:OD1	1.99	0.45
1:H:62:ASP:O	1:H:66:GLU:HG3	2.16	0.45
1:A:18:PHE:HE1	1:A:24:GLY:HA3	1.80	0.45
1:G:47:THR:HG22	1:G:49:VAL:H	1.81	0.45
1:H:140:LEU:HD23	1:H:141:VAL:N	2.31	0.45
1:F:88:THR:HA	1:F:89:PRO:HD2	1.84	0.45
1:G:148:ARG:NH2	1:G:156:ILE:HD13	2.31	0.45
1:G:12:PHE:HB2	1:G:110:ILE:HG12	1.98	0.45
1:I:61:LEU:HD12	1:I:99:LYS:HB2	1.98	0.45
1:G:36:TYR:OH	1:G:164:GLU:OE1	2.32	0.45
1:B:61:LEU:CD1	1:B:65:HIS:CE1	3.00	0.44
1:D:20:ASP:O	1:D:21:ASN:HB2	2.17	0.44
1:I:57:LEU:HB3	1:I:71:LEU:HD11	1.99	0.44
1:E:63:ALA:O	1:E:67:ARG:HG2	2.18	0.44
1:B:171:PRO:HB2	1:B:172:ALA:CA	2.47	0.44
1:J:76:VAL:CG2	1:J:108:LYS:HG2	2.48	0.44
1:E:142:ASN:OD1	1:F:138:HIS:HD2	2.01	0.44
1:B:12:PHE:HB2	1:B:110:ILE:HG12	1.99	0.44
1:C:71:LEU:HD13	1:C:100:HIS:CG	2.52	0.44
1:J:23:PHE:CD2	1:J:79:LYS:HD2	2.53	0.44
1:I:35:LYS:HE2	1:I:68:ASN:HD22	1.80	0.44
1:D:131:ASP:HB2	1:D:135:ILE:H	1.83	0.43
1:J:67:ARG:NH1	1:J:158:ASP:OD1	2.50	0.43
1:G:150:VAL:HA	1:G:153:ILE:HD12	2.00	0.43
1:J:18:PHE:HA	1:J:101:THR:HB	1.98	0.43
1:D:129:LEU:HD23	1:D:160:ILE:HD12	1.99	0.43
1:C:76:VAL:HG22	1:C:108:LYS:HG2	2.00	0.43
1:A:16:ALA:HB2	1:A:103:LEU:HD23	2.00	0.43
1:H:107:THR:O	1:H:108:LYS:HB2	2.18	0.43
1:F:63:ALA:O	1:F:67:ARG:HG2	2.18	0.43
1:B:39:LEU:HD13	1:B:41:PHE:CE1	2.53	0.43
1:B:153:ILE:O	1:B:157:ILE:HG13	2.18	0.43
1:E:101:THR:HG22	2:E:197:HOH:O	2.18	0.43
1:A:148:ARG:HD3	1:A:153:ILE:HG13	2.00	0.43
1:J:57:LEU:HB3	1:J:71:LEU:HD11	2.00	0.43
1:B:61:LEU:HD13	1:B:65:HIS:CE1	2.53	0.43
1:E:47:THR:HG23	1:E:49:VAL:H	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:8:GLU:CD	1:I:8:GLU:H	2.22	0.43
1:I:76:VAL:HG22	1:I:108:LYS:HG2	1.99	0.43
1:H:76:VAL:CG2	1:H:108:LYS:HG2	2.49	0.43
1:J:11:PHE:CE1	1:J:29:THR:HG23	2.53	0.43
1:G:47:THR:CG2	1:G:49:VAL:H	2.32	0.43
1:D:131:ASP:HB3	1:D:133:ASN:N	2.30	0.43
1:F:29:THR:HA	1:F:32:ILE:HG12	2.00	0.42
1:C:140:LEU:HD12	1:D:140:LEU:HD12	2.01	0.42
1:J:105:ASP:OD2	1:J:110:ILE:HG12	2.19	0.42
1:G:67:ARG:HD3	1:G:67:ARG:N	2.34	0.42
1:F:126:ALA:HA	1:F:140:LEU:O	2.19	0.42
1:I:5:VAL:HG11	1:J:141:VAL:HG12	2.00	0.42
1:J:12:PHE:HB2	1:J:110:ILE:CD1	2.40	0.42
1:G:131:ASP:HB2	1:G:135:ILE:H	1.84	0.42
1:I:53:GLU:OE1	1:I:148:ARG:O	2.37	0.42
1:E:4:TYR:CD2	1:E:136:VAL:HG21	2.55	0.42
