



Full wwPDB X-ray Structure Validation Report ⓘ

May 12, 2020 – 11:10 pm BST

PDB ID : 2V64
Title : Crystallographic structure of the conformational dimer of the Spindle Assembly Checkpoint protein Mad2.
Authors : Mapelli, M.; Massimiliano, L.; Santaguida, S.; Musacchio, A.
Deposited on : 2007-07-13
Resolution : 2.90 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	:	2.11
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)	:	2.11

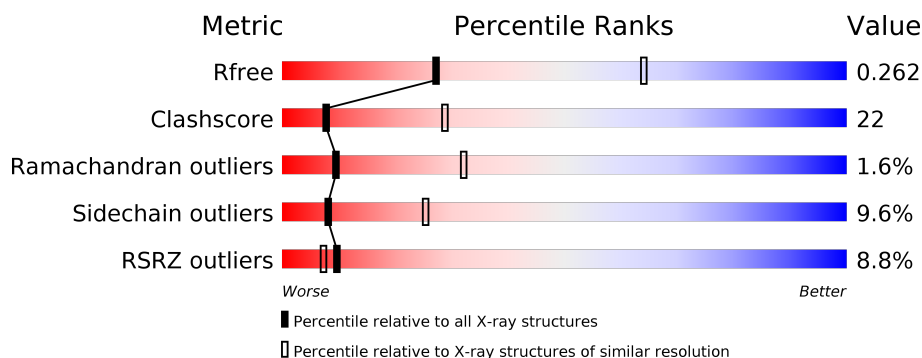
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 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	213	<div> <div>6%</div> <div> <div></div> <div>67%</div> <div>26%</div> <div>6%</div> </div> </div>
1	C	213	<div> <div>7%</div> <div> <div></div> <div>63%</div> <div>28%</div> <div>8%</div> </div> </div>
1	F	213	<div> <div>5%</div> <div> <div></div> <div>69%</div> <div>22%</div> <div>8%</div> </div> </div>
2	B	12	<div> <div></div> <div> <div></div> <div>75%</div> <div>17%</div> <div>8%</div> </div> </div>
2	G	12	<div> <div>17%</div> <div> <div></div> <div>83%</div> <div>8%</div> <div>8%</div> </div> </div>
2	I	12	<div> <div></div> <div> <div></div> <div>75%</div> <div>25%</div> </div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	D	207	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>9%47%29%5%17%</div></div>
3	E	207	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>12%44%29%9%15%</div></div>
3	H	207	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>12%47%30%10%13%</div></div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9648 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 MITOTIC SPINDLE ASSEMBLY CHECKPOINT PROTEIN MAD2A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	211	Total	C	N	O	S	0	0	1
			1700	1085	287	324	4			
1	C	211	Total	C	N	O	S	0	0	1
			1700	1085	287	324	4			
1	F	211	Total	C	N	O	S	0	0	1
			1700	1085	287	324	4			

- Molecule 2 is a protein called MBP1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	11	Total	C	N	O	0	0	1
			92	61	16	15			
2	G	11	Total	C	N	O	0	0	1
			92	61	16	15			
2	I	12	Total	C	N	O	0	0	1
			97	64	17	16			

- Molecule 3 is a protein called MITOTIC SPINDLE ASSEMBLY CHECKPOINT PROTEIN MAD2A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	172	Total	C	N	O	S	0	0	1
			1383	887	226	267	3			
3	E	176	Total	C	N	O	S	0	0	1
			1423	916	231	273	3			
3	H	181	Total	C	N	O	S	0	0	1
			1455	934	237	281	3			

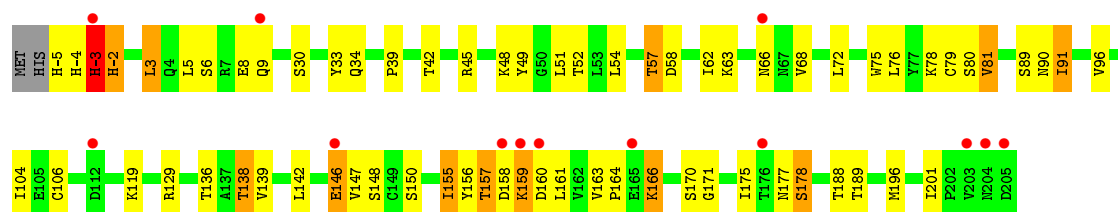
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	3	Total 3	O 3	0	0
4	F	2	Total 2	O 2	0	0
4	H	1	Total 1	O 1	0	0

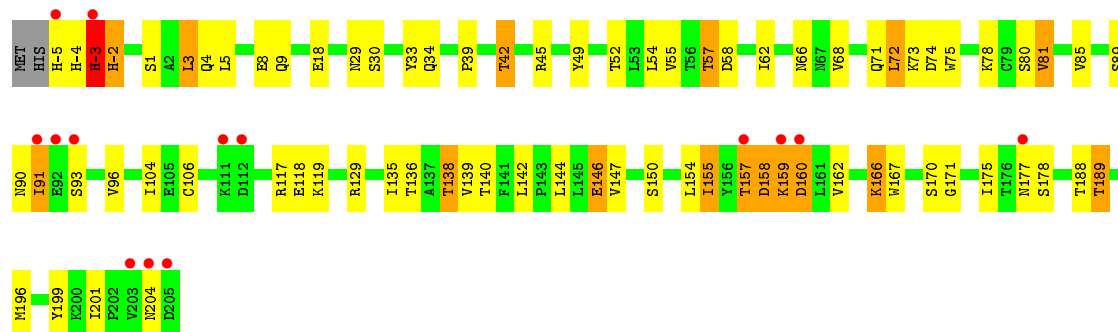
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

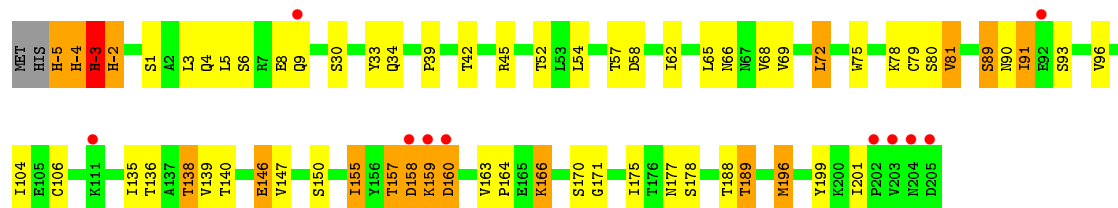
• Molecule 1: MITOTIC SPINDLE ASSEMBLY CHECKPOINT PROTEIN MAD2A



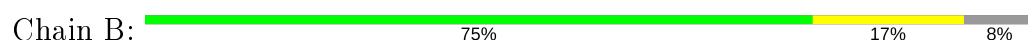
• Molecule 1: MITOTIC SPINDLE ASSEMBLY CHECKPOINT PROTEIN MAD2A



• Molecule 1: MITOTIC SPINDLE ASSEMBLY CHECKPOINT PROTEIN MAD2A

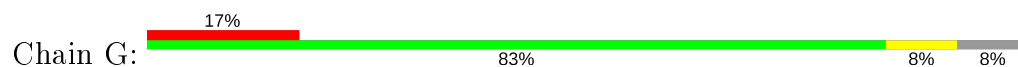


• Molecule 2: MBP1





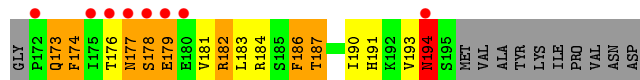
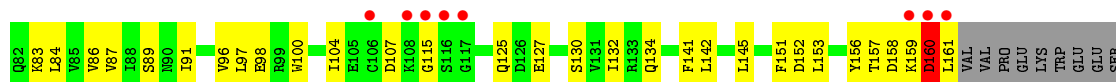
- Molecule 2: MBP1



