



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 5, 2023 – 04:21 am GMT

PDB ID : 1GO4  
Title : Crystal structure of Mad1-Mad2 reveals a conserved Mad2 binding motif in Mad1 and Cdc20.  
Authors : Sironi, L.; Mapelli, M.; Jeang, K.T.; Musacchio, A.  
Deposited on : 2001-10-17  
Resolution : 2.05 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

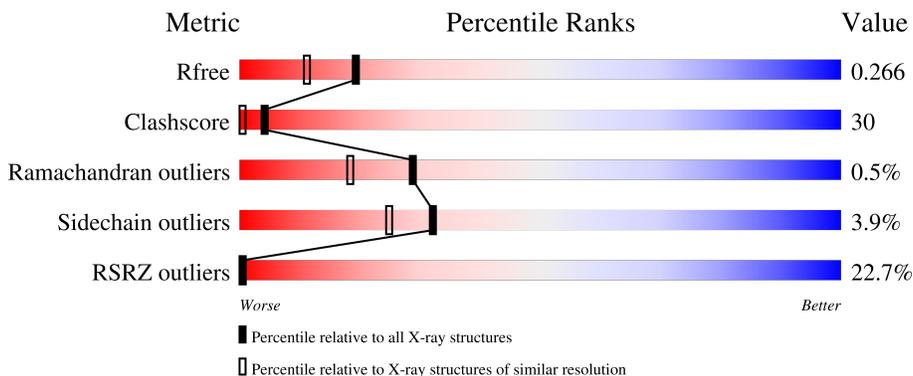
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.05 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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  $\geq 3$ , 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	205	
1	B	205	
1	C	205	
1	D	205	
2	E	100	

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Mol	Chain	Length	Quality of chain
2	F	100	
2	G	100	
2	H	100	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 9928 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
			Total	C	N	O	S			
1	A	196	Total 1578	C 1014	N 254	O 306	S 4	0	0	0
1	B	195	Total 1568	C 1008	N 253	O 303	S 4	0	0	0
1	C	195	Total 1568	C 1008	N 253	O 303	S 4	0	0	0
1	D	193	Total 1556	C 1002	N 250	O 300	S 4	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	133	ALA	ARG	engineered mutation	UNP Q13257
B	133	ALA	ARG	engineered mutation	UNP Q13257
C	133	ALA	ARG	engineered mutation	UNP Q13257
D	133	ALA	ARG	engineered mutation	UNP Q13257

- Molecule 2 is a protein called Mitotic spindle assembly checkpoint protein MAD1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	E	87	Total 722	C 433	N 143	O 142	S 4	0	0	0
2	F	87	Total 722	C 433	N 143	O 142	S 4	0	0	0
2	G	100	Total 816	C 489	N 160	O 163	S 4	0	0	0
2	H	93	Total 770	C 464	N 150	O 152	S 4	0	0	0

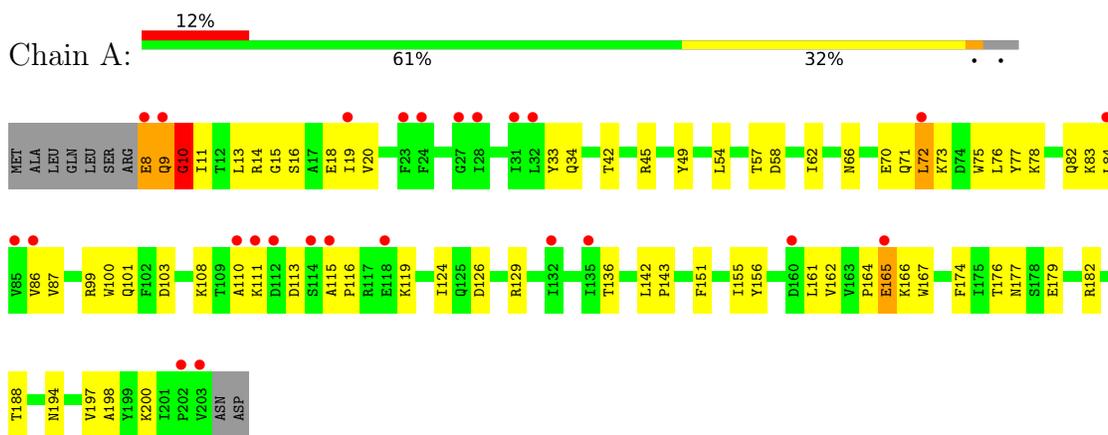
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	88	Total O 88 88	0	0
3	B	124	Total O 124 124	0	0
3	C	225	Total O 225 225	0	0
3	D	45	Total O 45 45	0	0
3	E	56	Total O 56 56	0	0
3	F	35	Total O 35 35	0	0
3	G	24	Total O 24 24	0	0
3	H	31	Total O 31 31	0	0

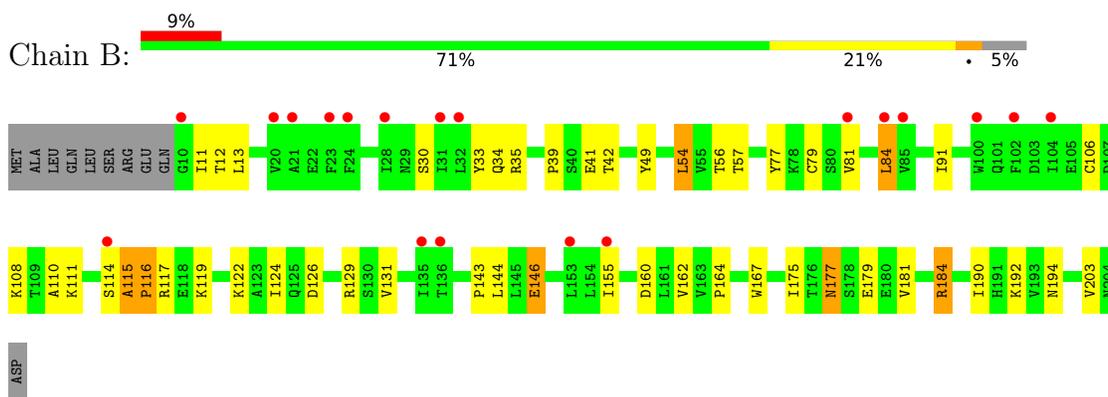
### 3 Residue-property plots [i](#)

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.

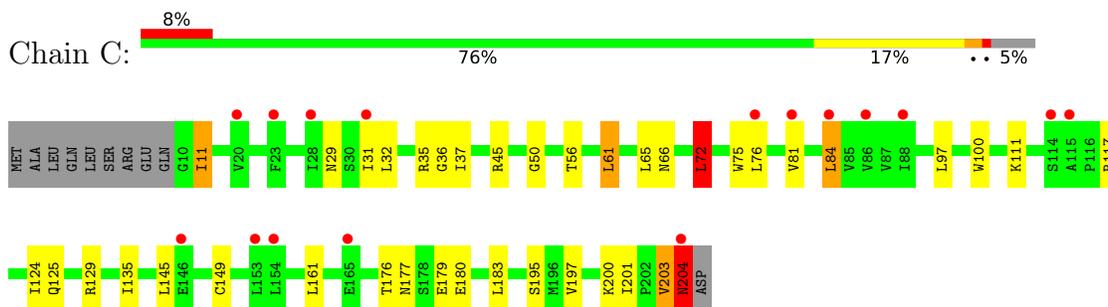
- Molecule 1: Mitotic spindle assembly checkpoint protein MAD2A



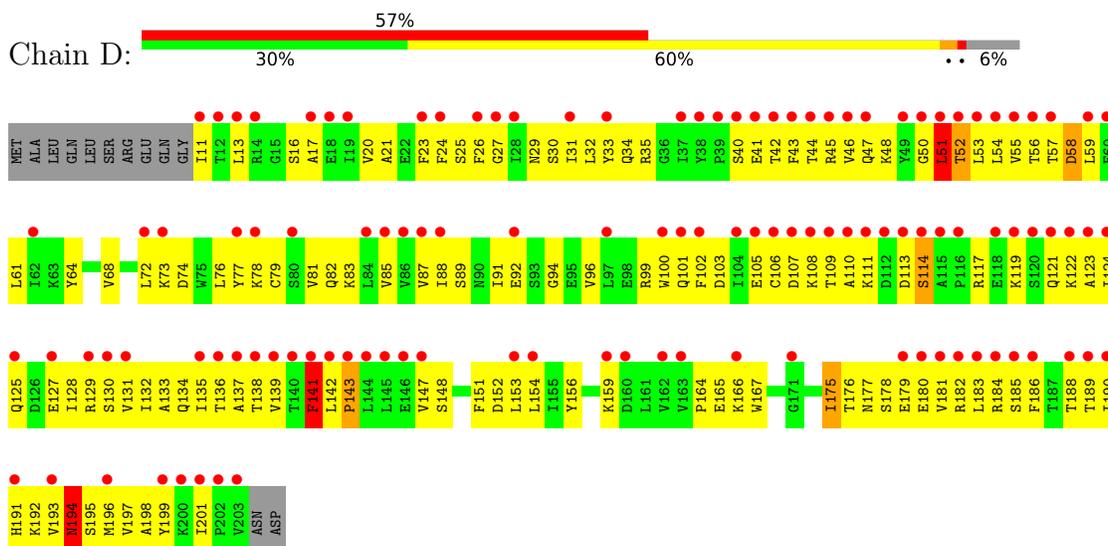
- Molecule 1: Mitotic spindle assembly checkpoint protein MAD2A



