



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:41 PM 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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

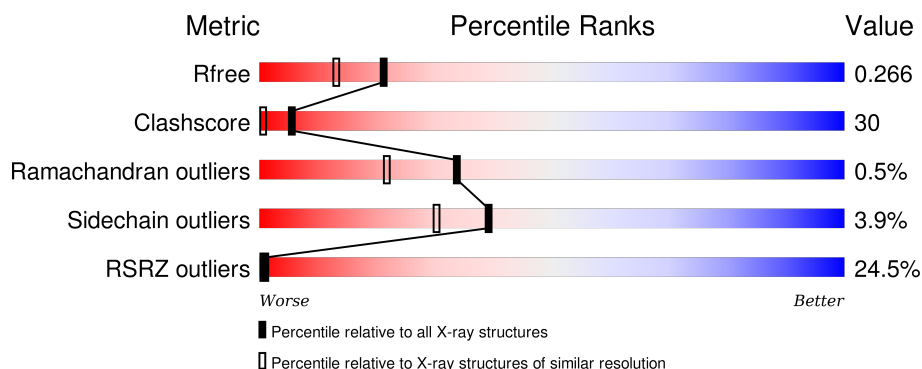
1 Overall quality at a glance ⓘ

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}	91344	1192 (2.04-2.04)
Clashscore	102246	1269 (2.04-2.04)
Ramachandran outliers	100387	1258 (2.04-2.04)
Sidechain outliers	100360	1258 (2.04-2.04)
RSRZ outliers	91569	1194 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	205	<div> <div>13%</div> <div>61%</div> <div>32%</div> <div>• •</div> </div>
1	B	205	<div> <div>10%</div> <div>71%</div> <div>21%</div> <div>• 5%</div> </div>
1	C	205	<div> <div>10%</div> <div>76%</div> <div>17%</div> <div>• • 5%</div> </div>
1	D	205	<div> <div>60%</div> <div>30%</div> <div>60%</div> <div>• • 6%</div> </div>
2	E	100	<div> <div>16%</div> <div>51%</div> <div>34%</div> <div>• • 13%</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	100	<div><div></div><div>22%</div><div>57%</div><div>26%</div><div>•</div><div>13%</div></div>
2	G	100	<div><div></div><div>21%</div><div>51%</div><div>42%</div><div>6%</div><div>•</div></div>
2	H	100	<div><div></div><div>31%</div><div>42%</div><div>47%</div><div>• •</div><div>7%</div></div>

2 Entry composition

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
1	A	196	Total	C	N	O	S	0	0	0
			1578	1014	254	306	4			
1	B	195	Total	C	N	O	S	0	0	0
			1568	1008	253	303	4			
1	C	195	Total	C	N	O	S	0	0	0
			1568	1008	253	303	4			
1	D	193	Total	C	N	O	S	0	0	0
			1556	1002	250	300	4			

There are 4 discrepancies between the modelled and reference sequences:

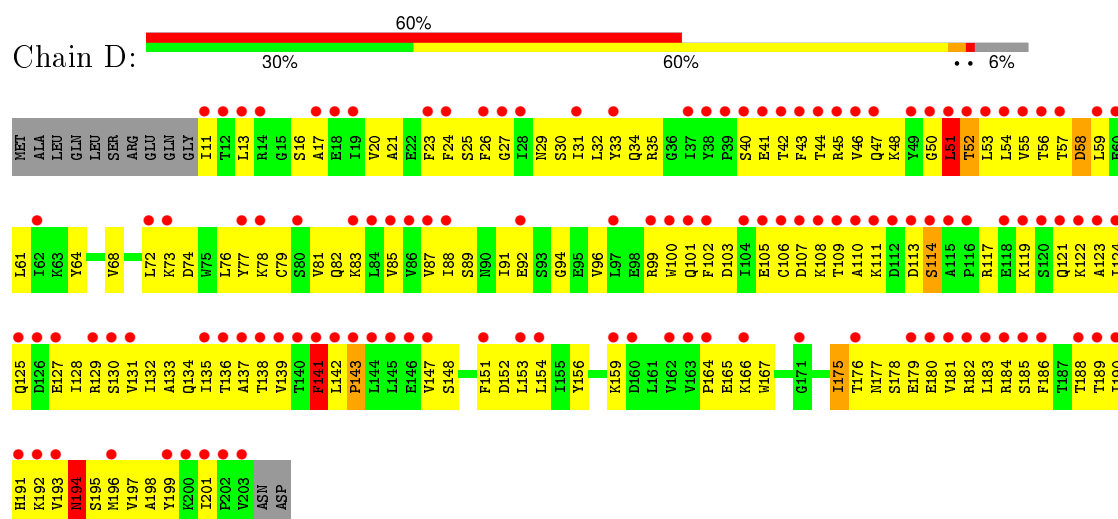
Chain	Residue	Modelled	Actual	Comment	Reference
A	133	ALA	ARG	ENGINEERED MUTATION	UNP Q13257
B	133	ALA	ARG	ENGINEERED MUTATION	UNP Q13257
C	133	ALA	ARG	ENGINEERED MUTATION	UNP Q13257
D	133	ALA	ARG	ENGINEERED MUTATION	UNP Q13257