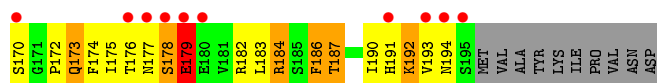
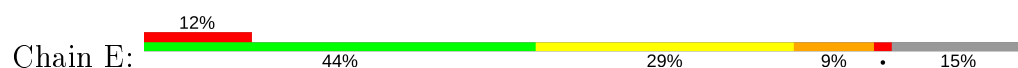
- Molecule 2: MBP1



- Molecule 3: MITOTIC SPINDLE ASSEMBLY CHECKPOINT PROTEIN MAD2A

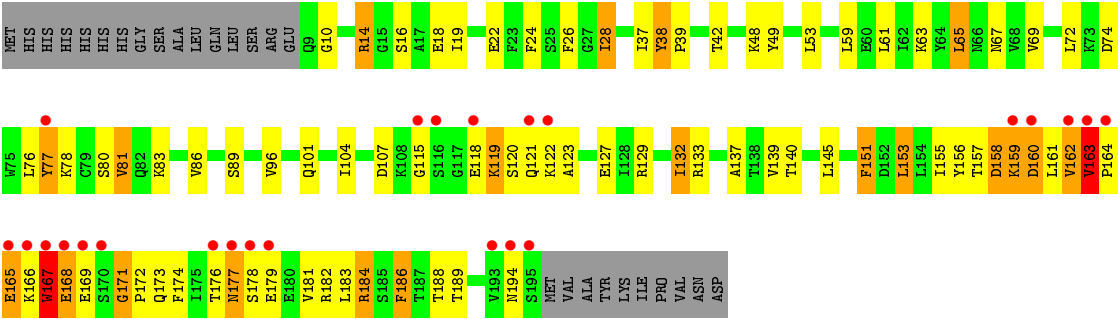


- Molecule 3: MITOTIC SPINDLE ASSEMBLY CHECKPOINT PROTEIN MAD2A



- Molecule 3: MITOTIC SPINDLE ASSEMBLY CHECKPOINT PROTEIN MAD2A





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	112.58Å 111.88Å 131.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.44 – 2.90 29.44 – 2.90	Depositor EDS
% Data completeness (in resolution range)	94.8 (29.44-2.90) 94.9 (29.44-2.90)	Depositor EDS
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.60 (at 2.90Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.233 , 0.273 0.221 , 0.262	Depositor DCC
R_{free} test set	1766 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	43.8	Xtriage
Anisotropy	0.176	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 53.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.014 for k,h,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	9648	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% 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	0.70	1/1733 (0.1%)	0.90	4/2350 (0.2%)
1	C	0.72	2/1733 (0.1%)	0.94	7/2350 (0.3%)
1	F	0.71	2/1733 (0.1%)	0.96	5/2350 (0.2%)
2	B	0.69	0/98	0.63	0/136
2	G	0.73	0/98	0.68	0/136
2	I	0.73	0/103	0.71	0/143
3	D	0.97	11/1404 (0.8%)	1.09	10/1899 (0.5%)
3	E	1.00	10/1447 (0.7%)	1.11	11/1962 (0.6%)
3	H	0.97	8/1480 (0.5%)	1.11	9/2006 (0.4%)
All	All	0.84	34/9829 (0.3%)	1.01	46/13332 (0.3%)

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	A	0	2
1	C	0	1
1	F	1	3
3	E	0	1
3	H	0	4
All	All	1	11

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	18	GLU	CB-CG	-10.80	1.31	1.52
3	E	77	TYR	CD1-CE1	-10.62	1.23	1.39
3	E	70	GLU	CG-CD	-8.74	1.38	1.51
3	D	77	TYR	CD1-CE1	-8.49	1.26	1.39
1	F	-3	HIS	C-O	-8.42	1.07	1.23
3	H	18	GLU	CD-OE2	-8.16	1.16	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	-3	HIS	C-O	-7.80	1.08	1.23
3	E	122	LYS	CB-CG	-7.67	1.31	1.52
3	H	158	ASP	CB-CG	-7.66	1.35	1.51
3	E	158	ASP	CB-CG	-7.30	1.36	1.51
3	H	159	LYS	CD-CE	-7.23	1.33	1.51
3	D	54	LEU	CG-CD1	-7.01	1.25	1.51
3	H	160	ASP	CB-CG	-7.01	1.37	1.51
3	E	18	GLU	CB-CG	-6.98	1.38	1.52
1	A	-4	HIS	CB-CG	6.78	1.62	1.50
3	E	160	ASP	CB-CG	-6.77	1.37	1.51
3	E	159	LYS	CB-CG	-6.67	1.34	1.52
3	E	77	TYR	CE2-CZ	-6.58	1.29	1.38
3	D	78	LYS	CD-CE	-6.39	1.35	1.51
3	D	77	TYR	CD2-CE2	-6.38	1.29	1.39
3	D	160	ASP	CB-CG	-6.27	1.38	1.51
3	H	159	LYS	CB-CG	-6.22	1.35	1.52
1	F	-4	HIS	CB-CG	6.17	1.61	1.50
1	C	-4	HIS	CB-CG	6.17	1.61	1.50
3	E	122	LYS	CD-CE	-6.12	1.35	1.51
3	H	122	LYS	CB-CG	-6.12	1.36	1.52
3	D	54	LEU	CG-CD2	-6.11	1.29	1.51
3	D	18	GLU	CB-CG	-6.00	1.40	1.52
3	D	158	ASP	CB-CG	-5.76	1.39	1.51
3	E	77	TYR	CG-CD1	-5.54	1.31	1.39
3	D	78	LYS	CB-CG	-5.49	1.37	1.52
3	D	77	TYR	CE2-CZ	-5.44	1.31	1.38
3	D	77	TYR	CB-CG	-5.43	1.43	1.51
3	H	122	LYS	CD-CE	-5.30	1.38	1.51

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	158	ASP	CB-CG-OD1	-19.52	100.73	118.30
1	F	-3	HIS	N-CA-C	15.57	153.03	111.00
3	E	160	ASP	CB-CG-OD1	-14.85	104.94	118.30
1	C	-3	HIS	N-CA-C	14.55	150.28	111.00
3	D	158	ASP	CB-CG-OD1	-14.49	105.26	118.30
3	E	158	ASP	CB-CG-OD1	-13.21	106.41	118.30
1	A	-3	HIS	N-CA-C	11.62	142.38	111.00
3	H	160	ASP	CB-CG-OD1	-11.05	108.35	118.30
3	D	158	ASP	CB-CG-OD2	10.96	128.17	118.30
3	E	77	TYR	CB-CG-CD1	-10.66	114.61	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	158	ASP	CB-CG-OD2	10.40	127.66	118.30
3	D	14	ARG	NE-CZ-NH2	-10.34	115.13	120.30
1	F	-2	HIS	N-CA-CB	-9.78	92.99	110.60
1	C	-2	HIS	N-CA-CB	-9.20	94.05	110.60
3	D	160	ASP	CB-CG-OD1	-9.03	110.17	118.30
3	H	18	GLU	OE1-CD-OE2	-8.64	112.93	123.30
3	E	159	LYS	CB-CG-CD	-8.46	89.62	111.60
3	D	54	LEU	CD1-CG-CD2	-8.43	85.20	110.50
3	E	70	GLU	CA-CB-CG	-7.82	96.19	113.40
3	D	160	ASP	CB-CG-OD2	7.82	125.33	118.30
3	E	77	TYR	CB-CG-CD2	7.73	125.64	121.00
1	F	-3	HIS	O-C-N	-7.51	110.69	122.70
3	H	18	GLU	CG-CD-OE1	7.16	132.61	118.30
3	H	159	LYS	CB-CG-CD	-7.11	93.12	111.60
3	E	160	ASP	CB-CG-OD2	6.92	124.53	118.30
3	D	14	ARG	CD-NE-CZ	-6.54	114.44	123.60
1	C	-4	HIS	C-N-CA	-6.44	105.61	121.70
3	E	122	LYS	CG-CD-CE	-6.36	92.83	111.90
1	A	-2	HIS	N-CA-CB	-6.17	99.50	110.60
3	D	78	LYS	CB-CG-CD	-6.15	95.61	111.60
3	D	160	ASP	N-CA-CB	-5.99	99.83	110.60
1	C	-3	HIS	CB-CA-C	-5.91	98.59	110.40
3	E	70	GLU	OE1-CD-OE2	5.87	130.34	123.30
1	F	158	ASP	CB-CG-OD1	5.84	123.56	118.30
1	C	158	ASP	CB-CG-OD2	-5.76	113.12	118.30
1	F	-3	HIS	CB-CA-C	-5.74	98.92	110.40
1	A	-4	HIS	CB-CA-C	-5.72	98.97	110.40
1	C	-3	HIS	O-C-N	-5.69	113.60	122.70
3	E	18	GLU	OE1-CD-OE2	-5.49	116.71	123.30
3	H	132	ILE	CG1-CB-CG2	-5.42	99.46	111.40
3	D	18	GLU	OE1-CD-OE2	-5.36	116.86	123.30
3	E	14	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	A	178	SER	N-CA-C	5.30	125.31	111.00
1	C	158	ASP	CB-CG-OD1	5.25	123.02	118.30
3	H	14	ARG	NE-CZ-NH2	-5.21	117.70	120.30
3	H	67	ASN	N-CA-CB	-5.17	101.30	110.60