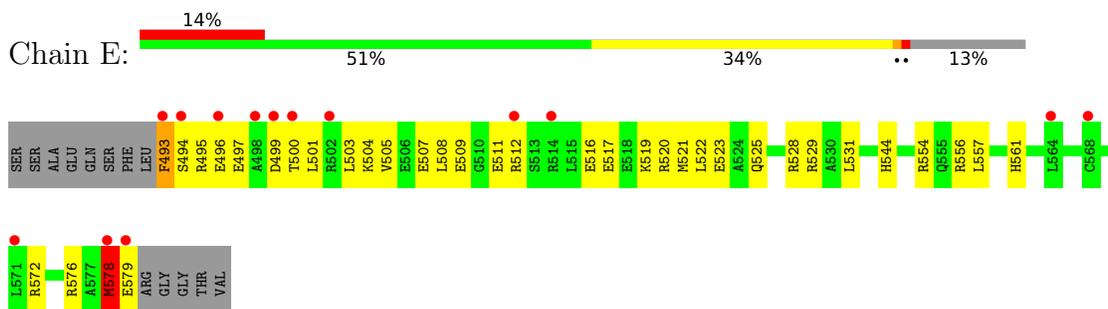
- Molecule 1: Mitotic spindle assembly checkpoint protein MAD2A



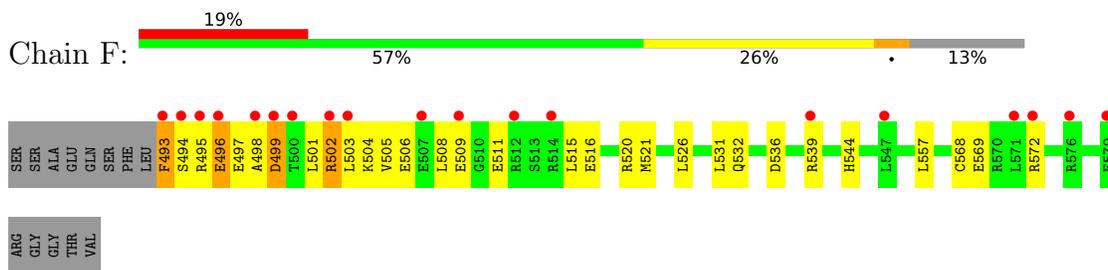
- Molecule 1: Mitotic spindle assembly checkpoint protein MAD2A



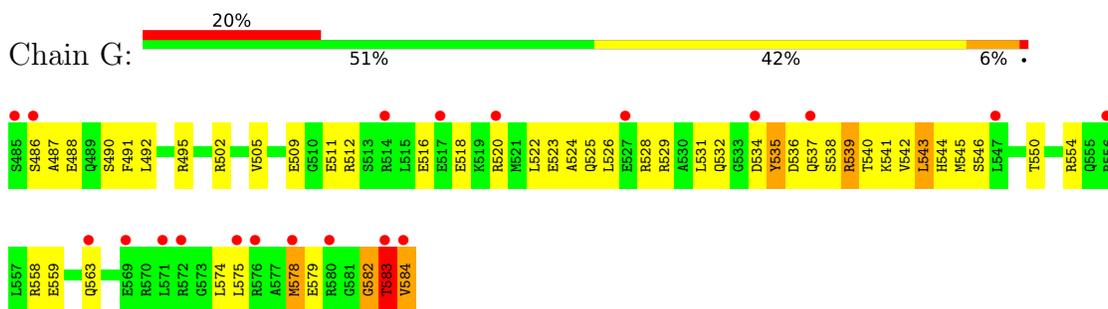
- Molecule 2: Mitotic spindle assembly checkpoint protein MAD1



- Molecule 2: Mitotic spindle assembly checkpoint protein MAD1

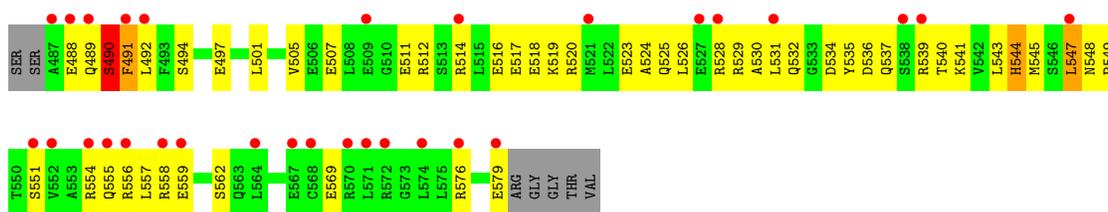


- Molecule 2: Mitotic spindle assembly checkpoint protein MAD1



- Molecule 2: Mitotic spindle assembly checkpoint protein MAD1

Chain H: 30% 42% 47% 7%



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	111.04Å 63.02Å 139.51Å 90.00° 111.65° 90.00°	Depositor
Resolution (Å)	24.50 – 2.05 24.50 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.6 (24.50-2.05) 99.8 (24.50-2.05)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.32 (at 2.04Å)	Xtrriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.240 , 0.268 0.238 , 0.266	Depositor DCC
$R_{free}$ test set	5665 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	41.5	Xtrriage
Anisotropy	0.081	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 59.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.011 for h,-k,-h-l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9928	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.17% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 i

### 5.1 Standard geometry i

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	0.85	3/1606 (0.2%)	0.83	2/2179 (0.1%)
1	B	0.66	0/1596	0.81	3/2166 (0.1%)
1	C	0.86	0/1596	0.99	7/2166 (0.3%)
1	D	0.42	0/1584	1.05	9/2150 (0.4%)
2	E	0.61	0/726	0.94	7/966 (0.7%)
2	F	0.46	0/726	0.62	0/966
2	G	0.48	0/821	0.83	3/1092 (0.3%)
2	H	0.39	0/775	0.77	2/1032 (0.2%)
All	All	0.65	3/9430 (0.0%)	0.89	33/12717 (0.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	10	GLY	N-CA	21.90	1.78	1.46
1	A	8	GLU	CG-CD	-8.78	1.38	1.51
1	A	9	GLN	CG-CD	-6.40	1.36	1.51

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	195	SER	N-CA-CB	-28.89	67.16	110.50
1	C	203	VAL	CA-C-N	-15.38	83.37	117.20
1	A	9	GLN	C-N-CA	-13.24	94.50	122.30
1	D	59	LEU	N-CA-CB	-12.80	84.80	110.40
1	C	203	VAL	O-C-N	11.13	140.51	122.70
2	E	578	MET	CA-C-N	-10.86	93.30	117.20
2	G	584	VAL	N-CA-C	-9.79	84.58	111.00
1	D	194	ASN	CB-CA-C	-9.70	91.00	110.40
1	A	10	GLY	N-CA-C	9.50	136.84	113.10
1	D	52	THR	N-CA-CB	-9.36	92.51	110.30
2	G	583	THR	N-CA-C	-8.41	88.28	111.00
1	C	203	VAL	C-N-CA	8.18	142.14	121.70
1	D	195	SER	N-CA-C	8.15	133.02	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	203	VAL	CA-C-O	7.63	136.12	120.10
1	D	51	LEU	N-CA-C	-7.29	91.32	111.00
2	E	578	MET	O-C-N	7.21	134.23	122.70
2	E	493	PHE	CB-CG-CD1	-6.95	115.93	120.80
2	E	578	MET	N-CA-C	-6.48	93.50	111.00
2	E	493	PHE	CB-CA-C	6.38	123.15	110.40
2	E	493	PHE	CB-CG-CD2	6.27	125.19	120.80
2	E	578	MET	CA-C-O	5.89	132.47	120.10
1	D	175	ILE	N-CA-C	-5.76	95.44	111.00
2	H	491	PHE	CA-C-N	-5.72	104.61	117.20
1	D	141	PHE	CB-CG-CD2	5.72	124.80	120.80
1	C	84	LEU	CA-CB-CG	5.69	128.39	115.30
2	H	492	LEU	CA-CB-CG	5.55	128.06	115.30
1	B	175	ILE	N-CA-C	-5.54	96.05	111.00
1	B	179	GLU	N-CA-C	-5.50	96.15	111.00
1	C	204	ASN	CB-CA-C	5.45	121.30	110.40
1	C	72	LEU	CA-CB-CG	5.24	127.36	115.30
1	B	164	PRO	CA-N-CD	-5.24	104.17	111.50
1	D	58	ASP	N-CA-C	-5.20	96.97	111.00
2	G	535	TYR	CA-CB-CG	5.10	123.09	113.40

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	1578	0	1596	73	0
1	B	1568	0	1588	46	0
1	C	1568	0	1587	38	0
1	D	1556	0	1579	202	0
2	E	722	0	720	58	0
2	F	722	0	722	40	0
2	G	816	0	811	61	0
2	H	770	0	766	79	0
3	A	88	0	0	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	124	0	0	17	0
3	C	225	0	0	18	0
3	D	45	0	0	69	0
3	E	56	0	0	13	0
3	F	35	0	0	4	0
3	G	24	0	0	7	0
3	H	31	0	0	24	0
All	All	9928	0	9369	553	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 30.