- Molecule 2 is a protein called MAD1 (MITOTIC ARREST DEFICIENT)-LIKE 1.

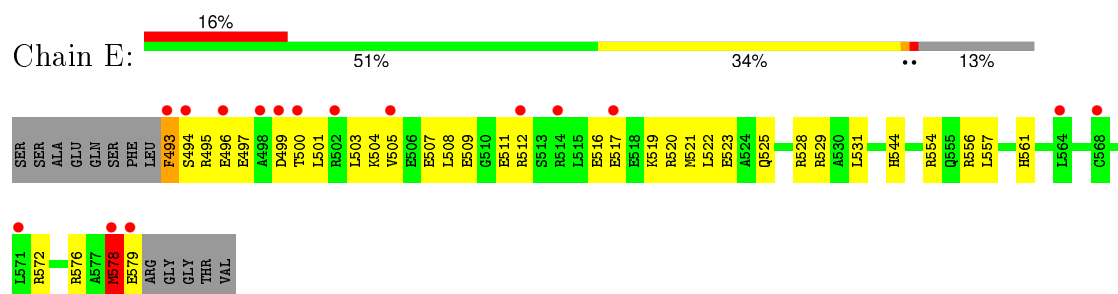
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	87	Total	C	N	O	S	0	0	0
			722	433	143	142	4			
2	F	87	Total	C	N	O	S	0	0	0
			722	433	143	142	4			
2	G	100	Total	C	N	O	S	0	0	0
			816	489	160	163	4			
2	H	93	Total	C	N	O	S	0	0	0
			770	464	150	152	4			

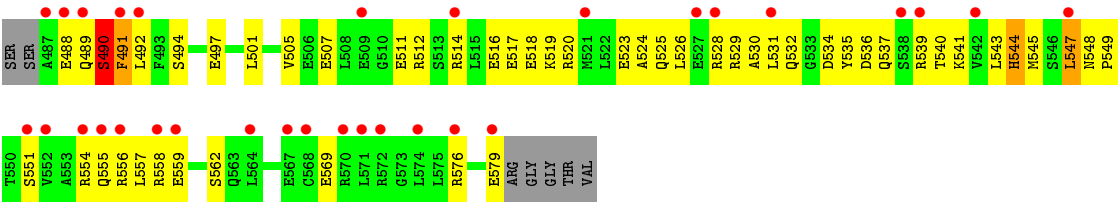
- Molecule 3 is water.