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	F	-3	HIS	CA

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	-3	HIS	Sidechain,Mainchain
1	C	-3	HIS	Mainchain
3	E	184	ARG	Sidechain
1	F	-2	HIS	Sidechain
1	F	-3	HIS	Mainchain
1	F	-5	HIS	Sidechain
3	H	162	VAL	Peptide
3	H	163	VAL	Peptide
3	H	164	PRO	Peptide
3	H	184	ARG	Sidechain

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	1700	0	1707	61	0
1	C	1700	0	1707	61	2
1	F	1700	0	1707	59	0
2	B	92	0	82	1	0
2	G	92	0	82	1	0
2	I	97	0	87	5	0
3	D	1383	0	1399	75	0
3	E	1423	0	1438	96	2
3	H	1455	0	1469	88	0
4	C	3	0	0	0	0
4	F	2	0	0	0	0
4	H	1	0	0	0	0
All	All	9648	0	9678	420	2

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 22.

All (420) 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)
3:H:184:ARG:HH11	3:H:184:ARG:CB	1.39	1.34

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:184:ARG:HB3	3:H:184:ARG:NH1	1.44	1.28
1:A:-3:HIS:NE2	1:F:-3:HIS:CE1	2.16	1.14
1:A:-3:HIS:CE1	1:C:-5:HIS:HE1	1.67	1.12
3:D:14:ARG:HH21	3:D:14:ARG:HB3	1.10	1.09
3:H:184:ARG:CA	3:H:184:ARG:HH11	1.65	1.09
3:D:14:ARG:NH2	3:D:14:ARG:HB3	1.68	1.07
1:A:-3:HIS:CE1	1:C:-5:HIS:CE1	2.45	1.04
1:A:-3:HIS:CE1	1:C:-3:HIS:NE2	2.26	1.04
3:D:14:ARG:CB	3:D:14:ARG:HH21	1.72	1.02
1:C:-3:HIS:CE1	1:F:-3:HIS:NE2	2.30	1.00
3:D:181:VAL:O	3:D:182:ARG:HB3	1.62	0.99
3:H:184:ARG:HB3	3:H:184:ARG:HH11	1.01	0.99
3:E:166:LYS:O	3:E:167:TRP:HB2	1.60	0.98
3:H:160:ASP:O	3:H:161:LEU:HG	1.63	0.98
3:H:159:LYS:NZ	3:H:194:ASN:HD22	1.63	0.96
3:D:173:GLN:HB2	3:D:187:THR:HB	1.49	0.94
3:E:177:ASN:HA	3:E:184:ARG:NH2	1.84	0.93
1:A:-3:HIS:ND1	1:C:-5:HIS:CE1	2.38	0.92
3:E:163:VAL:HG21	3:E:190:ILE:CD1	1.99	0.91
1:A:-3:HIS:ND1	1:C:-5:HIS:HE1	1.68	0.91
1:A:-3:HIS:CE1	1:F:-3:HIS:HE1	1.91	0.89
3:D:84:LEU:HG	3:D:104:ILE:HD11	1.55	0.88
1:A:-3:HIS:HD1	1:C:-5:HIS:CE1	1.92	0.87
1:A:-3:HIS:HE1	1:C:-3:HIS:CE1	1.92	0.87
1:A:-3:HIS:CE1	1:C:-3:HIS:CE1	2.63	0.87
1:C:-3:HIS:CE1	1:F:-3:HIS:CE1	2.61	0.87
3:E:14:ARG:H	3:E:14:ARG:NH2	1.73	0.86
3:H:167:TRP:CE3	3:H:168:GLU:N	2.43	0.86
3:D:176:THR:HG22	3:D:177:ASN:H	1.40	0.86
3:E:14:ARG:H	3:E:14:ARG:HH21	1.18	0.86
3:H:184:ARG:NH1	3:H:184:ARG:CB	2.15	0.86
3:D:177:ASN:ND2	3:D:184:ARG:HD3	1.90	0.85
3:E:178:SER:O	3:E:179:GLU:HB2	1.76	0.85
1:A:-3:HIS:CE1	1:F:-3:HIS:CE1	2.64	0.85
3:H:81:VAL:HG22	3:H:104:ILE:HD12	1.61	0.82
3:E:165:GLU:O	3:E:166:LYS:HB2	1.78	0.82
3:H:14:ARG:NH2	3:H:14:ARG:HG2	1.94	0.81
3:H:14:ARG:HG2	3:H:14:ARG:HH21	1.43	0.81
3:E:108:LYS:HB3	3:E:108:LYS:NZ	1.95	0.81
3:E:177:ASN:HA	3:E:184:ARG:HH21	1.46	0.80
3:H:159:LYS:HZ1	3:H:194:ASN:HD22	1.29	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:83:LYS:HG3	3:D:156:TYR:HD1	1.47	0.79
3:E:160:ASP:C	3:E:161:LEU:HG	2.03	0.79
3:H:157:THR:OG1	3:H:161:LEU:HD11	1.82	0.79
3:E:108:LYS:HZ3	3:E:108:LYS:HB3	1.48	0.78
1:F:157:THR:OG1	1:F:158:ASP:N	2.15	0.77
1:F:33:TYR:CZ	1:F:54:LEU:HD22	2.20	0.77
3:E:14:ARG:NH1	3:E:127:GLU:OE1	2.18	0.77
3:E:177:ASN:C	3:E:179:GLU:H	1.89	0.76
3:H:59:LEU:HG	3:H:63:LYS:HE3	1.69	0.75
1:C:30:SER:O	1:C:34:GLN:HG3	1.87	0.74
1:A:96:VAL:HG12	1:A:175:ILE:HG12	1.69	0.74
3:D:174:PHE:CE1	3:D:186:PHE:HB3	2.22	0.74
3:E:163:VAL:HG21	3:E:190:ILE:HD12	1.69	0.73
3:H:24:PHE:O	3:H:28:ILE:HG22	1.88	0.73
1:C:-3:HIS:HE1	1:F:-3:HIS:CE1	2.05	0.73
1:A:39:PRO:O	1:A:42:THR:HB	1.89	0.72
3:E:166:LYS:O	3:E:167:TRP:CB	2.35	0.72
3:H:184:ARG:CA	3:H:184:ARG:NH1	2.45	0.72
3:E:145:LEU:HD22	3:E:182:ARG:HD3	1.71	0.72
3:H:89:SER:HB3	3:H:96:VAL:HA	1.71	0.72
3:D:58:ASP:O	3:D:62:ILE:HG13	1.90	0.71
1:A:80:SER:O	1:A:157:THR:HB	1.88	0.71
3:D:176:THR:O	3:D:177:ASN:HB2	1.89	0.71
1:F:39:PRO:O	1:F:42:THR:HB	1.91	0.71
1:A:-3:HIS:HE1	1:C:-5:HIS:CE1	2.08	0.71
1:F:80:SER:O	1:F:157:THR:HB	1.90	0.70
3:D:173:GLN:CB	3:D:187:THR:HB	2.22	0.70
3:E:14:ARG:HH21	3:E:14:ARG:N	1.89	0.70
1:C:39:PRO:O	1:C:42:THR:HB	1.92	0.70
1:A:158:ASP:O	1:A:160:ASP:N	2.23	0.70
3:E:14:ARG:HG2	3:E:14:ARG:NH2	2.06	0.70
3:H:163:VAL:HG23	3:H:165:GLU:N	2.07	0.70
3:H:167:TRP:HE3	3:H:168:GLU:H	1.35	0.69
1:A:-3:HIS:NE2	1:F:-3:HIS:HE1	1.78	0.69
3:E:177:ASN:O	3:E:179:GLU:N	2.23	0.69
3:H:159:LYS:NZ	3:H:194:ASN:ND2	2.39	0.69
1:C:96:VAL:HG12	1:C:175:ILE:HG12	1.74	0.69
1:F:135:ILE:O	1:F:138:THR:HB	1.93	0.69
1:C:166:LYS:HB3	1:C:166:LYS:NZ	2.08	0.68
1:F:96:VAL:HG12	1:F:175:ILE:HG12	1.75	0.68
1:F:158:ASP:O	1:F:160:ASP:N	2.26	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:192:LYS:H	3:E:192:LYS:HZ2	1.39	0.68
3:H:160:ASP:O	3:H:161:LEU:CG	2.39	0.68
3:E:71:GLN:HG2	3:E:167:TRP:CZ2	2.28	0.67
3:H:78:LYS:HE3	3:H:80:SER:OG	1.94	0.67
1:C:80:SER:O	1:C:157:THR:HB	1.94	0.67
3:H:177:ASN:HB2	3:H:184:ARG:NH2	2.09	0.67
1:F:140:THR:HB	3:H:132:ILE:HG21	1.77	0.66