1:H:45:ASP:O	1:H:46:PHE:HB2	2.20	0.42
1:A:67:ARG:HB2	1:A:69:VAL:CG1	2.51	0.41
1:F:83:LEU:HD11	1:F:87:LYS:HE3	2.02	0.41
1:B:59:LYS:HA	1:B:59:LYS:HD3	1.94	0.41
1:H:27:ASN:H	1:H:30:GLN:NE2	2.17	0.41
1:G:27:ASN:O	1:G:30:GLN:HG2	2.20	0.41
1:G:142:ASN:OD1	1:H:138:HIS:HD2	2.03	0.41
1:A:36:TYR:OH	1:A:164:GLU:OE1	2.37	0.41
1:E:71:LEU:HD13	1:E:100:HIS:CG	2.56	0.41
1:I:144:LEU:HD12	1:J:160:ILE:HG12	2.03	0.41
1:I:21:ASN:HD21	1:I:86:LYS:NZ	2.19	0.41
1:C:129:LEU:HD23	1:C:160:ILE:HD12	2.03	0.41
1:E:107:THR:O	1:E:108:LYS:HB2	2.21	0.41
1:J:132:MET:CE	2:J:203:HOH:O	2.68	0.41
1:E:20:ASP:OD1	1:E:22:SER:CB	2.68	0.41
1:A:107:THR:O	1:A:108:LYS:HB2	2.20	0.41
1:H:138:HIS:HE1	1:H:148:ARG:HH12	1.68	0.41
1:G:8:GLU:HG2	1:G:8:GLU:H	1.52	0.41
1:D:18:PHE:CE1	1:D:24:GLY:HA3	2.56	0.41
1:E:140:LEU:CD2	1:E:148:ARG:HG3	2.51	0.40
1:I:114:TYR:O	1:I:115:ASN:HB2	2.22	0.40
1:B:58:ASP:O	1:B:61:LEU:HB2	2.21	0.40
1:G:20:ASP:CG	1:G:20:ASP:O	2.60	0.40
1:J:18:PHE:HE1	1:J:24:GLY:HA3	1.87	0.40
1:J:125:ARG:CZ	1:J:145:ALA:HB2	2.52	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:51:PRO:O	1:C:55:ILE:HG12	2.21	0.40
1:A:4:TYR:CD2	1:A:136:VAL:HG21	2.57	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	165/213 (78%)	153 (93%)	10 (6%)	2 (1%)	16	29
1	B	169/213 (79%)	158 (94%)	8 (5%)	3 (2%)	11	18
1	C	168/213 (79%)	157 (94%)	9 (5%)	2 (1%)	16	29
1	D	167/213 (78%)	160 (96%)	7 (4%)	0	100	100
1	E	159/213 (75%)	153 (96%)	6 (4%)	0	100	100
1	F	166/213 (78%)	156 (94%)	10 (6%)	0	100	100
1	G	169/213 (79%)	162 (96%)	6 (4%)	1 (1%)	30	50
1	H	165/213 (78%)	160 (97%)	5 (3%)	0	100	100
1	I	175/213 (82%)	166 (95%)	8 (5%)	1 (1%)	30	50
1	J	161/213 (76%)	155 (96%)	5 (3%)	1 (1%)	30	50
All	All	1664/2130 (78%)	1580 (95%)	74 (4%)	10 (1%)	30	50

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	167	GLY
1	C	168	ASP
1	G	21	ASN
1	I	145	ALA
1	C	167	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	131	ASP
1	A	50	CYS
1	B	43	PRO
1	B	51	PRO
1	B	171	PRO

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	145/184 (79%)	124 (86%)	21 (14%)	4 7
1	B	147/184 (80%)	125 (85%)	22 (15%)	3 6
1	C	144/184 (78%)	125 (87%)	19 (13%)	5 9
1	D	145/184 (79%)	135 (93%)	10 (7%)	19 35