All (553) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:141:PHE:HE2	1:D:199:TYR:CE2	1.30	1.47
1:A:10:GLY:N	1:A:10:GLY:CA	1.78	1.46
2:E:529:ARG:CZ	3:E:2018:HOH:O	1.81	1.26
1:D:141:PHE:CE2	1:D:199:TYR:CE2	2.22	1.25
1:D:152:ASP:OD2	3:D:2030:HOH:O	1.57	1.16
2:E:493:PHE:O	2:E:497:GLU:HG2	1.48	1.14
1:C:37:ILE:N	3:C:2035:HOH:O	1.79	1.13
1:A:19:ILE:HD11	1:A:188:THR:CG2	1.80	1.12
1:D:58:ASP:O	3:D:2011:HOH:O	1.71	1.08
1:A:166:LYS:O	3:A:2075:HOH:O	1.70	1.06
1:B:39:PRO:O	1:B:42:THR:HG22	1.57	1.04
2:F:499:ASP:HA	2:F:502:ARG:HD3	1.38	1.04
1:A:19:ILE:HD11	1:A:188:THR:HG21	1.06	1.03
2:F:502:ARG:HB2	2:F:502:ARG:NH1	1.74	1.03
2:E:529:ARG:NE	3:E:2018:HOH:O	1.85	1.02
1:D:138:THR:HG22	1:D:142:LEU:HG	1.39	1.01
1:D:194:ASN:O	3:D:2043:HOH:O	1.76	1.00
1:D:47:GLN:HE22	1:D:52:THR:HG22	1.20	0.99
1:A:162:VAL:O	1:A:164:PRO:HD3	1.61	0.99
2:G:579:GLU:HA	2:G:584:VAL:OXT	1.61	0.99
1:A:9:GLN:C	1:A:10:GLY:CA	2.30	0.99
1:D:117:ARG:CD	1:D:189:THR:HG21	1.92	0.98
1:D:131:VAL:HG21	1:D:186:PHE:HD2	1.24	0.98
1:D:117:ARG:HD2	1:D:189:THR:HG21	1.46	0.96
1:D:100:TRP:CZ2	3:D:2018:HOH:O	2.20	0.93
1:D:117:ARG:HD2	1:D:189:THR:CG2	1.97	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:29:ASN:OD1	1:D:56:THR:HG23	1.69	0.92
1:B:177:ASN:H	1:B:177:ASN:HD22	1.15	0.91
1:D:124:ILE:HD11	3:D:2041:HOH:O	1.69	0.91
1:D:51:LEU:HD12	1:D:129:ARG:HG3	1.50	0.91
2:G:578:MET:O	2:G:584:VAL:OXT	1.87	0.91
2:F:502:ARG:HB2	2:F:502:ARG:HH11	1.34	0.90
2:E:529:ARG:NH2	3:E:2018:HOH:O	1.93	0.90
1:D:42:THR:O	1:D:57:THR:HG22	1.72	0.90
2:G:531:LEU:HD23	2:G:532:GLN:N	1.88	0.89
2:G:536:ASP:OD2	2:G:538:SER:HB2	1.72	0.88
1:D:43:PHE:HB3	3:D:2009:HOH:O	1.72	0.88
2:E:493:PHE:CE2	2:E:496:GLU:HG2	2.08	0.88
1:D:141:PHE:CE2	1:D:199:TYR:HE2	1.72	0.88
1:A:165:GLU:O	1:A:166:LYS:HB2	1.72	0.87
1:D:52:THR:HA	3:D:2008:HOH:O	1.72	0.87
2:F:521:MET:HE3	3:F:2006:HOH:O	1.74	0.87
1:D:30:SER:O	1:D:34:GLN:HG2	1.74	0.86
1:A:19:ILE:CD1	1:A:188:THR:HG21	2.01	0.85
1:D:73:LYS:HA	1:D:76:LEU:HD12	1.58	0.85
2:E:576:ARG:O	2:E:579:GLU:HA	1.74	0.85
2:G:558:ARG:HD2	3:G:2020:HOH:O	1.76	0.85
1:D:11:ILE:HG13	3:D:2041:HOH:O	1.77	0.85
1:D:83:LYS:HG2	1:D:103:ASP:HA	1.58	0.85
1:D:194:ASN:HB2	3:D:2043:HOH:O	1.76	0.84
1:B:42:THR:O	1:B:57:THR:HG22	1.78	0.84
1:C:36:GLY:C	3:C:2035:HOH:O	2.06	0.84
2:E:554:ARG:HD3	3:E:2039:HOH:O	1.77	0.84
1:D:99:ARG:HB2	1:D:175:ILE:HD11	1.60	0.83
1:D:35:ARG:NH2	1:D:143:PRO:O	2.12	0.83
2:H:579:GLU:HB2	3:H:2030:HOH:O	1.78	0.83
1:C:195:SER:HB2	3:C:2208:HOH:O	1.79	0.83
1:B:160:ASP:OD2	3:B:2083:HOH:O	1.97	0.83
1:D:47:GLN:HA	3:D:2008:HOH:O	1.78	0.82
1:C:203:VAL:HG13	1:C:204:ASN:OD1	1.79	0.82
1:C:36:GLY:CA	3:C:2035:HOH:O	2.27	0.82
2:G:539:ARG:N	3:G:2014:HOH:O	2.11	0.82
2:G:574:LEU:O	2:G:578:MET:HB2	1.80	0.82
3:B:2107:HOH:O	2:F:532:GLN:HG2	1.80	0.81
1:D:136:THR:O	1:D:139:VAL:HG23	1.80	0.81
1:A:13:LEU:HD22	1:A:111:LYS:HG2	1.63	0.81
2:F:493:PHE:CE1	2:F:495:ARG:HB2	2.15	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:VAL:O	1:A:164:PRO:CD	2.29	0.81
1:D:180:GLU:OE1	3:D:2037:HOH:O	1.99	0.80
2:E:493:PHE:HZ	2:H:528:ARG:HH22	1.28	0.80
1:D:188:THR:HG21	3:D:2001:HOH:O	1.81	0.79
1:B:56:THR:OG1	3:B:2031:HOH:O	1.69	0.79
1:A:11:ILE:HD11	1:A:124:ILE:HD11	1.65	0.78
1:A:45:ARG:HD2	3:A:2023:HOH:O	1.82	0.78
1:C:177:ASN:HB2	3:C:2221:HOH:O	1.83	0.78
1:D:197:VAL:HG21	3:D:2018:HOH:O	1.84	0.78
2:H:554:ARG:O	2:H:558:ARG:HG3	1.85	0.77
2:E:493:PHE:CD2	2:E:496:GLU:HG2	2.19	0.77
2:E:505:VAL:CG2	2:F:505:VAL:HG22	2.15	0.77
2:E:556:ARG:CG	3:E:2047:HOH:O	2.33	0.76
1:D:51:LEU:HD11	3:D:2022:HOH:O	1.85	0.76
3:A:2075:HOH:O	2:G:546:SER:N	1.76	0.76
1:D:131:VAL:HG21	1:D:186:PHE:CD2	2.16	0.75
2:E:503:LEU:HD23	3:E:2011:HOH:O	1.85	0.75
1:D:132:ILE:HA	1:D:135:ILE:HD12	1.69	0.75
2:H:559:GLU:HB3	3:H:2027:HOH:O	1.86	0.75
1:D:117:ARG:CD	1:D:189:THR:CG2	2.60	0.74
1:D:54:LEU:HB3	3:D:2009:HOH:O	1.86	0.74
1:B:11:ILE:HG22	1:B:190:ILE:HD12	1.68	0.74
1:D:141:PHE:HE2	1:D:199:TYR:CZ	2.02	0.74
1:D:131:VAL:HG22	3:D:2040:HOH:O	1.87	0.74
2:E:505:VAL:HG22	2:F:505:VAL:HG22	1.68	0.74
1:D:94:GLY:HA2	2:H:554:ARG:HH22	1.53	0.73
1:D:141:PHE:CE2	1:D:199:TYR:CZ	2.76	0.73
1:A:11:ILE:CD1	1:A:124:ILE:HD11	2.17	0.73
2:H:547:LEU:HD23	2:H:547:LEU:H	1.52	0.73
1:D:32:LEU:HB3	3:D:2003:HOH:O	1.87	0.73
2:G:541:LYS:HG3	2:G:543:LEU:HD11	1.70	0.73
1:C:179:GLU:HG3	1:C:201:ILE:HG12	1.70	0.73
1:C:135:ILE:HB	3:C:2137:HOH:O	1.87	0.73
2:G:536:ASP:O	3:G:2014:HOH:O	2.07	0.73
1:B:203:VAL:HG21	3:B:2121:HOH:O	1.88	0.72
1:A:82:GLN:HB3	3:A:2041:HOH:O	1.89	0.72
1:C:100:TRP:CE3	1:C:197:VAL:HG22	2.24	0.72
1:D:47:GLN:NE2	1:D:52:THR:HG22	2.01	0.72
1:D:56:THR:HA	3:D:2006:HOH:O	1.89	0.72
1:A:19:ILE:CD1	1:A:188:THR:CG2	2.63	0.72
1:D:128:ILE:HD13	3:D:2007:HOH:O	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:ASN:H	1:B:177:ASN:ND2	1.87	0.71
1:D:35:ARG:HH12	1:D:142:LEU:HB2	1.55	0.71
2:E:493:PHE:O	2:E:497:GLU:CG	2.34	0.71
2:E:556:ARG:HG3	3:E:2047:HOH:O	1.88	0.71
1:C:111:LYS:HG2	3:C:2099:HOH:O	1.90	0.71
1:C:183:LEU:HB2	3:C:2208:HOH:O	1.89	0.71
2:H:541:LYS:HD3	2:H:543:LEU:HD21	1.73	0.71
1:A:9:GLN:O	1:A:10:GLY:CA	2.38	0.70
2:F:539:ARG:NH1	3:F:2021:HOH:O	2.24	0.70
1:D:94:GLY:HA2	2:H:554:ARG:NH2	2.06	0.70
2:F:511:GLU:O	2:F:515:LEU:HD13	1.92	0.70
1:D:20:VAL:HG23	3:D:2001:HOH:O	1.91	0.69
1:A:165:GLU:O	1:A:166:LYS:CB	2.40	0.69
2:E:493:PHE:HE2	2:E:496:GLU:HG2	1.57	0.69
1:D:176:THR:HG22	3:D:2036:HOH:O	1.92	0.69
1:D:142:LEU:HD21	1:D:197:VAL:HG11	1.74	0.69
1:D:50:GLY:HA3	1:D:129:ARG:NH2	2.07	0.69
1:D:89:SER:HA	3:D:2015:HOH:O	1.92	0.69
1:C:125:GLN:O	1:C:129:ARG:HG3	1.92	0.69
2:E:503:LEU:HD12	3:H:2008:HOH:O	1.90	0.69
1:D:129:ARG:HA	3:D:2022:HOH:O	1.92	0.68
2:G:525:GLN:HE21	2:H:526:LEU:HD13	1.58	0.68
2:G:528:ARG:O	2:H:537:GLN:HG2	1.94	0.68
1:C:177:ASN:N	3:C:2190:HOH:O	2.27	0.68
2:E:528:ARG:HD2	2:F:536:ASP:OD2	1.93	0.68
2:H:576:ARG:HB2	3:H:2029:HOH:O	1.95	0.67
1:A:126:ASP:OD1	1:A:129:ARG:NH2	2.26	0.67
2:G:536:ASP:OD2	2:G:538:SER:CB	2.43	0.67
1:C:180:GLU:OE1	3:C:2197:HOH:O	2.12	0.66
1:A:16:SER:O	1:A:19:ILE:HG12	1.95	0.66
2:E:528:ARG:NH1	3:E:2015:HOH:O	2.26	0.66
1:D:132:ILE:HD12	3:D:2022:HOH:O	1.94	0.66
2:H:557:LEU:C	2:H:557:LEU:HD23	2.16	0.66
3:A:2075:HOH:O	2:G:545:MET:HA	1.96	0.66
1:D:139:VAL:HG22	3:D:2027:HOH:O	1.95	0.66
2:G:525:GLN:HE21	2:H:526:LEU:CD1	2.09	0.66
2:G:528:ARG:NE	3:G:2010:HOH:O	2.29	0.66
1:A:100:TRP:CE3	1:A:197:VAL:HG22	2.30	0.65
2:G:511:GLU:OE1	2:H:512:ARG:NH2	2.26	0.65
1:D:184:ARG:N	3:D:2038:HOH:O	2.28	0.65
1:D:119:LYS:HB3	3:D:2041:HOH:O	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:141:PHE:C	1:D:141:PHE:CD2	2.70	0.65
2:E:493:PHE:CD2	2:E:496:GLU:HB2	2.31	0.65
2:H:529:ARG:HD3	3:H:2018:HOH:O	1.97	0.65
1:A:19:ILE:HG13	1:A:20:VAL:N	2.11	0.65
1:A:87:VAL:HG13	3:A:2049:HOH:O	1.96	0.65
1:A:87:VAL:HA	3:A:2049:HOH:O	1.95	0.65
2:F:569:GLU:O	2:F:572:ARG:HB3	1.97	0.64
2:H:514:ARG:O	2:H:518:GLU:HG3	1.98	0.64
1:C:66:ASN:HB2	3:C:2081:HOH:O	1.96	0.64
2:G:505:VAL:O	2:G:509:GLU:HG3	1.97	0.64
1:D:106:CYS:HB2	3:D:2019:HOH:O	1.98	0.64
2:E:512:ARG:O	2:E:516:GLU:HG3	1.98	0.64
1:D:68:VAL:HG11	1:D:153:LEU:HD13	1.80	0.63
1:D:72:LEU:O	1:D:76:LEU:HG	1.98	0.63
2:F:493:PHE:HE1	2:F:495:ARG:HB2	1.63	0.63
2:H:497:GLU:HG3	3:H:2007:HOH:O	1.96	0.63
2:G:579:GLU:CA	2:G:584:VAL:OXT	2.43	0.63
2:H:569:GLU:HB2	3:H:2028:HOH:O	1.97	0.63
1:D:178:SER:HA	1:D:201:ILE:HG13	1.79	0.63
1:D:103:ASP:HB2	3:D:2043:HOH:O	1.98	0.63
1:D:58:ASP:HB2	1:D:61:LEU:HB3	1.81	0.63
2:G:582:GLY:HA2	2:G:584:VAL:O	1.99	0.62
1:A:13:LEU:HD21	1:A:111:LYS:HE2	1.79	0.62
1:D:51:LEU:CD1	1:D:129:ARG:HG3	2.28	0.62
1:D:117:ARG:CB	1:D:189:THR:HG21	2.28	0.62
1:D:131:VAL:HA	3:D:2023:HOH:O	1.98	0.62
1:D:176:THR:HG23	1:D:177:ASN:N	2.13	0.62
1:A:11:ILE:HD11	1:A:119:LYS:HB3	1.81	0.62
1:D:159:LYS:HA	2:H:541:LYS:HE3	1.82	0.62
2:E:493:PHE:CD2	2:E:496:GLU:CG	2.82	0.62
2:H:554:ARG:HG3	2:H:554:ARG:HH11	1.64	0.61
2:H:557:LEU:HD23	2:H:557:LEU:O	2.01	0.61
1:D:151:PHE:CE1	3:D:2012:HOH:O	2.54	0.61
1:B:131:VAL:HG22	1:B:184:ARG:HB3	1.82	0.61
3:B:2099:HOH:O	1:C:176:THR:HG22	1.99	0.61
1:D:185:SER:HB3	1:D:194:ASN:HA	1.82	0.61
2:H:489:GLN:C	2:H:491:PHE:H	2.04	0.61
1:D:33:TYR:HA	3:D:2005:HOH:O	2.00	0.61