1:F:-5:HIS:ND1	1:F:-4:HIS:N	2.43	0.66
3:E:14:ARG:NE	3:E:127:GLU:OE2	2.28	0.66
1:F:30:SER:O	1:F:34:GLN:HG3	1.96	0.66
1:C:188:THR:O	1:C:189:THR:HG23	1.97	0.65
3:D:174:PHE:HE1	3:D:186:PHE:HB3	1.61	0.65
3:H:39:PRO:O	3:H:42:THR:HB	1.97	0.65
3:E:39:PRO:O	3:E:42:THR:HB	1.97	0.65
3:H:153:LEU:HD22	3:H:155:ILE:HD13	1.79	0.65
3:E:173:GLN:HG3	3:E:174:PHE:N	2.11	0.64
1:C:81:VAL:HG22	1:C:104:ILE:HD12	1.79	0.64
1:C:158:ASP:O	1:C:160:ASP:N	2.29	0.64
3:H:81:VAL:HG22	3:H:104:ILE:CD1	2.26	0.64
1:C:135:ILE:O	1:C:138:THR:HB	1.97	0.64
3:H:163:VAL:O	3:H:163:VAL:HG22	1.96	0.64
3:D:39:PRO:O	3:D:42:THR:HB	1.99	0.63
3:E:81:VAL:HG22	3:E:104:ILE:HD12	1.79	0.63
3:E:14:ARG:HH21	3:E:14:ARG:CG	2.12	0.62
1:F:1:SER:HB3	1:F:4:GLN:HG3	1.80	0.62
1:F:188:THR:O	1:F:189:THR:HG23	2.00	0.62
1:A:157:THR:OG1	1:A:158:ASP:N	2.30	0.62
3:E:14:ARG:NH1	3:E:127:GLU:CD	2.53	0.62
3:D:156:TYR:HE2	3:D:191:HIS:ND1	1.98	0.62
1:F:136:THR:O	1:F:139:VAL:HG23	1.98	0.62
3:E:192:LYS:H	3:E:192:LYS:NZ	1.98	0.61
3:H:184:ARG:HB3	3:H:184:ARG:CZ	2.23	0.61
1:C:42:THR:O	1:C:57:THR:HB	1.99	0.61
3:D:159:LYS:NZ	3:D:194:ASN:HB2	2.15	0.61
3:D:178:SER:O	3:D:179:GLU:HG2	2.00	0.61
1:F:42:THR:O	1:F:57:THR:HB	2.00	0.61
1:A:89:SER:HB3	1:A:96:VAL:HA	1.83	0.61
1:C:89:SER:HB3	1:C:96:VAL:HA	1.83	0.61
3:H:14:ARG:CG	3:H:14:ARG:HH21	2.05	0.61
3:H:145:LEU:CD2	3:H:182:ARG:HD3	2.31	0.61
1:F:33:TYR:CE1	1:F:54:LEU:HD22	2.36	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:49:TYR:O	1:C:129:ARG:HD3	2.01	0.60
3:D:173:GLN:HB2	3:D:187:THR:CB	2.28	0.60
2:I:8:PRO:C	2:I:10:ARG:H	2.04	0.60
1:C:162:VAL:HG12	1:C:162:VAL:O	1.99	0.60
3:H:171:GLY:HA3	3:H:188:THR:O	2.00	0.60
1:C:3:LEU:CD1	3:E:10:GLY:HA2	2.30	0.60
1:F:-5:HIS:HE1	1:F:-3:HIS:CE1	2.19	0.60
3:D:193:VAL:O	3:D:194:ASN:HB2	2.01	0.60
3:E:58:ASP:O	3:E:62:ILE:HG13	2.02	0.59
3:H:184:ARG:HH11	3:H:184:ARG:HA	1.61	0.59
3:D:14:ARG:CB	3:D:14:ARG:NH2	2.45	0.59
1:A:33:TYR:CZ	1:A:54:LEU:HD22	2.37	0.59
1:C:178:SER:HA	1:C:201:ILE:HG13	1.85	0.59
3:E:148:SER:HB3	3:E:184:ARG:HG3	1.84	0.59
1:F:8:GLU:O	1:F:9:GLN:HB2	2.03	0.59
3:H:174:PHE:CE1	3:H:186:PHE:HB3	2.37	0.59
1:C:146:GLU:OE2	1:C:147:VAL:HG13	2.03	0.58
2:I:10:ARG:HG2	2:I:10:ARG:O	2.04	0.58
1:C:136:THR:O	1:C:139:VAL:HG23	2.03	0.58
3:H:22:GLU:OE1	3:H:49:TYR:HE1	1.87	0.58
1:A:-5:HIS:HE1	1:F:-3:HIS:CE1	2.22	0.58
3:D:89:SER:HB3	3:D:96:VAL:HA	1.86	0.57
3:H:166:LYS:O	3:H:167:TRP:CB	2.52	0.57
1:A:-2:HIS:O	1:A:119:LYS:HE3	2.05	0.57
1:C:157:THR:OG1	1:C:158:ASP:N	2.38	0.57
3:D:179:GLU:HB2	3:D:181:VAL:HG23	1.86	0.57
3:H:179:GLU:HB2	3:H:181:VAL:HG23	1.86	0.57
3:E:178:SER:O	3:E:179:GLU:CB	2.49	0.57
1:F:166:LYS:NZ	1:F:166:LYS:HB3	2.20	0.57
1:F:58:ASP:O	1:F:62:ILE:HG13	2.05	0.57
3:H:14:ARG:CZ	3:H:127:GLU:OE2	2.53	0.57
3:H:165:GLU:O	3:H:166:LYS:HB2	2.04	0.57
3:H:176:THR:C	3:H:178:SER:H	2.07	0.57
3:H:22:GLU:OE1	3:H:49:TYR:CE1	2.57	0.57
1:C:118:GLU:HG2	3:E:141:PHE:CE1	2.40	0.56
3:H:184:ARG:NH1	3:H:184:ARG:O	2.38	0.56
2:I:10:ARG:CG	2:I:10:ARG:O	2.53	0.56
1:F:188:THR:C	1:F:189:THR:HG23	2.25	0.56
1:C:138:THR:HG23	1:C:142:LEU:CD1	2.35	0.56
3:D:12:THR:HG21	3:D:14:ARG:HH22	1.71	0.56
1:A:146:GLU:CD	1:A:146:GLU:H	2.09	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1:SER:HB3	1:F:4:GLN:CG	2.35	0.56
1:A:90:ASN:ND2	1:A:147:VAL:HG21	2.20	0.56
3:E:37:ILE:HG22	3:E:183:LEU:HB2	1.87	0.55
1:F:178:SER:HA	1:F:201:ILE:HG13	1.88	0.55
1:F:90:ASN:ND2	1:F:147:VAL:HG21	2.21	0.55
1:F:68:VAL:HG12	1:F:72:LEU:HD22	1.88	0.55
3:H:157:THR:CB	3:H:161:LEU:HD11	2.35	0.55
3:H:167:TRP:HE3	3:H:168:GLU:N	1.97	0.55
3:E:89:SER:HB3	3:E:96:VAL:HA	1.87	0.54
1:A:51:LEU:HD11	1:A:129:ARG:HG3	1.90	0.54
3:D:193:VAL:HG23	3:D:193:VAL:O	2.06	0.54
3:E:108:LYS:CB	3:E:108:LYS:NZ	2.69	0.54
3:D:12:THR:CG2	3:D:14:ARG:HH22	2.21	0.54
3:E:14:ARG:HG2	3:E:14:ARG:HH21	1.68	0.54
3:D:177:ASN:CG	3:D:184:ARG:CD	2.76	0.54
3:E:177:ASN:C	3:E:179:GLU:N	2.59	0.54
3:H:145:LEU:HD21	3:H:182:ARG:HD3	1.90	0.54
3:H:38:TYR:HE1	3:H:183:LEU:HD23	1.72	0.54
3:E:13:LEU:HD22	3:E:23:PHE:HB3	1.90	0.54
1:F:196:MET:O	1:F:196:MET:HG3	2.07	0.53
1:A:42:THR:O	1:A:42:THR:CG2	2.55	0.53
3:E:165:GLU:O	3:E:166:LYS:CB	2.55	0.53
3:E:82:GLN:OE1	3:E:193:VAL:HG11	2.08	0.53
1:C:177:ASN:OD1	1:C:201:ILE:HD12	2.08	0.53
1:C:45:ARG:HG2	1:C:52:THR:CG2	2.38	0.53
3:E:168:GLU:O	3:E:169:GLU:HB2	2.07	0.53
3:E:40:SER:C	3:E:42:THR:H	2.11	0.53
3:D:23:PHE:CE2	3:D:127:GLU:HB3	2.44	0.53
1:A:178:SER:HA	1:A:201:ILE:HG13	1.91	0.53
1:F:1:SER:CB	1:F:4:GLN:HG3	2.39	0.53
3:H:76:LEU:HD21	3:H:104:ILE:HD13	1.90	0.53
1:C:33:TYR:CZ	1:C:54:LEU:HD22	2.44	0.53
1:C:188:THR:C	1:C:189:THR:HG23	2.28	0.53
3:E:59:LEU:HG	3:E:63:LYS:HE2	1.90	0.53
1:F:45:ARG:HG2	1:F:52:THR:CG2	2.39	0.53
3:E:145:LEU:HD22	3:E:182:ARG:CD	2.37	0.52