1	E	140/184 (76%)	122 (87%)	18 (13%)	5 10
1	F	146/184 (79%)	123 (84%)	23 (16%)	3 5
1	G	147/184 (80%)	124 (84%)	23 (16%)	3 6
1	H	144/184 (78%)	126 (88%)	18 (12%)	6 10
1	I	151/184 (82%)	135 (89%)	16 (11%)	8 16
1	J	141/184 (77%)	126 (89%)	15 (11%)	8 16
All	All	1450/1840 (79%)	1265 (87%)	185 (13%)	5 10

All (185) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	LEU
1	A	29	THR
1	A	32	ILE
1	A	35	LYS
1	A	38	LEU
1	A	39	LEU
1	A	50	CYS
1	A	54	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	55	ILE
1	A	59	LYS
1	A	61	LEU
1	A	69	VAL
1	A	71	LEU
1	A	76	VAL
1	A	87	LYS
1	A	92	LYS
1	A	109	SER
1	A	117	LEU
1	A	131	ASP
1	A	150	VAL
1	A	154	LEU
1	B	27	ASN
1	B	28	LEU
1	B	32	ILE
1	B	35	LYS
1	B	38	LEU
1	B	39	LEU
1	B	54	ILE
1	B	59	LYS
1	B	61	LEU
1	B	69	VAL
1	B	71	LEU
1	B	90	LEU
1	B	119	ASP
1	B	120	ASP
1	B	139	LEU
1	B	140	LEU
1	B	146	ILE
1	B	148	ARG
1	B	150	VAL
1	B	154	LEU
1	B	169	VAL
1	B	170	CYS
1	C	8	GLU
1	C	15	GLU
1	C	27	ASN
1	C	29	THR
1	C	34	LYS
1	C	38	LEU
1	C	39	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	61	LEU
1	C	67	ARG
1	C	69	VAL
1	C	71	LEU
1	C	76	VAL
1	C	87	LYS
1	C	101	THR
1	C	110	ILE
1	C	117	LEU
1	C	139	LEU
1	C	154	LEU
1	C	168	ASP
1	D	30	GLN
1	D	35	LYS
1	D	38	LEU
1	D	39	LEU
1	D	69	VAL
1	D	71	LEU
1	D	101	THR
1	D	117	LEU
1	D	148	ARG
1	D	154	LEU
1	E	7	LYS
1	E	28	LEU
1	E	35	LYS
1	E	39	LEU
1	E	47	THR
1	E	61	LEU
1	E	71	LEU
1	E	75	SER
1	E	87	LYS
1	E	99	LYS
1	E	101	THR
1	E	117	LEU
1	E	125	ARG
1	E	148	ARG
1	E	150	VAL
1	E	154	LEU
1	E	155	ARG
1	E	162	HIS
1	F	3	THR
1	F	27	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	28	LEU
1	F	29	THR
1	F	30	GLN
1	F	35	LYS
1	F	38	LEU
1	F	39	LEU
1	F	47	THR
1	F	52	SER
1	F	55	ILE
1	F	59	LYS
1	F	61	LEU
1	F	67	ARG
1	F	71	LEU
1	F	101	THR
1	F	117	LEU
1	F	119	ASP
1	F	146	ILE
1	F	148	ARG
1	F	154	LEU
1	F	160	ILE
1	F	170	CYS
1	G	8	GLU
1	G	20	ASP
1	G	27	ASN
1	G	28	LEU
1	G	32	ILE
1	G	35	LYS
1	G	38	LEU
1	G	39	LEU
1	G	47	THR
1	G	54	ILE
1	G	61	LEU
1	G	69	VAL
1	G	71	LEU
1	G	90	LEU
1	G	97	ASN
1	G	101	THR
1	G	106	ILE
1	G	117	LEU
1	G	146	ILE
1	G	148	ARG
1	G	150	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	154	LEU
1	G	168	ASP
1	H	13	LYS
1	H	27	ASN
1	H	28	LEU
1	H	29	THR
1	H	34	LYS
1	H	35	LYS
1	H	38	LEU