1:A:18:GLU:HA	1:A:73:LYS:HE2	1.83	0.60
2:G:543:LEU:HD12	2:G:543:LEU:N	2.15	0.60
1:D:20:VAL:HB	3:D:2002:HOH:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:151:PHE:CZ	3:D:2012:HOH:O	2.51	0.60
2:E:554:ARG:CZ	3:E:2040:HOH:O	2.49	0.60
1:B:203:VAL:HG22	3:B:2123:HOH:O	2.01	0.60
1:D:134:GLN:HB2	3:D:2023:HOH:O	2.02	0.60
1:C:200:LYS:NZ	3:C:2221:HOH:O	2.35	0.60
2:E:505:VAL:CG2	2:F:505:VAL:CG2	2.79	0.59
2:H:547:LEU:HD23	2:H:547:LEU:N	2.17	0.59
1:D:141:PHE:CZ	1:D:181:VAL:HG21	2.37	0.59
1:D:164:PRO:HG2	1:D:167:TRP:CG	2.36	0.59
1:D:194:ASN:HB3	3:D:2039:HOH:O	2.01	0.59
1:C:11:ILE:HD12	1:C:11:ILE:H	1.67	0.59
2:H:545:MET:HE3	3:H:2023:HOH:O	2.03	0.59
1:D:83:LYS:HB3	3:D:2014:HOH:O	2.02	0.59
1:D:91:ILE:HG13	1:D:148:SER:O	2.02	0.59
2:E:493:PHE:N	2:G:537:GLN:OE1	2.35	0.59
2:F:539:ARG:HD3	3:F:2021:HOH:O	2.02	0.59
1:A:9:GLN:O	1:A:10:GLY:O	2.20	0.58
1:A:49:TYR:O	1:A:129:ARG:HD3	2.03	0.58
1:C:29:ASN:ND2	1:C:56:THR:H	2.01	0.58
1:D:178:SER:HB2	3:D:2045:HOH:O	2.02	0.58
1:D:13:LEU:CD2	1:D:111:LYS:HG2	2.33	0.58
2:F:502:ARG:HB2	2:F:502:ARG:CZ	2.34	0.58
1:D:185:SER:CB	1:D:194:ASN:HA	2.34	0.58
2:G:512:ARG:O	2:G:516:GLU:HG3	2.04	0.58
1:D:147:VAL:HG22	3:D:2016:HOH:O	2.04	0.58
2:E:500:THR:HG22	3:H:2008:HOH:O	2.03	0.58
2:E:493:PHE:HD2	2:E:496:GLU:CG	2.16	0.58
1:B:30:SER:O	1:B:34:GLN:HG3	2.04	0.58
1:D:68:VAL:HG11	1:D:153:LEU:CD1	2.33	0.58
1:D:180:GLU:CD	2:H:532:GLN:HG2	2.24	0.58
1:D:17:ALA:O	1:D:73:LYS:HG3	2.04	0.57
2:E:493:PHE:HD2	2:E:496:GLU:HB2	1.68	0.57
2:G:529:ARG:HD2	2:H:534:ASP:OD2	2.04	0.57
2:G:578:MET:HE2	2:G:583:THR:HG21	1.84	0.57
1:C:203:VAL:HA	1:C:204:ASN:ND2	2.19	0.57
1:D:108:LYS:HG3	3:D:2019:HOH:O	2.05	0.57
1:B:146:GLU:HB3	3:B:2076:HOH:O	2.04	0.57
1:D:25:SER:O	1:D:29:ASN:ND2	2.36	0.57
2:E:505:VAL:HG22	2:F:505:VAL:CG2	2.35	0.57
2:E:505:VAL:HG23	2:F:505:VAL:HG22	1.87	0.57
1:C:179:GLU:CD	3:C:2194:HOH:O	2.42	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:540:THR:N	3:G:2014:HOH:O	2.19	0.57
1:D:51:LEU:C	1:D:51:LEU:HD22	2.25	0.56
3:D:2037:HOH:O	2:E:495:ARG:NH1	2.37	0.56
1:D:122:LYS:HA	3:D:2020:HOH:O	2.04	0.56
2:E:495:ARG:HE	2:H:528:ARG:NH2	2.03	0.56
2:F:495:ARG:O	2:F:495:ARG:HG2	2.05	0.56
2:G:518:GLU:O	2:G:522:LEU:HB2	2.05	0.56
1:B:34:GLN:NE2	3:B:2015:HOH:O	2.38	0.56
1:A:34:GLN:HE22	1:A:136:THR:HA	1.71	0.56
1:D:35:ARG:NH1	1:D:142:LEU:HB2	2.20	0.56
2:H:529:ARG:HB3	3:H:2018:HOH:O	2.06	0.56
1:D:83:LYS:HD2	1:D:101:GLN:CG	2.35	0.55
2:E:556:ARG:HG2	3:E:2047:HOH:O	1.99	0.55
2:G:578:MET:C	2:G:584:VAL:OXT	2.44	0.55
1:D:33:TYR:CE1	1:D:40:SER:HA	2.40	0.55
1:D:134:GLN:HA	1:D:137:ALA:HB3	1.89	0.55
1:D:101:GLN:HB3	3:D:2044:HOH:O	2.05	0.55
2:H:557:LEU:C	2:H:557:LEU:CD2	2.75	0.55
1:A:11:ILE:CD1	1:A:119:LYS:HB3	2.35	0.55
1:A:15:GLY:O	1:A:19:ILE:HG23	2.06	0.55
1:D:164:PRO:HG2	1:D:167:TRP:CD1	2.41	0.55
1:A:9:GLN:O	1:A:10:GLY:C	2.45	0.55
1:D:136:THR:HB	3:D:2024:HOH:O	2.06	0.55
1:D:176:THR:CG2	1:D:177:ASN:N	2.70	0.55
2:F:503:LEU:O	2:F:506:GLU:HG2	2.07	0.54
1:D:117:ARG:HD3	1:D:189:THR:HG21	1.86	0.54
2:H:523:GLU:OE1	3:H:2010:HOH:O	2.18	0.54
1:B:177:ASN:ND2	3:B:2105:HOH:O	2.35	0.54
2:G:524:ALA:C	3:G:2010:HOH:O	2.45	0.54
1:D:43:PHE:HD2	3:D:2009:HOH:O	1.91	0.54
1:D:51:LEU:HD22	1:D:51:LEU:O	2.08	0.54
2:E:493:PHE:CD2	2:E:496:GLU:CB	2.90	0.54
1:D:179:GLU:O	1:D:198:ALA:HA	2.07	0.54
1:C:45:ARG:HD3	3:C:2048:HOH:O	2.07	0.54
1:D:87:VAL:O	1:D:151:PHE:HA	2.07	0.54
1:D:130:SER:O	1:D:133:ALA:HB3	2.07	0.54
2:E:500:THR:HA	3:H:2008:HOH:O	2.08	0.54
1:B:119:LYS:HD2	1:B:124:ILE:CG1	2.38	0.54
1:D:94:GLY:CA	2:H:554:ARG:NH2	2.71	0.54
1:D:27:GLY:O	1:D:31:ILE:HG13	2.08	0.53
2:F:497:GLU:O	2:F:497:GLU:HG2	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:196:MET:HG3	3:D:2044:HOH:O	2.09	0.53
1:A:99:ARG:HH12	1:A:101:GLN:NE2	2.07	0.53
1:D:34:GLN:OE1	1:D:136:THR:HG23	2.08	0.53
1:D:79:CYS:HB3	3:D:2019:HOH:O	2.08	0.53
1:A:14:ARG:HG3	3:A:2001:HOH:O	2.07	0.53
1:D:45:ARG:HG2	1:D:54:LEU:HG	1.91	0.53
2:E:494:SER:OG	2:F:495:ARG:HA	2.08	0.53
2:G:525:GLN:NE2	2:H:526:LEU:HD13	2.24	0.53
2:G:542:VAL:C	2:G:543:LEU:HD12	2.29	0.53
1:D:175:ILE:HG21	3:D:2045:HOH:O	2.07	0.53
1:A:83:LYS:HB2	1:A:156:TYR:HB2	1.91	0.53
1:D:99:ARG:HB2	1:D:175:ILE:CD1	2.35	0.53
1:D:134:GLN:HB3	3:D:2029:HOH:O	2.09	0.53
1:D:142:LEU:HD21	1:D:197:VAL:CG1	2.38	0.53
2:G:578:MET:HG3	2:G:583:THR:HG22	1.91	0.53
1:D:138:THR:CG2	1:D:142:LEU:HG	2.28	0.52
1:D:159:LYS:N	3:D:2031:HOH:O	2.41	0.52
1:D:175:ILE:CD1	3:D:2045:HOH:O	2.57	0.52
2:G:526:LEU:HD11	2:G:534:ASP:OD2	2.09	0.52
2:G:502:ARG:NH2	2:H:497:GLU:CD	2.62	0.52
1:B:114:SER:O	1:B:115:ALA:HB2	2.09	0.52
2:H:517:GLU:HB3	2:H:520:ARG:NH1	2.24	0.52
1:A:14:ARG:HG2	1:A:77:TYR:CE1	2.44	0.52
1:A:78:LYS:HA	1:A:111:LYS:NZ	2.24	0.52
1:D:165:GLU:O	1:D:166:LYS:HB2	2.10	0.52
2:H:528:ARG:HG3	3:H:2013:HOH:O	2.10	0.52
2:F:516:GLU:HB3	2:F:520:ARG:NH2	2.25	0.51
1:B:144:LEU:HB3	3:B:2076:HOH:O	2.11	0.51
2:E:554:ARG:NH1	3:E:2040:HOH:O	2.43	0.51
1:D:196:MET:CG	3:D:2044:HOH:O	2.59	0.51
2:E:556:ARG:NH2	3:E:2043:HOH:O	2.42	0.51
1:D:131:VAL:O	1:D:135:ILE:HG13	2.10	0.51
1:D:194:ASN:N	1:D:194:ASN:HD22	2.07	0.51
2:H:530:ALA:HB2	3:H:2012:HOH:O	2.10	0.51
1:A:99:ARG:HH12	1:A:101:GLN:HE21	1.57	0.51
1:A:110:ALA:HA	1:A:113:ASP:OD2	2.10	0.51
1:A:182:ARG:HG2	3:A:2078:HOH:O	2.10	0.51
1:D:87:VAL:HG21	1:D:154:LEU:HD11	1.91	0.51
1:D:138:THR:OG1	3:D:2029:HOH:O	2.19	0.51
2:E:557:LEU:C	2:E:557:LEU:HD23	2.31	0.51
2:H:501:LEU:O	2:H:505:VAL:HG23	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:34:GLN:OE1	1:D:136:THR:HA	2.12	0.50
2:F:496:GLU:C	2:F:498:ALA:H	2.14	0.50
2:E:503:LEU:HA	3:E:2011:HOH:O	2.11	0.50
2:E:517:GLU:HA	2:E:520:ARG:HH21	1.75	0.50
2:F:501:LEU:O	2:F:505:VAL:HG23	2.11	0.50
2:H:544:HIS:NE2	3:H:2021:HOH:O	2.35	0.50
1:B:79:CYS:HA	1:B:106:CYS:SG	2.51	0.50
2:E:495:ARG:NE	2:H:528:ARG:NH2	2.59	0.50
1:B:146:GLU:HG2	3:B:2075:HOH:O	2.11	0.50
1:D:54:LEU:N	1:D:54:LEU:HD12	2.27	0.50
2:G:574:LEU:O	2:G:578:MET:N	2.44	0.50
2:H:494:SER:HA	3:H:2006:HOH:O	2.10	0.50
2:F:505:VAL:O	2:F:509:GLU:HG3	2.12	0.50
2:H:489:GLN:C	2:H:491:PHE:N	2.65	0.50
1:A:33:TYR:CE2	1:A:54:LEU:HD13	2.47	0.50
1:A:177:ASN:ND2	3:H:2020:HOH:O	2.45	0.50
1:A:78:LYS:HA	1:A:111:LYS:HZ1	1.77	0.49
1:A:82:GLN:OE1	2:G:540:THR:HG22	2.12	0.49
2:H:488:GLU:O	2:H:491:PHE:HB2	2.12	0.49
1:D:165:GLU:HG3	1:D:166:LYS:HG3	1.93	0.49
2:E:507:GLU:O	2:E:511:GLU:HG3	2.13	0.49
2:H:531:LEU:HB2	3:H:2014:HOH:O	2.11	0.49
2:E:493:PHE:HD2	2:E:496:GLU:CB	2.25	0.49
2:H:507:GLU:O	2:H:511:GLU:HG3	2.13	0.49
1:C:50:GLY:HA3	1:C:129:ARG:NH1	2.27	0.49
1:D:56:THR:HG21	1:D:61:LEU:CD2	2.42	0.49
2:G:559:GLU:O	2:G:563:GLN:HG3	2.12	0.49
1:B:119:LYS:HD2	1:B:124:ILE:HG13	1.93	0.49
1:D:35:ARG:NH1	1:D:142:LEU:CB	2.75	0.49
1:D:83:LYS:HB2	1:D:156:TYR:HB2	1.93	0.49
1:C:61:LEU:HD22	1:C:65:LEU:HG	1.94	0.49
1:A:45:ARG:CD	3:A:2023:HOH:O	2.52	0.49
1:A:176:THR:O	1:A:200:LYS:HE2	2.12	0.49
1:D:85:VAL:HA	1:D:100:TRP:O	2.12	0.49
2:G:526:LEU:O	2:G:526:LEU:HD23	2.12	0.49
1:B:184:ARG:HG3	1:B:184:ARG:HH11	1.76	0.49
1:D:64:TYR:OH	3:D:2030:HOH:O	2.19	0.49
1:D:50:GLY:HA3	1:D:129:ARG:CZ	2.42	0.49
2:G:491:PHE:O	2:G:495:ARG:HG3	2.13	0.49
1:A:108:LYS:HE2	2:G:539:ARG:HH22	1.78	0.48
1:D:156:TYR:HD2	2:H:540:THR:HG21	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:136:THR:HA	3:D:2027:HOH:O	2.13	0.48
1:B:12:THR:HG22	1:B:116:PRO:HG3	1.95	0.48
1:C:11:ILE:CD1	1:C:117:ARG:HB2	2.44	0.48
1:D:166:LYS:HB3	2:H:547:LEU:HD21	1.94	0.48
2:G:516:GLU:O	2:G:520:ARG:HG3	2.13	0.48
1:D:76:LEU:HD23	1:D:81:VAL:HG11	1.95	0.48
1:A:87:VAL:O	1:A:151:PHE:HA	2.14	0.48
1:D:188:THR:OG1	1:D:189:THR:N	2.46	0.48
2:H:536:ASP:HB3	2:H:539:ARG:HB2	1.96	0.48
2:H:531:LEU:N	3:H:2014:HOH:O	2.45	0.48
2:F:521:MET:HB2	3:F:2006:HOH:O	2.13	0.48
2:G:511:GLU:OE1	2:H:512:ARG:NE	2.47	0.48
1:A:19:ILE:CD1	1:A:188:THR:HG22	2.44	0.48
1:B:177:ASN:HD22	1:B:177:ASN:N	1.96	0.48
1:D:83:LYS:HD2	1:D:101:GLN:HG3	1.94	0.48
2:E:508:LEU:HB3	2:F:508:LEU:HB3	1.96	0.48
1:B:33:TYR:CE2	1:B:54:LEU:HD13	2.49	0.47
1:B:56:THR:CB	3:B:2031:HOH:O	2.46	0.47
2:H:555:GLN:O	2:H:559:GLU:HG3	2.13	0.47
2:H:491:PHE:N	2:H:491:PHE:CD2	2.79	0.47
2:H:519:LYS:O	2:H:523:GLU:HG3	2.14	0.47