1:A:136:THR:O	1:A:139:VAL:HG23	2.09	0.52
3:H:120:SER:O	3:H:121:GLN:C	2.45	0.52
3:H:166:LYS:O	3:H:167:TRP:HB2	2.09	0.52
3:D:14:ARG:CG	3:D:14:ARG:NH2	2.66	0.52
3:E:163:VAL:HG21	3:E:190:ILE:HD11	1.88	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:173:GLN:HB2	3:E:187:THR:HB	1.91	0.52
1:C:140:THR:HB	3:D:132:ILE:HG21	1.92	0.52
3:D:177:ASN:CG	3:D:184:ARG:HD3	2.30	0.52
3:E:64:TYR:O	3:E:68:VAL:HG12	2.09	0.52
1:F:68:VAL:O	1:F:72:LEU:HB2	2.09	0.52
3:H:174:PHE:HE1	3:H:186:PHE:HB3	1.74	0.52
3:H:167:TRP:CD1	3:H:172:PRO:HD2	2.45	0.52
1:A:30:SER:O	1:A:34:GLN:HG3	2.09	0.51
1:A:138:THR:HG23	1:A:142:LEU:HD12	1.92	0.51
3:E:14:ARG:CZ	3:E:127:GLU:OE2	2.59	0.51
3:D:161:LEU:HG	3:D:190:ILE:HD13	1.93	0.51
3:H:129:ARG:O	3:H:133:ARG:HB2	2.11	0.51
1:A:177:ASN:OD1	1:A:201:ILE:HD12	2.11	0.51
1:A:166:LYS:HB3	1:A:166:LYS:NZ	2.26	0.50
3:H:159:LYS:HZ2	3:H:194:ASN:ND2	2.07	0.50
3:E:14:ARG:CZ	3:E:127:GLU:CD	2.80	0.50
3:D:14:ARG:HG2	3:D:127:GLU:OE2	2.12	0.50
1:F:91:ILE:HG12	1:F:150:SER:HB3	1.93	0.50
3:D:181:VAL:O	3:D:182:ARG:CB	2.44	0.50
3:H:72:LEU:HG	3:H:76:LEU:CD1	2.41	0.50
3:E:127:GLU:OE1	3:E:127:GLU:HA	2.11	0.50
3:E:168:GLU:O	3:E:169:GLU:CB	2.60	0.50
3:E:38:TYR:HE1	3:E:183:LEU:HD23	1.77	0.49
1:F:65:LEU:O	1:F:69:VAL:HG23	2.12	0.49
1:C:170:SER:OG	1:C:171:GLY:N	2.44	0.49
3:E:10:GLY:N	3:E:103:ASP:OD2	2.44	0.49
3:E:163:VAL:HG21	3:E:166:LYS:O	2.12	0.49
3:H:120:SER:O	3:H:123:ALA:N	2.45	0.49
3:D:176:THR:O	3:D:177:ASN:CB	2.60	0.49
1:A:3:LEU:O	1:A:6:SER:OG	2.27	0.49
3:E:159:LYS:NZ	3:E:194:ASN:HB2	2.27	0.49
1:C:1:SER:HB3	1:C:4:GLN:HG3	1.94	0.49
3:E:77:TYR:HD2	3:E:77:TYR:O	1.96	0.49
3:D:48:LYS:HG3	3:D:49:TYR:CD1	2.47	0.49
3:D:49:TYR:O	3:D:125:GLN:NE2	2.34	0.49
3:E:14:ARG:CB	3:E:105:GLU:HB3	2.43	0.49
1:F:57:THR:CG2	1:F:57:THR:O	2.60	0.49
3:D:178:SER:O	3:D:179:GLU:CG	2.61	0.48
1:A:75:TRP:NE1	1:A:161:LEU:HD21	2.28	0.48
1:C:-2:HIS:O	1:C:119:LYS:HE3	2.14	0.48
3:H:37:ILE:HG22	3:H:183:LEU:HB2	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:79:CYS:SG	3:E:106:CYS:HB3	2.53	0.48
3:H:26:PHE:HZ	3:H:48:LYS:HG2	1.79	0.48
3:D:174:PHE:HD1	3:D:174:PHE:H	1.61	0.48
3:E:173:GLN:CG	3:E:174:PHE:N	2.77	0.48
3:E:175:ILE:HG22	3:E:176:THR:N	2.29	0.48
1:A:42:THR:O	1:A:57:THR:HB	2.14	0.48
1:A:8:GLU:O	1:A:9:GLN:HB2	2.13	0.48
1:A:138:THR:HG23	1:A:142:LEU:CD1	2.43	0.48
1:F:177:ASN:OD1	1:F:201:ILE:HD12	2.13	0.48
3:D:178:SER:O	3:D:179:GLU:CB	2.61	0.48
3:E:145:LEU:CD2	3:E:182:ARG:HD3	2.41	0.48
3:D:72:LEU:HG	3:D:76:LEU:HD11	1.96	0.47
1:A:45:ARG:HG2	1:A:52:THR:CG2	2.45	0.47
1:C:167:TRP:CD2	2:I:5:TYR:HB2	2.49	0.47
3:D:74:ASP:O	3:D:77:TYR:HB3	2.14	0.47
3:E:82:GLN:HE22	3:E:193:VAL:CG1	2.27	0.47
3:H:159:LYS:HA	3:H:159:LYS:HD2	1.55	0.47
1:C:138:THR:HG23	1:C:142:LEU:HD12	1.96	0.47
3:D:83:LYS:HG2	3:D:156:TYR:HB2	1.97	0.47
1:A:-5:HIS:CE1	1:F:-3:HIS:CE1	3.03	0.47
1:A:81:VAL:HG22	1:A:104:ILE:HD12	1.96	0.47
3:D:160:ASP:C	3:D:160:ASP:OD2	2.53	0.47
3:D:159:LYS:HZ2	3:D:194:ASN:HB2	1.80	0.47
3:E:167:TRP:CD1	3:E:168:GLU:N	2.83	0.47
3:E:72:LEU:HG	3:E:76:LEU:HD11	1.96	0.47
1:F:155:ILE:HD13	1:F:155:ILE:HA	1.65	0.47
3:H:38:TYR:CE1	3:H:61:LEU:HD22	2.50	0.47
3:D:161:LEU:O	3:D:161:LEU:HD12	2.15	0.47
3:D:193:VAL:O	3:D:194:ASN:CB	2.61	0.47
3:E:163:VAL:HG22	3:E:166:LYS:C	2.35	0.47
3:D:141:PHE:CE2	1:F:6:SER:HA	2.49	0.47
1:A:51:LEU:CG	1:A:129:ARG:HG3	2.45	0.47
3:E:77:TYR:CD2	3:E:77:TYR:O	2.67	0.47
1:C:146:GLU:H	1:C:146:GLU:CD	2.19	0.46
3:D:177:ASN:ND2	3:D:184:ARG:CD	2.70	0.46
1:F:146:GLU:H	1:F:146:GLU:CD	2.18	0.46
1:A:170:SER:OG	1:A:171:GLY:N	2.47	0.46
3:E:159:LYS:HZ1	3:E:194:ASN:HB2	1.80	0.46
1:A:51:LEU:CD1	1:A:129:ARG:HG3	2.46	0.46
1:A:33:TYR:CE1	1:A:54:LEU:HD22	2.51	0.46
3:E:153:LEU:HD22	3:E:155:ILE:HD13	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:42:THR:O	3:H:42:THR:CG2	2.64	0.46
1:A:91:ILE:HB	1:A:148:SER:O	2.15	0.46
3:D:156:TYR:CE2	3:D:191:HIS:ND1	2.82	0.46
3:D:59:LEU:HG	3:D:63:LYS:HE3	1.98	0.46
3:D:83:LYS:HG3	3:D:156:TYR:CD1	2.37	0.46
3:E:72:LEU:HG	3:E:76:LEU:CD1	2.46	0.46
1:F:159:LYS:HE2	1:F:159:LYS:HB3	1.79	0.46
1:C:166:LYS:HZ3	1:C:166:LYS:HB3	1.78	0.46
1:A:48:LYS:HG3	1:A:49:TYR:CD1	2.51	0.45
1:C:66:ASN:N	1:C:66:ASN:HD22	2.14	0.45
3:E:157:THR:OG1	3:E:161:LEU:HD21	2.16	0.45
3:E:77:TYR:C	3:E:77:TYR:CD2	2.89	0.45
3:H:14:ARG:NH1	3:H:127:GLU:OE1	2.49	0.45
1:C:155:ILE:HA	1:C:155:ILE:HD13	1.66	0.45
1:F:81:VAL:HG22	1:F:104:ILE:HD12	1.98	0.45
3:H:28:ILE:O	3:H:28:ILE:HG12	2.14	0.45
1:A:-5:HIS:HE1	1:F:-3:HIS:HE1	1.64	0.45
3:D:81:VAL:O	3:D:81:VAL:HG22	2.16	0.45
3:H:184:ARG:NH1	3:H:184:ARG:HA	2.25	0.45
1:C:58:ASP:O	1:C:62:ILE:HG13	2.15	0.45
3:H:158:ASP:OD1	3:H:158:ASP:C	2.52	0.45
3:H:118:GLU:CD	3:H:118:GLU:H	2.20	0.45