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



• Molecule 2: MAD1 (MITOTIC ARREST DEFICIENT)-LIKE 1





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	2.32 (at 2.04Å)	Xtriage
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%)	DCC
Wilson B-factor (Å ²)	41.5	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 59.3	EDS
Estimated twinning fraction	0.011 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 112653 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9928	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.85	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:CA	1:A:10:GLY:N	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:NH1	2:F:502:ARG:HB2	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
2:G:579:GLU:HA	2:G:584:VAL:OXT	1.61	0.99
1:A:162:VAL:O	1:A:164:PRO:HD3	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:HD22	1:B:177:ASN:H	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:HH11	2:F:502:ARG:HB2	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:G:558:ARG:HD2	3:G:2020:HOH:O	1.76	0.85
2:E:576:ARG:O	2:E:579:GLU:HA	1.74	0.85
1:D:83:LYS:HG2	1:D:103:ASP:HA	1.58	0.85
1:D:11:ILE:HG13	3:D:2041:HOH:O	1.77	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
1:D:136:THR:O	1:D:139:VAL:HG23	1.80	0.81
3:B:2107:HOH:O	2:F:532:GLN:HG2	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:D:141:PHE:HE2	1:D:199:TYR:CZ	2.02	0.74
1:B:11:ILE:HG22	1:B:190:ILE:HD12	1.68	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
2:G:536:ASP:O	3:G:2014:HOH:O	2.07	0.73
1:C:135:ILE:HB	3:C:2137:HOH:O	1.87	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:D:56:THR:HA	3:D:2006:HOH:O	1.89	0.72
1:D:47:GLN:NE2	1:D:52:THR:HG22	2.01	0.72
1:C:100:TRP:CE3	1:C:197:VAL:HG22	2.24	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:D:35:ARG:HH12	1:D:142:LEU:HB2	1.55	0.71
1:B:177:ASN:ND2	1:B:177:ASN:H	1.87	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
2:E:493:PHE:HE2	2:E:496:GLU:HG2	1.57	0.69
1:A:165:GLU:O	1:A:166:LYS:CB	2.40	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
2:E:503:LEU:HD12	3:H:2008:HOH:O	1.90	0.69
1:C:125:GLN:O	1:C:129:ARG:HG3	1.92	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:HD23	2:H:557:LEU:C	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:141:PHE:CD2	1:D:141:PHE:C	2.70	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:493:PHE:CD2	2:E:496:GLU:HB2	2.31	0.65
1:D:119:LYS:HB3	3:D:2041:HOH:O	1.97	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
2:G:505:VAL:O	2:G:509:GLU:HG3	1.97	0.64
1:C:66:ASN:HB2	3:C:2081:HOH:O	1.96	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:131:VAL:HA	3:D:2023:HOH:O	1.98	0.62
1:D:117:ARG:CB	1:D:189:THR:HG21	2.28	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:HH11	2:H:554:ARG:HG3	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
1:D:185:SER:HB3	1:D:194:ASN:HA	1.82	0.61
3:B:2099:HOH:O	1:C:176:THR:HG22	1.99	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:194:ASN:HB3	3:D:2039:HOH:O	2.01	0.59
1:D:164:PRO:HG2	1:D:167:TRP:CG	2.36	0.59
2:H:545:MET:HE3	3:H:2023:HOH:O	2.03	0.59
1:C:11:ILE:H	1:C:11:ILE:HD12	1.67	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:D:178:SER:HB2	3:D:2045:HOH:O	2.02	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
2:F:502:ARG:CZ	2:F:502:ARG:HB2	2.34	0.58
1:D:13:LEU:CD2	1:D:111:LYS:HG2	2.33	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
2:E:500:THR:HG22	3:H:2008:HOH:O	2.03	0.58
1:D:147:VAL:HG22	3:D:2016:HOH:O	2.04	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
2:E:505:VAL:HG23	2:F:505:VAL:HG22	1.87	0.57
2:E:505:VAL:HG22	2:F:505:VAL:CG2	2.35	0.57
1:D:25:SER:O	1:D:29:ASN:ND2	2.36	0.57