1:D:151:PHE:O	2:H:549:PRO:HB2	2.14	0.47
1:A:177:ASN:HA	3:H:2020:HOH:O	2.13	0.47
1:C:36:GLY:HA2	3:C:2035:HOH:O	2.05	0.47
1:A:42:THR:O	1:A:57:THR:HG22	2.14	0.47
1:D:23:PHE:HB2	3:D:2007:HOH:O	2.14	0.47
1:D:13:LEU:HD22	1:D:111:LYS:HG2	1.95	0.47
1:B:143:PRO:HD2	3:B:2017:HOH:O	2.15	0.47
1:D:44:THR:HG23	1:D:44:THR:O	2.15	0.47
1:D:176:THR:CG2	1:D:177:ASN:H	2.27	0.47
2:E:501:LEU:HD13	2:F:501:LEU:HB2	1.96	0.47
1:A:8:GLU:O	1:A:9:GLN:CG	2.62	0.47
1:C:72:LEU:HD22	1:C:76:LEU:HG	1.97	0.47
1:C:203:VAL:HG13	1:C:204:ASN:CG	2.34	0.47
1:D:129:ARG:HH11	1:D:129:ARG:CB	2.28	0.47
2:E:499:ASP:OD1	2:H:528:ARG:HD2	2.15	0.47
2:H:490:SER:C	2:H:491:PHE:CD2	2.89	0.47
1:A:99:ARG:HG3	3:A:2049:HOH:O	2.14	0.47
1:D:20:VAL:HG12	1:D:24:PHE:HE1	1.80	0.47
1:D:185:SER:N	3:D:2040:HOH:O	2.48	0.47
1:D:110:ALA:HB1	1:D:190:ILE:HD13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:29:ASN:HD21	1:C:56:THR:HG22	1.81	0.46
1:D:105:GLU:O	1:D:191:HIS:HA	2.15	0.46
1:B:110:ALA:HA	1:B:117:ARG:HH21	1.80	0.46
1:D:178:SER:CB	3:D:2045:HOH:O	2.62	0.46
1:D:199:TYR:C	3:D:2045:HOH:O	2.53	0.46
2:G:487:ALA:O	2:G:490:SER:HB2	2.15	0.46
2:H:545:MET:N	3:H:2022:HOH:O	2.18	0.46
1:A:72:LEU:HD22	1:A:76:LEU:HG	1.97	0.46
2:H:548:ASN:HB2	2:H:549:PRO:HD2	1.98	0.46
1:A:34:GLN:NE2	1:A:136:THR:HA	2.31	0.46
2:F:568:CYS:O	2:F:572:ARG:HB2	2.15	0.46
1:A:161:LEU:HD23	1:A:162:VAL:O	2.16	0.46
2:G:520:ARG:HA	2:G:523:GLU:HG2	1.97	0.46
2:G:543:LEU:N	2:G:543:LEU:CD1	2.77	0.46
1:A:86:VAL:HB	1:A:100:TRP:HB2	1.97	0.46
1:D:16:SER:HA	3:D:2001:HOH:O	2.15	0.46
1:D:26:PHE:HB3	1:D:53:LEU:HD13	1.98	0.46
1:D:117:ARG:HB3	1:D:189:THR:HG21	1.98	0.46
2:F:499:ASP:O	2:F:503:LEU:HG	2.16	0.46
1:D:33:TYR:HE1	1:D:40:SER:HA	1.81	0.46
1:D:48:LYS:HB3	1:D:53:LEU:HD12	1.98	0.46
2:H:512:ARG:O	2:H:516:GLU:HG3	2.15	0.46
1:B:39:PRO:HB3	1:B:41:GLU:CD	2.36	0.45
1:A:11:ILE:HD13	1:A:124:ILE:HD11	1.96	0.45
1:A:71:GLN:NE2	1:A:75:TRP:NE1	2.63	0.45
2:H:490:SER:O	2:H:491:PHE:HD2	1.99	0.45
1:D:76:LEU:HD13	3:D:2002:HOH:O	2.16	0.45
1:C:32:LEU:O	3:C:2035:HOH:O	2.21	0.45
1:D:26:PHE:CE2	1:D:48:LYS:HG2	2.51	0.45
1:D:33:TYR:CE1	1:D:40:SER:CB	3.00	0.45
1:B:167:TRP:CB	3:B:2087:HOH:O	2.65	0.45
1:D:51:LEU:C	1:D:51:LEU:CD2	2.84	0.45
1:D:175:ILE:HD13	3:D:2045:HOH:O	2.17	0.45
1:A:179:GLU:O	1:A:198:ALA:HA	2.17	0.45
1:D:40:SER:C	1:D:42:THR:H	2.20	0.45
2:G:531:LEU:HD23	2:G:531:LEU:C	2.37	0.45
1:A:176:THR:HG22	1:A:177:ASN:OD1	2.16	0.45
1:D:55:VAL:N	3:D:2009:HOH:O	2.49	0.45
2:H:528:ARG:C	3:H:2014:HOH:O	2.55	0.45
1:B:91:ILE:HG22	2:F:557:LEU:CD1	2.47	0.45
1:D:50:GLY:HA3	1:D:129:ARG:HH21	1.78	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:64:TYR:HE1	2:H:545:MET:HG3	1.82	0.45
1:B:49:TYR:O	1:B:129:ARG:HD2	2.16	0.45
1:D:96:VAL:CG1	1:D:175:ILE:HG12	2.47	0.45
2:G:579:GLU:HA	2:G:584:VAL:C	2.32	0.45
1:B:167:TRP:HB2	3:B:2087:HOH:O	2.16	0.44
1:A:161:LEU:HD23	1:A:161:LEU:C	2.38	0.44
2:G:538:SER:N	3:G:2014:HOH:O	2.49	0.44
1:A:155:ILE:HD12	1:A:167:TRP:CH2	2.52	0.44
1:B:84:LEU:HD22	1:B:155:ILE:CD1	2.47	0.44
1:D:88:ILE:HG12	3:D:2017:HOH:O	2.17	0.44
1:A:66:ASN:O	1:A:70:GLU:HG2	2.17	0.44
1:B:192:LYS:HE2	1:B:194:ASN:OD1	2.18	0.44
1:D:117:ARG:HD3	1:D:189:THR:CG2	2.42	0.44
2:F:493:PHE:HD1	2:F:494:SER:N	2.16	0.44
1:A:13:LEU:HD23	1:A:77:TYR:CE1	2.52	0.44
3:A:2075:HOH:O	2:G:545:MET:CA	2.53	0.44
2:E:497:GLU:O	2:E:501:LEU:HG	2.18	0.44
2:G:531:LEU:HD23	2:G:532:GLN:H	1.78	0.44
1:B:122:LYS:O	1:B:126:ASP:OD2	2.36	0.44
1:B:108:LYS:O	1:B:111:LYS:HG2	2.18	0.43
1:C:97:LEU:HD12	1:C:149:CYS:SG	2.58	0.43
1:D:92:GLU:OE2	1:D:92:GLU:N	2.50	0.43
1:D:182:ARG:HH21	2:H:531:LEU:HD21	1.82	0.43
1:D:73:LYS:O	1:D:76:LEU:HB2	2.18	0.43
2:E:504:LYS:O	2:E:508:LEU:HG	2.17	0.43
1:D:44:THR:O	1:D:46:VAL:HG13	2.19	0.43
1:D:105:GLU:HB3	1:D:192:LYS:HB3	2.01	0.43
2:E:522:LEU:HD22	2:F:526:LEU:HD12	2.00	0.43
2:G:502:ARG:NH2	2:H:497:GLU:OE2	2.51	0.43
1:A:58:ASP:O	1:A:62:ILE:HG13	2.17	0.43
2:G:486:SER:HB3	2:G:488:GLU:OE1	2.17	0.43
2:H:524:ALA:HB2	3:H:2008:HOH:O	2.17	0.43
1:B:181:VAL:HG21	2:G:492:LEU:HD13	1.99	0.43
2:H:535:TYR:CD1	2:H:540:THR:HB	2.54	0.43
1:A:174:PHE:HB3	2:G:532:GLN:O	2.19	0.43
1:D:51:LEU:HD12	1:D:129:ARG:CG	2.35	0.43
2:G:575:LEU:HD23	2:G:575:LEU:HA	1.88	0.43
2:H:528:ARG:O	2:H:528:ARG:CG	2.67	0.43
1:D:74:ASP:OD1	1:D:78:LYS:HE3	2.18	0.43
2:H:535:TYR:HD1	2:H:540:THR:HB	1.83	0.43
1:C:66:ASN:CB	3:C:2081:HOH:O	2.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:196:MET:CE	2:H:531:LEU:HD22	2.49	0.43
1:B:162:VAL:HG23	3:B:2084:HOH:O	2.19	0.43
1:D:88:ILE:HD13	1:D:151:PHE:HB2	2.01	0.43
1:D:123:ALA:O	1:D:127:GLU:HG3	2.19	0.43
2:G:502:ARG:HE	2:G:502:ARG:HB2	1.54	0.42
1:D:30:SER:C	1:D:34:GLN:HG2	2.38	0.42
1:D:152:ASP:OD2	1:D:153:LEU:N	2.52	0.42
1:D:180:GLU:OE2	2:H:532:GLN:HG2	2.19	0.42
2:F:504:LYS:O	2:F:508:LEU:HD23	2.19	0.42
1:C:100:TRP:CD2	1:C:197:VAL:HG22	2.54	0.42
1:D:134:GLN:HB3	1:D:183:LEU:HD13	2.01	0.42
1:B:35:ARG:HD2	1:B:35:ARG:HA	1.81	0.42
2:E:517:GLU:HA	2:E:520:ARG:HE	1.84	0.42
2:E:521:MET:O	2:E:525:GLN:HG3	2.20	0.42
2:H:554:ARG:HG3	2:H:554:ARG:NH1	2.32	0.42
1:D:31:ILE:HD13	1:D:100:TRP:CE3	2.54	0.42
2:H:525:GLN:O	2:H:529:ARG:HG3	2.20	0.42
1:D:128:ILE:HG21	3:D:2007:HOH:O	2.19	0.42
1:D:184:ARG:C	3:D:2040:HOH:O	2.57	0.42
2:F:502:ARG:CZ	2:F:502:ARG:CB	2.98	0.42
1:B:146:GLU:HG2	1:B:146:GLU:H	1.63	0.42
1:D:117:ARG:CG	1:D:189:THR:HG21	2.48	0.42
2:G:550:THR:O	2:G:554:ARG:HG3	2.19	0.42
1:C:75:TRP:CE2	1:C:161:LEU:HD21	2.54	0.42
1:D:13:LEU:HG	1:D:77:TYR:CD1	2.55	0.42
1:D:136:THR:O	1:D:139:VAL:CG2	2.61	0.42
2:E:579:GLU:HA	2:E:579:GLU:OE1	2.20	0.42
1:D:184:ARG:CA	3:D:2038:HOH:O	2.67	0.42
2:G:488:GLU:CD	2:G:488:GLU:H	2.23	0.42
1:A:142:LEU:HA	1:A:143:PRO:HD3	1.79	0.41
1:D:113:ASP:HB3	1:D:114:SER:H	1.66	0.41
1:D:117:ARG:HD2	1:D:189:THR:HG22	1.92	0.41
2:E:505:VAL:HG23	2:F:505:VAL:CG2	2.48	0.41
1:C:145:LEU:HD23	1:C:145:LEU:HA	1.84	0.41
2:F:496:GLU:C	2:F:498:ALA:N	2.74	0.41
2:H:559:GLU:O	2:H:562:SER:HB2	2.21	0.41
1:A:115:ALA:HB1	1:A:116:PRO:HD2	2.02	0.41
1:D:53:LEU:C	1:D:54:LEU:HD12	2.40	0.41
1:B:84:LEU:HD22	1:B:155:ILE:HD13	2.01	0.41
1:D:193:VAL:C	1:D:194:ASN:HD22	2.24	0.41
2:E:517:GLU:CA	2:E:520:ARG:HH21	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:498:ALA:O	2:F:502:ARG:HG3	2.20	0.41
2:G:511:GLU:CD	2:H:512:ARG:HH21	2.18	0.41
1:A:8:GLU:O	1:A:9:GLN:HG3	2.20	0.41
1:D:176:THR:HG23	1:D:177:ASN:H	1.85	0.41
2:E:578:MET:HE2	2:E:578:MET:HB3	1.81	0.41
1:C:11:ILE:HG12	1:C:124:ILE:HD11	2.03	0.41
1:D:50:GLY:C	1:D:51:LEU:HD13	2.40	0.41
1:D:102:PHE:N	1:D:102:PHE:CD1	2.89	0.41
2:H:489:GLN:O	2:H:491:PHE:N	2.54	0.41
2:H:516:GLU:O	2:H:519:LYS:HB2	2.19	0.41
1:A:13:LEU:CD2	1:A:111:LYS:HG2	2.43	0.41
1:A:103:ASP:HB2	1:A:194:ASN:HB2	2.02	0.41
1:B:13:LEU:HG	1:B:77:TYR:CD1	2.56	0.41
1:B:194:ASN:HB3	3:B:2115:HOH:O	2.21	0.41
2:G:578:MET:HG3	2:G:583:THR:CG2	2.51	0.41
1:A:71:GLN:NE2	1:A:75:TRP:CE2	2.89	0.40
1:B:91:ILE:HG22	2:F:557:LEU:HD11	2.03	0.40
1:D:82:GLN:O	1:D:83:LYS:HG3	2.21	0.40
1:D:179:GLU:HG3	1:D:201:ILE:HG12	2.02	0.40
2:E:517:GLU:HA	2:E:520:ARG:NH2	2.36	0.40
2:G:488:GLU:CD	2:G:488:GLU:N	2.74	0.40
1:B:81:VAL:HG23	1:B:155:ILE:CG2	2.52	0.40
1:C:31:ILE:O	1:C:35:ARG:HG2	2.21	0.40
1:D:21:ALA:HB2	1:D:76:LEU:HD12	2.04	0.40
1:D:121:GLN:O	1:D:125:GLN:HG2	2.21	0.40
1:D:132:ILE:O	1:D:135:ILE:HB	2.21	0.40
3:D:2031:HOH:O	2:H:540:THR:CA	2.69	0.40
1:C:129:ARG:HD2	3:C:2133:HOH:O	2.20	0.40
1:D:107:ASP:OD1	1:D:109:THR:HG23	2.20	0.40
1:D:117:ARG:HH11	1:D:189:THR:HG22	1.87	0.40
2:E:519:LYS:O	2:E:523:GLU:HG3	2.21	0.40
1:B:11:ILE:CG2	1:B:190:ILE:HD12	2.45	0.40
3:D:2031:HOH:O	2:H:540:THR:C	2.59	0.40
2:H:532:GLN:HG3	3:H:2014:HOH:O	2.21	0.40
2:H:551:SER:O	2:H:555:GLN:HG3	2.21	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	194/205 (95%)	185 (95%)	8 (4%)	1 (0%)	29	18
1	B	193/205 (94%)	187 (97%)	5 (3%)	1 (0%)	29	18
1	C	193/205 (94%)	190 (98%)	3 (2%)	0	100	100
1	D	191/205 (93%)	167 (87%)	22 (12%)	2 (1%)	15	6
2	E	85/100 (85%)	82 (96%)	3 (4%)	0	100	100
2	F	85/100 (85%)	80 (94%)	5 (6%)	0	100	100
2	G	98/100 (98%)	95 (97%)	2 (2%)	1 (1%)	15	6
2	H	91/100 (91%)	84 (92%)	6 (7%)	1 (1%)	14	5
All	All	1130/1220 (93%)	1070 (95%)	54 (5%)	6 (0%)	29	18