3:H:145:LEU:C	3:H:145:LEU:HD23	2.37	0.45
3:E:10:GLY:HA3	3:E:101:GLN:O	2.16	0.45
3:H:10:GLY:N	3:H:101:GLN:NE2	2.65	0.45
3:H:178:SER:O	3:H:179:GLU:HB2	2.17	0.45
2:I:8:PRO:C	2:I:10:ARG:N	2.69	0.45
3:D:65:LEU:O	3:D:69:VAL:HG23	2.16	0.45
3:E:14:ARG:HA	3:E:105:GLU:HB3	1.98	0.44
3:H:14:ARG:CG	3:H:127:GLU:OE2	2.65	0.44
3:H:145:LEU:HD22	3:H:182:ARG:HD3	1.98	0.44
3:E:75:TRP:O	3:E:80:SER:HB2	2.17	0.44
1:C:18:GLU:HG2	1:C:73:LYS:HD2	1.99	0.44
1:F:78:LYS:HE3	1:F:78:LYS:HB2	1.74	0.44
1:F:8:GLU:O	1:F:9:GLN:CB	2.65	0.44
1:A:146:GLU:N	1:A:146:GLU:CD	2.70	0.44
3:E:26:PHE:HZ	3:E:48:LYS:HG2	1.82	0.44
1:F:89:SER:HB3	1:F:96:VAL:HA	1.99	0.44
2:G:10:ARG:H	2:G:10:ARG:HG3	1.51	0.44
1:C:29:ASN:OD1	1:C:55:VAL:HA	2.18	0.44
1:C:78:LYS:HE3	1:C:78:LYS:HB2	1.75	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:157:THR:HG21	3:D:161:LEU:HD23	1.99	0.44
3:D:86:VAL:HB	3:D:100:TRP:HB2	2.00	0.44
1:A:91:ILE:HG12	1:A:150:SER:HB3	2.00	0.44
3:H:14:ARG:NH2	3:H:14:ARG:CG	2.62	0.44
3:E:163:VAL:CG2	3:E:167:TRP:HB2	2.48	0.43
1:A:159:LYS:HB3	1:A:159:LYS:HE2	1.80	0.43
1:C:158:ASP:C	1:C:160:ASP:H	2.21	0.43
1:F:75:TRP:HB3	1:F:81:VAL:HG12	2.01	0.43
1:F:78:LYS:O	1:F:79:CYS:HB2	2.18	0.43
1:A:78:LYS:HB2	1:A:78:LYS:HE3	1.66	0.43
3:E:42:THR:CG2	3:E:42:THR:O	2.65	0.43
3:E:166:LYS:HB2	3:E:170:SER:HA	2.01	0.43
1:C:85:VAL:HB	1:C:154:LEU:HB2	2.00	0.43
3:E:167:TRP:CE3	3:E:172:PRO:HD2	2.54	0.43
3:D:157:THR:HG21	3:D:161:LEU:CD2	2.49	0.43
3:D:186:PHE:C	3:D:186:PHE:CD2	2.92	0.43
3:H:74:ASP:O	3:H:77:TYR:HD2	2.01	0.43
1:F:166:LYS:HZ3	1:F:166:LYS:HB3	1.82	0.43
1:C:8:GLU:O	1:C:9:GLN:HB2	2.18	0.43
3:E:176:THR:HG23	3:E:178:SER:H	1.84	0.43
1:F:178:SER:HB2	1:F:199:TYR:O	2.18	0.42
3:H:42:THR:O	3:H:42:THR:HG22	2.19	0.42
1:A:51:LEU:HG	1:A:129:ARG:HG3	2.01	0.42
1:A:58:ASP:O	1:A:62:ILE:HG13	2.19	0.42
1:C:159:LYS:HB3	1:C:159:LYS:HE2	1.81	0.42
3:H:163:VAL:HG23	3:H:165:GLU:H	1.79	0.42
3:D:186:PHE:C	3:D:186:PHE:HD2	2.22	0.42
3:H:160:ASP:OD1	3:H:160:ASP:N	2.45	0.42
3:H:59:LEU:HA	3:H:59:LEU:HD12	1.70	0.42
3:E:193:VAL:O	3:E:194:ASN:HB2	2.18	0.42
3:E:82:GLN:HE22	3:E:193:VAL:HG11	1.83	0.42
3:D:42:THR:O	3:D:42:THR:CG2	2.66	0.42
3:D:97:LEU:O	3:D:98:GLU:HB3	2.18	0.42
3:E:174:PHE:CE1	3:E:186:PHE:HB3	2.55	0.42
3:E:40:SER:C	3:E:42:THR:N	2.70	0.42
1:C:117:ARG:HD2	1:C:189:THR:OG1	2.20	0.42
3:D:130:SER:O	3:D:134:GLN:HG3	2.20	0.42
3:D:178:SER:C	3:D:179:GLU:HG2	2.39	0.42
3:H:137:ALA:O	3:H:140:THR:HB	2.19	0.42
3:D:91:ILE:HG12	3:D:184:ARG:HG3	2.01	0.42
3:E:186:PHE:HD2	3:E:187:THR:N	2.17	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:10:GLY:H	3:H:101:GLN:NE2	2.17	0.42
1:C:68:VAL:HG12	1:C:72:LEU:HD22	2.01	0.42
1:F:-5:HIS:CE1	1:F:-3:HIS:CE1	3.03	0.42
3:H:65:LEU:HD23	3:H:65:LEU:HA	1.81	0.42
3:E:190:ILE:HG22	3:E:191:HIS:N	2.34	0.42
3:H:72:LEU:HG	3:H:76:LEU:HD12	2.01	0.42
1:A:68:VAL:O	1:A:72:LEU:HB2	2.20	0.42
3:D:75:TRP:CZ2	3:D:161:LEU:HD11	2.54	0.42
3:H:77:TYR:CD2	3:H:78:LYS:HG2	2.54	0.41
1:A:188:THR:C	1:A:189:THR:HG23	2.39	0.41
3:E:81:VAL:HG22	3:E:104:ILE:CD1	2.49	0.41
1:F:158:ASP:C	1:F:160:ASP:H	2.21	0.41
1:F:163:VAL:HA	1:F:164:PRO:HD3	1.89	0.41
1:F:90:ASN:HB3	1:F:93:SER:OG	2.20	0.41
3:H:26:PHE:CE2	3:H:53:LEU:HD13	2.55	0.41
1:A:78:LYS:O	1:A:79:CYS:HB2	2.21	0.41
3:E:166:LYS:O	3:E:190:ILE:HD12	2.20	0.41
3:E:190:ILE:CG2	3:E:191:HIS:N	2.83	0.41
1:F:170:SER:OG	1:F:171:GLY:N	2.52	0.41
1:A:158:ASP:C	1:A:160:ASP:H	2.20	0.41
3:D:176:THR:CG2	3:D:177:ASN:H	2.18	0.41
3:D:72:LEU:HD11	3:D:84:LEU:HD21	2.01	0.41
3:H:65:LEU:O	3:H:69:VAL:HG23	2.19	0.41
1:A:72:LEU:O	1:A:76:LEU:HG	2.21	0.41
3:D:87:VAL:HB	3:D:152:ASP:HB2	2.02	0.41
1:C:71:GLN:NE2	1:C:75:TRP:CE2	2.89	0.41
3:E:82:GLN:NE2	3:E:193:VAL:HG11	2.35	0.41
3:H:83:LYS:HG2	3:H:156:TYR:HB2	2.02	0.41
1:C:91:ILE:HG12	1:C:150:SER:HB3	2.03	0.41
3:D:37:ILE:HG22	3:D:183:LEU:HB2	2.03	0.41
3:D:156:TYR:HA	3:D:191:HIS:O	2.20	0.41
3:D:19:ILE:HD12	3:D:19:ILE:HA	1.82	0.41
3:E:136:THR:HA	3:E:139:VAL:HG13	2.02	0.41
3:D:81:VAL:HG22	3:D:104:ILE:CD1	2.51	0.41
3:E:163:VAL:CG2	3:E:166:LYS:O	2.69	0.41
3:H:178:SER:O	3:H:179:GLU:CB	2.69	0.41
3:E:192:LYS:HB2	3:E:192:LYS:HZ2	1.86	0.41
1:A:163:VAL:HA	1:A:164:PRO:HD3	1.85	0.40
3:H:119:LYS:HE3	3:H:119:LYS:N	2.36	0.40
1:A:156:TYR:CD1	2:B:2:TRP:CE2	3.09	0.40
3:E:100:TRP:CZ2	3:E:142:LEU:HD11	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:118:GLU:HG2	3:E:141:PHE:CD1	2.55	0.40
1:C:178:SER:HB2	1:C:199:TYR:O	2.22	0.40
3:D:19:ILE:CG2	3:D:20:VAL:N	2.83	0.40
3:D:18:GLU:HG2	3:D:73:LYS:HE2	2.04	0.40
1:C:90:ASN:HB3	1:C:93:SER:OG	2.22	0.40
3:H:86:VAL:HG11	3:H:151:PHE:CE2	2.56	0.40
1:A:155:ILE:HD13	1:A:155:ILE:HA	1.64	0.40
3:D:35:ARG:NH1	3:D:142:LEU:HB2	2.37	0.40
3:H:176:THR:C	3:H:178:SER:N	2.74	0.40