1	H	39	LEU
1	H	61	LEU
1	H	67	ARG
1	H	71	LEU
1	H	76	VAL
1	H	97	ASN
1	H	99	LYS
1	H	101	THR
1	H	117	LEU
1	H	150	VAL
1	H	154	LEU
1	I	28	LEU
1	I	38	LEU
1	I	39	LEU
1	I	61	LEU
1	I	69	VAL
1	I	71	LEU
1	I	76	VAL
1	I	101	THR
1	I	117	LEU
1	I	120	ASP
1	I	146	ILE
1	I	148	ARG
1	I	153	ILE
1	I	154	LEU
1	I	164	GLU
1	I	175	GLN
1	J	3	THR
1	J	38	LEU
1	J	39	LEU
1	J	59	LYS
1	J	67	ARG
1	J	69	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	71	LEU
1	J	76	VAL
1	J	97	ASN
1	J	101	THR
1	J	117	LEU
1	J	121	SER
1	J	150	VAL
1	J	154	LEU
1	J	155	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	65	HIS
1	A	68	ASN
1	A	115	ASN
1	A	138	HIS
1	A	163	HIS
1	B	27	ASN
1	B	65	HIS
1	B	138	HIS
1	C	27	ASN
1	C	30	GLN
1	C	138	HIS
1	D	30	GLN
1	D	138	HIS
1	D	163	HIS
1	E	27	ASN
1	E	65	HIS
1	E	68	ASN
1	F	27	ASN
1	F	30	GLN
1	F	68	ASN
1	F	97	ASN
1	F	138	HIS
1	F	163	HIS
1	G	30	GLN
1	G	65	HIS
1	G	68	ASN
1	G	138	HIS
1	H	27	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	30	GLN
1	H	68	ASN
1	H	138	HIS
1	I	21	ASN
1	I	27	ASN
1	I	68	ASN
1	I	138	HIS
1	I	163	HIS
1	I	175	GLN
1	J	30	GLN
1	J	68	ASN
1	J	138	HIS
1	J	162	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, 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	167/213 (78%)	-0.11	2 (1%) 81 83	34, 49, 67, 84	0
1	B	171/213 (80%)	-0.10	3 (1%) 71 75	36, 47, 67, 85	0
1	C	170/213 (79%)	-0.16	1 (0%) 90 91	30, 41, 59, 73	0
1	D	169/213 (79%)	-0.17	0 100 100	32, 48, 61, 70	0
1	E	161/213 (75%)	-0.26	0 100 100	33, 45, 61, 76	0
1	F	168/213 (78%)	-0.08	4 (2%) 62 66	33, 46, 65, 86	0
1	G	171/213 (80%)	-0.13	0 100 100	33, 47, 62, 67	0
1	H	167/213 (78%)	-0.30	2 (1%) 81 83	26, 41, 61, 84	0
1	I	177/213 (83%)	-0.16	3 (1%) 73 76	30, 43, 58, 65	0
1	J	163/213 (76%)	-0.36	0 100 100	27, 37, 51, 64	0
All	All	1684/2130 (79%)	-0.18	15 (0%) 85 88	26, 44, 62, 86	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	166	TYR	3.6
1	I	92	LYS	3.4
1	F	92	LYS	3.0
1	A	11	PHE	3.0
1	B	91	ALA	2.9
1	I	91	ALA	2.7
1	F	170	CYS	2.7
1	A	166	TYR	2.6
1	H	165	LYS	2.6
1	C	1	SER	2.5
1	F	169	VAL	2.4
1	F	91	ALA	2.3
1	B	34	LYS	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	1	SER	2.0
1	B	90	LEU	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.