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	10	GLY
1	D	41	GLU
1	D	114	SER
2	G	582	GLY
2	H	490	SER
1	B	115	ALA

### 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	181/189 (96%)	178 (98%)	3 (2%)	60	57
1	B	180/189 (95%)	174 (97%)	6 (3%)	38	31
1	C	180/189 (95%)	174 (97%)	6 (3%)	38	31
1	D	179/189 (95%)	175 (98%)	4 (2%)	52	46
2	E	78/88 (89%)	72 (92%)	6 (8%)	13	5
2	F	78/88 (89%)	72 (92%)	6 (8%)	13	5
2	G	88/88 (100%)	82 (93%)	6 (7%)	16	8
2	H	83/88 (94%)	79 (95%)	4 (5%)	25	18
All	All	1047/1108 (94%)	1006 (96%)	41 (4%)	32	25

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	LEU
1	A	84	LEU
1	A	165	GLU
1	B	54	LEU
1	B	84	LEU
1	B	116	PRO
1	B	146	GLU
1	B	177	ASN
1	B	184	ARG
1	C	11	ILE
1	C	61	LEU
1	C	72	LEU
1	C	81	VAL
1	C	84	LEU
1	C	204	ASN
1	D	51	LEU
1	D	141	PHE
1	D	143	PRO
1	D	194	ASN
2	E	509	GLU
2	E	531	LEU
2	E	544	HIS
2	E	561	HIS
2	E	572	ARG
2	E	578	MET
2	F	493	PHE
2	F	496	GLU