All (2) 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:C:204:ASN:N	3:E:78:LYS:NZ[4_545]	2.13	0.07
1:C:74:ASP:OD1	3:E:63:LYS:NZ[2_455]	2.16	0.04

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	209/213 (98%)	199 (95%)	9 (4%)	1 (0%)	29	61
1	C	209/213 (98%)	200 (96%)	8 (4%)	1 (0%)	29	61
1	F	209/213 (98%)	199 (95%)	9 (4%)	1 (0%)	29	61
2	B	9/12 (75%)	7 (78%)	2 (22%)	0	100	100
2	G	9/12 (75%)	7 (78%)	2 (22%)	0	100	100
2	I	10/12 (83%)	9 (90%)	1 (10%)	0	100	100
3	D	168/207 (81%)	149 (89%)	14 (8%)	5 (3%)	4	17
3	E	172/207 (83%)	147 (86%)	19 (11%)	6 (4%)	3	14

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	H	179/207 (86%)	160 (89%)	14 (8%)	5 (3%)	5	19
All	All	1174/1296 (91%)	1077 (92%)	78 (7%)	19 (2%)	9	32

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	159	LYS
1	C	159	LYS
3	D	179	GLU
3	D	194	ASN
3	E	167	TRP
3	E	169	GLU
3	E	178	SER
3	E	179	GLU
1	F	159	LYS
3	H	167	TRP
3	D	177	ASN
3	D	182	ARG
3	E	166	LYS
3	H	115	GLY
3	H	165	GLU
3	H	168	GLU
3	E	106	CYS
3	D	115	GLY
3	H	171	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	194/197 (98%)	180 (93%)	14 (7%)	14	39
1	C	194/197 (98%)	177 (91%)	17 (9%)	10	30
1	F	194/197 (98%)	178 (92%)	16 (8%)	11	32
2	B	10/11 (91%)	9 (90%)	1 (10%)	7	23