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Mol	Chain	Res	Type
2	F	499	ASP
2	F	502	ARG
2	F	531	LEU
2	F	544	HIS
2	G	535	TYR
2	G	539	ARG
2	G	543	LEU
2	G	544	HIS
2	G	578	MET
2	G	583	THR
2	H	490	SER
2	H	544	HIS
2	H	547	LEU
2	H	556	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	101	GLN
1	B	47	GLN
1	B	177	ASN
1	C	29	ASN
1	D	47	GLN
1	D	66	ASN
1	D	71	GLN
1	D	125	GLN
1	D	134	GLN
1	D	194	ASN
2	E	525	GLN
2	E	563	GLN
2	G	525	GLN
2	G	561	HIS
2	H	525	GLN
2	H	561	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	196/205 (95%)	0.65	25 (12%) 3 3	34, 53, 80, 95	0
1	B	195/205 (95%)	0.54	19 (9%) 7 8	29, 45, 69, 86	0
1	C	195/205 (95%)	0.40	16 (8%) 11 12	21, 33, 61, 87	0
1	D	193/205 (94%)	3.18	117 (60%) 0 0	80, 98, 103, 105	0
2	E	87/100 (87%)	0.92	14 (16%) 1 1	27, 68, 94, 100	0
2	F	87/100 (87%)	1.08	19 (21%) 0 0	30, 69, 100, 104	0
2	G	100/100 (100%)	1.25	20 (20%) 1 0	49, 78, 92, 95	0
2	H	93/100 (93%)	1.58	30 (32%) 0 0	52, 82, 95, 101	0
All	All	1146/1220 (93%)	1.20	260 (22%) 0 0	21, 62, 100, 105	0