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	G	10/11 (91%)	10 (100%)	0	100	100
2	I	10/11 (91%)	10 (100%)	0	100	100
3	D	159/191 (83%)	145 (91%)	14 (9%)	10	30
3	E	164/191 (86%)	140 (85%)	24 (15%)	3	9
3	H	167/191 (87%)	147 (88%)	20 (12%)	5	15
All	All	1102/1197 (92%)	996 (90%)	106 (10%)	8	25

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	5	LEU
1	A	57	THR
1	A	63	LYS
1	A	66	ASN
1	A	81	VAL
1	A	91	ILE
1	A	106	CYS
1	A	138	THR
1	A	146	GLU
1	A	155	ILE
1	A	157	THR
1	A	166	LYS
1	A	196	MET
2	B	5	TYR
1	C	3	LEU
1	C	5	LEU
1	C	42	THR
1	C	57	THR
1	C	72	LEU
1	C	81	VAL
1	C	91	ILE
1	C	106	CYS
1	C	138	THR
1	C	144	LEU
1	C	146	GLU
1	C	155	ILE
1	C	157	THR
1	C	160	ASP
1	C	166	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	189	THR
1	C	196	MET
3	D	14	ARG
3	D	70	GLU
3	D	81	VAL
3	D	107	ASP
3	D	145	LEU
3	D	151	PHE
3	D	153	LEU
3	D	160	ASP
3	D	173	GLN
3	D	174	PHE
3	D	178	SER
3	D	186	PHE
3	D	187	THR
3	D	194	ASN
3	E	14	ARG
3	E	19	ILE
3	E	30	SER
3	E	42	THR
3	E	55	VAL
3	E	66	ASN
3	E	77	TYR
3	E	81	VAL
3	E	89	SER
3	E	107	ASP
3	E	108	LYS
3	E	151	PHE
3	E	153	LEU
3	E	158	ASP
3	E	159	LYS
3	E	161	LEU
3	E	165	GLU
3	E	168	GLU
3	E	169	GLU
3	E	173	GLN
3	E	179	GLU
3	E	186	PHE
3	E	187	THR
3	E	192	LYS
1	F	3	LEU
1	F	5	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	66	ASN
1	F	72	LEU
1	F	81	VAL
1	F	89	SER
1	F	91	ILE
1	F	106	CYS
1	F	138	THR
1	F	146	GLU
1	F	155	ILE
1	F	157	THR
1	F	160	ASP
1	F	166	LYS
1	F	189	THR
1	F	196	MET
3	H	16	SER
3	H	19	ILE
3	H	28	ILE
3	H	38	TYR
3	H	65	LEU
3	H	77	TYR
3	H	81	VAL
3	H	107	ASP
3	H	119	LYS
3	H	139	VAL
3	H	151	PHE
3	H	153	LEU
3	H	162	VAL
3	H	163	VAL
3	H	167	TRP
3	H	169	GLU
3	H	173	GLN
3	H	177	ASN
3	H	186	PHE
3	H	189	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	-5	HIS
1	A	66	ASN
1	A	125	GLN
1	C	-5	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	-3	HIS
1	C	66	ASN
1	C	125	GLN
3	D	66	ASN
3	D	67	ASN
3	D	173	GLN
3	D	177	ASN
3	D	194	ASN
3	E	66	ASN
3	E	82	GLN
3	E	101	GLN
3	E	121	GLN
3	E	177	ASN
1	F	-5	HIS
1	F	-3	HIS
1	F	66	ASN
1	F	125	GLN
3	H	66	ASN
3	H	101	GLN
3	H	121	GLN
3	H	194	ASN

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	211/213 (99%)	0.26	13 (6%) 20 16	16, 31, 61, 100	0
1	C	211/213 (99%)	0.30	14 (6%) 18 14	16, 32, 61, 100	0
1	F	211/213 (99%)	0.19	10 (4%) 31 28	16, 30, 61, 100	0
2	B	11/12 (91%)	0.37	0 100 100	36, 43, 67, 69	0
2	G	11/12 (91%)	0.62	2 (18%) 1 1	37, 43, 66, 68	0
2	I	12/12 (100%)	0.38	0 100 100	38, 42, 69, 69	0
3	D	172/207 (83%)	0.38	18 (10%) 6 5	14, 37, 88, 96	0
3	E	176/207 (85%)	0.41	24 (13%) 3 2	17, 38, 94, 98	0
3	H	181/207 (87%)	0.53	24 (13%) 3 2	15, 37, 92, 99	0
All	All	1196/1296 (92%)	0.34	105 (8%) 10 7	14, 34, 84, 100	0

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	205	ASP	15.9
1	A	205	ASP	9.1
1	C	204	ASN	9.0
1	A	204	ASN	8.1
1	F	204	ASN	8.1
3	H	170	SER	8.0
3	D	160	ASP	6.8
3	H	194	ASN	6.7
3	E	168	GLU	6.5
3	H	195	SER	6.3
3	H	169	GLU	6.1
3	E	178	SER	6.1
1	F	203	VAL	5.6
3	D	176	THR	5.5
1	F	160	ASP	5.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	H	116	SER	5.5
1	F	205	ASP	5.4
3	H	159	LYS	5.4
3	D	117	GLY	5.4
1	C	159	LYS	5.3
1	C	160	ASP	5.2
3	E	194	ASN	5.1
3	D	177	ASN	5.0
3	H	178	SER	4.9
1	A	203	VAL	4.8
3	H	168	GLU	4.7
1	A	159	LYS	4.7
3	D	106	CYS	4.6
3	E	177	ASN	4.6
3	H	167	TRP	4.5
3	E	107	ASP	4.4
3	D	178	SER	4.4
1	A	160	ASP	4.1
3	D	194	ASN	4.1
3	E	193	VAL	4.1
3	H	179	GLU	4.0
2	G	1	SER	3.9
3	H	177	ASN	3.9
1	C	91	ILE	3.9
3	E	77	TYR	3.9
3	D	116	SER	3.8
1	F	159	LYS	3.8
3	E	165	GLU	3.8
3	H	165	GLU	3.8
3	H	77	TYR	3.7
3	H	162	VAL	3.7
3	H	166	LYS	3.6
3	E	170	SER	3.6
3	D	115	GLY	3.6
3	E	179	GLU	3.4
3	E	164	PRO	3.3
3	H	121	GLN	3.2
3	E	195	SER	3.2
3	D	77	TYR	3.1
3	D	175	ILE	3.1
3	H	176	THR	3.1
3	D	159	LYS	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	D	172	PRO	2.9
3	E	159	LYS	2.9
3	E	176	THR	2.9
1	A	158	ASP	2.9
1	F	9	GLN	2.9
1	A	165	GLU	2.9
3	E	169	GLU	2.9
3	H	193	VAL	2.8
1	C	93	SER	2.8
3	H	164	PRO	2.8
3	H	118	GLU	2.7
1	C	177	ASN	2.6
1	C	-3	HIS	2.6
3	E	158	ASP	2.6
1	F	158	ASP	2.6
1	C	112	ASP	2.5
3	E	108	LYS	2.5
3	D	161	LEU	2.5
3	E	161	LEU	2.5
1	C	111	LYS	2.5
1	F	92	GLU	2.5
3	E	162	VAL	2.5
3	H	122	LYS	2.4
3	D	180	GLU	2.4
2	G	9	GLN	2.3
3	H	163	VAL	2.3
1	C	92	GLU	2.3
1	A	-3	HIS	2.3
3	E	121	GLN	2.3
1	A	9	GLN	2.2
1	C	157	THR	2.2
3	D	70	GLU	2.2
1	A	112	ASP	2.2
1	A	66	ASN	2.2
1	F	202	PRO	2.2
3	D	108	LYS	2.2
1	C	203	VAL	2.2
1	A	176	THR	2.1
3	E	160	ASP	2.1
3	E	9	GLN	2.1
3	H	115	GLY	2.1
1	C	-5	HIS	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	H	160	ASP	2.1
1	F	111	LYS	2.1
1	A	146	GLU	2.0
3	D	179	GLU	2.0
3	E	180	GLU	2.0
3	E	191	HIS	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.