All (260) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	114	SER	16.6
1	D	190	ILE	12.6
1	D	120	SER	9.4
1	D	123	ALA	9.2
1	D	44	THR	8.7
1	D	203	VAL	8.7
1	D	141	PHE	8.5
1	D	124	ILE	8.4
2	H	531	LEU	8.3
2	G	584	VAL	7.9
1	D	144	LEU	7.8
2	G	485	SER	7.7
1	D	86	VAL	7.7
1	D	11	ILE	7.6
1	D	112	ASP	7.3
1	D	115	ALA	7.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	113	ASP	6.9
1	D	202	PRO	6.8
1	D	45	ARG	6.8
1	D	119	LYS	6.7
2	F	503	LEU	6.4
1	D	52	THR	6.4
2	E	493	PHE	6.3
2	H	487	ALA	6.3
1	D	189	THR	6.2
1	D	38	TYR	6.2
1	D	129	ARG	6.1
1	D	142	LEU	6.1
1	D	125	GLN	6.0
1	D	183	LEU	6.0
1	D	184	ARG	5.9
2	F	493	PHE	5.7
1	D	47	GLN	5.7
1	D	154	LEU	5.7
1	A	202	PRO	5.6
1	D	138	THR	5.6
2	F	495	ARG	5.6
1	D	137	ALA	5.6
1	D	111	LYS	5.5
1	D	59	LEU	5.5
2	H	488	GLU	5.5
1	D	14	ARG	5.5
1	D	139	VAL	5.5
1	D	57	THR	5.4
1	D	85	VAL	5.4
2	E	494	SER	5.4
1	D	87	VAL	5.4
1	D	116	PRO	5.4
2	G	580	ARG	5.3
1	D	118	GLU	5.3
1	D	131	VAL	5.2
1	D	13	LEU	5.2
1	A	203	VAL	5.1
1	D	100	TRP	5.1
1	D	140	THR	5.1
2	H	547	LEU	5.1
2	H	489	GLN	5.0
1	D	49	TYR	5.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	G	534	ASP	5.0
1	D	53	LEU	5.0
2	F	502	ARG	4.9
2	H	527	GLU	4.9
2	H	555	GLN	4.9
2	G	576	ARG	4.8
1	D	121	GLN	4.7
2	G	527	GLU	4.7
1	D	26	PHE	4.7
1	D	122	LYS	4.6
2	F	499	ASP	4.6
1	D	181	VAL	4.5
1	A	8	GLU	4.5
1	C	204	ASN	4.5
2	F	496	GLU	4.5
1	D	43	PHE	4.5
2	H	568	CYS	4.4
1	D	153	LEU	4.3
1	D	77	TYR	4.3
1	D	41	GLU	4.3
1	D	109	THR	4.3
2	F	498	ALA	4.3
2	F	500	THR	4.3
1	C	114	SER	4.3
1	D	145	LEU	4.1
1	D	62	ILE	4.1
2	H	556	ARG	4.1
1	D	110	ALA	4.1
1	D	73	LYS	4.1
2	H	491	PHE	4.1
1	D	33	TYR	4.0
1	D	188	THR	4.0
2	F	579	GLU	4.0
1	D	28	ILE	4.0
1	D	135	ILE	3.9
1	D	182	ARG	3.9
2	E	498	ALA	3.9
1	D	46	VAL	3.8
1	D	193	VAL	3.8
1	D	92	GLU	3.8
1	D	84	LEU	3.8
1	B	84	LEU	3.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	50	GLY	3.7
1	A	31	ILE	3.7
1	D	102	PHE	3.7
1	D	18	GLU	3.7
2	G	575	LEU	3.7
1	A	114	SER	3.6
1	D	72	LEU	3.6
1	D	23	PHE	3.6
2	H	509	GLU	3.6
1	A	111	LYS	3.6
1	D	146	GLU	3.5
1	D	180	GLU	3.5
2	H	564	LEU	3.5
1	A	9	GLN	3.5
2	H	554	ARG	3.5
1	D	163	VAL	3.4
2	E	514	ARG	3.4
1	D	24	PHE	3.4
1	C	86	VAL	3.4
1	A	160	ASP	3.4
2	H	570	ARG	3.4
2	E	502	ARG	3.4
1	D	19	ILE	3.4
1	D	31	ILE	3.4
1	D	127	GLU	3.3
1	D	199	TYR	3.3
2	H	528	ARG	3.3
1	A	118	GLU	3.3
2	H	558	ARG	3.3
1	D	17	ALA	3.3
2	G	569	GLU	3.2
2	H	552	VAL	3.2
2	E	500	THR	3.2
2	E	578	MET	3.2
1	D	40	SER	3.2
1	A	32	LEU	3.2
2	F	571	LEU	3.1
1	B	104	ILE	3.1
1	D	42	THR	3.1
1	D	105	GLU	3.1
2	G	520	ARG	3.1
2	G	571	LEU	3.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	196	MET	3.1
1	A	72	LEU	3.0
1	C	115	ALA	3.0
1	D	39	PRO	3.0
2	H	538	SER	3.0
2	F	512	ARG	2.9
2	G	572	ARG	2.9
2	F	576	ARG	2.9
1	D	54	LEU	2.9
1	D	107	ASP	2.9
1	B	10	GLY	2.9
2	F	494	SER	2.9
1	B	23	PHE	2.9
1	D	185	SER	2.9
2	E	568	CYS	2.9
2	H	539	ARG	2.8
2	H	572	ARG	2.8
1	A	84	LEU	2.8
2	E	512	ARG	2.8
1	B	20	VAL	2.8
2	F	539	ARG	2.8
1	A	19	ILE	2.8
1	D	37	ILE	2.8
1	A	135	ILE	2.8
1	D	186	PHE	2.8
2	H	514	ARG	2.8
2	H	567	GLU	2.7
1	D	159	LYS	2.7
1	A	112	ASP	2.7
2	G	547	LEU	2.7
2	H	579	GLU	2.7
1	A	115	ALA	2.7
1	D	106	CYS	2.6
1	D	136	THR	2.6
2	F	514	ARG	2.6
1	C	23	PHE	2.6
2	G	486	SER	2.6
1	D	51	LEU	2.6
1	D	108	LYS	2.6
1	D	200	LYS	2.6
1	D	88	ILE	2.5
1	A	110	ALA	2.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	G	514	ARG	2.5
2	G	556	ARG	2.5
1	D	166	LYS	2.5
1	D	162	VAL	2.5
1	B	135	ILE	2.5
1	C	165	GLU	2.5
1	C	31	ILE	2.4
1	C	154	LEU	2.4
1	D	101	GLN	2.4
1	C	76	LEU	2.4
1	B	21	ALA	2.4
1	A	23	PHE	2.4
1	D	27	GLY	2.4
1	C	28	ILE	2.4
2	E	579	GLU	2.4
2	F	507	GLU	2.4
2	F	509	GLU	2.4
1	D	60	GLU	2.4
1	D	191	HIS	2.4
1	B	136	THR	2.4
1	D	104	ILE	2.4
1	C	81	VAL	2.3
1	D	80	SER	2.3
1	D	12	THR	2.3
1	D	160	ASP	2.3
1	B	28	ILE	2.3
2	H	574	LEU	2.3
2	H	521	MET	2.3
2	G	583	THR	2.3
1	C	153	LEU	2.3
2	H	571	LEU	2.3
1	D	55	VAL	2.3
1	D	147	VAL	2.3
1	D	56	THR	2.3
1	C	146	GLU	2.3
1	B	24	PHE	2.3
1	D	130	SER	2.3
2	H	576	ARG	2.3
2	E	564	LEU	2.2
2	G	578	MET	2.2
1	A	86	VAL	2.2
1	C	20	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	84	LEU	2.2
1	D	78	LYS	2.2
1	A	28	ILE	2.2
1	B	85	VAL	2.2
2	G	563	GLN	2.2
1	B	31	ILE	2.2
2	H	551	SER	2.2
1	D	201	ILE	2.1
1	D	97	LEU	2.1
2	F	547	LEU	2.1
1	A	24	PHE	2.1
2	H	559	GLU	2.1
1	A	132	ILE	2.1
1	B	155	ILE	2.1
1	A	165	GLU	2.1
1	A	27	GLY	2.1
1	D	143	PRO	2.1
2	G	517	GLU	2.1
2	E	571	LEU	2.1
1	B	81	VAL	2.1
2	F	572	ARG	2.1
2	E	496	GLU	2.0
1	B	32	LEU	2.0
1	B	153	LEU	2.0
2	G	537	GLN	2.0
1	B	100	TRP	2.0
1	B	114	SER	2.0
1	B	102	PHE	2.0
1	D	171	GLY	2.0
2	E	499	ASP	2.0
1	D	179	GLU	2.0
1	C	88	ILE	2.0
2	H	492	LEU	2.0
1	A	85	VAL	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains

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.