2:G:540:THR:N	3:G:2014:HOH:O	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:179:GLU:CD	3:C:2194:HOH:O	2.42	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
2:E:495:ARG:HE	2:H:528:ARG:NH2	2.03	0.56
1:D:122:LYS:HA	3:D:2020:HOH:O	2.04	0.56
2:F:495:ARG:HG2	2:F:495:ARG:O	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:G:578:MET:C	2:G:584:VAL:OXT	2.44	0.55
2:E:556:ARG:HG2	3:E:2047:HOH:O	1.99	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:CD2	2:H:557:LEU:C	2.75	0.55
1:A:15:GLY:O	1:A:19:ILE:HG23	2.06	0.55
1:A:11:ILE:CD1	1:A:119:LYS:HB3	2.35	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
2:E:500:THR:HA	3:H:2008:HOH:O	2.08	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
1:C:45:ARG:HD3	3:C:2048:HOH:O	2.07	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:D:34:GLN:OE1	1:D:136:THR:HG23	2.08	0.53
1:A:99:ARG:HH12	1:A:101:GLN:NE2	2.07	0.53
1:D:79:CYS:HB3	3:D:2019:HOH:O	2.08	0.53
1:D:45:ARG:HG2	1:D:54:LEU:HG	1.91	0.53
1:A:14:ARG:HG3	3:A:2001:HOH:O	2.07	0.53
2:E:494:SER:OG	2:F:495:ARG:HA	2.08	0.53
2:G:542:VAL:C	2:G:543:LEU:HD12	2.29	0.53
2:G:525:GLN:NE2	2:H:526:LEU:HD13	2.24	0.53
1:D:175:ILE:HG21	3:D:2045:HOH:O	2.07	0.53
1:D:99:ARG:HB2	1:D:175:ILE:CD1	2.35	0.53
1:A:83:LYS:HB2	1:A:156:TYR:HB2	1.91	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:175:ILE:CD1	3:D:2045:HOH:O	2.57	0.52
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
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:D:87:VAL:HG21	1:D:154:LEU:HD11	1.91	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:138:THR:OG1	3:D:2029:HOH:O	2.19	0.51
2:E:557:LEU:HD23	2:E:557:LEU:C	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)
2:F:496:GLU:C	2:F:498:ALA:H	2.14	0.50
1:D:34:GLN:OE1	1:D:136:THR:HA	2.12	0.50
2:F:501:LEU:O	2:F:505:VAL:HG23	2.11	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:H:544:HIS:NE2	3:H:2021:HOH:O	2.35	0.50
2:E:495:ARG:NE	2:H:528:ARG:NH2	2.59	0.50
1:B:79:CYS:HA	1:B:106:CYS:SG	2.51	0.50
2:G:574:LEU:O	2:G:578:MET:N	2.44	0.50
1:D:54:LEU:HD12	1:D:54:LEU:N	2.27	0.50
1:B:146:GLU:HG2	3:B:2075:HOH:O	2.11	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:82:GLN:OE1	2:G:540:THR:HG22	2.12	0.49
1:A:78:LYS:HA	1:A:111:LYS:HZ1	1.77	0.49
2:H:488:GLU:O	2:H:491:PHE:HB2	2.12	0.49
2:H:531:LEU:HB2	3:H:2014:HOH:O	2.11	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: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:D:56:THR:HG21	1:D:61:LEU:CD2	2.42	0.49
1:C:50:GLY:HA3	1:C:129:ARG:NH1	2.27	0.49
2:G:559:GLU:O	2:G:563:GLN:HG3	2.12	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:B:119:LYS:HD2	1:B:124:ILE:HG13	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:D:85:VAL:HA	1:D:100:TRP:O	2.12	0.49
2:G:526:LEU:HD23	2:G:526:LEU:O	2.12	0.49
1:A:176:THR:O	1:A:200:LYS:HE2	2.12	0.49
1:D:64:TYR:OH	3:D:2030:HOH:O	2.19	0.49
1:B:184:ARG:HH11	1:B:184:ARG:HG3	1.76	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:D:156:TYR:HD2	2:H:540:THR:HG21	1.78	0.48
1:A:108:LYS:HE2	2:G:539:ARG:HH22	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:D:166:LYS:HB3	2:H:547:LEU:HD21	1.94	0.48
1:C:11:ILE:CD1	1:C:117:ARG:HB2	2.44	0.48
2:G:516:GLU:O	2:G:520:ARG:HG3	2.13	0.48
1:B:12:THR:HG22	1:B:116:PRO:HG3	1.95	0.48
1:D:76:LEU:HD23	1:D:81:VAL:HG11	1.95	0.48
1:D:188:THR:OG1	1:D:189:THR:N	2.46	0.48
1:A:87:VAL:O	1:A:151:PHE:HA	2.14	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:D:83:LYS:HD2	1:D:101:GLN:HG3	1.94	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
2:E:508:LEU:HB3	2:F:508:LEU:HB3	1.96	0.48
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
1:B:33:TYR:CE2	1:B:54:LEU:HD13	2.49	0.47
2:H:519:LYS:O	2:H:523:GLU:HG3	2.14	0.47
2:H:491:PHE:CD2	2:H:491:PHE:N	2.79	0.47
1:D:151:PHE:O	2:H:549:PRO:HB2	2.14	0.47
1:C:36:GLY:HA2	3:C:2035:HOH:O	2.05	0.47
1:A:177:ASN:HA	3:H:2020:HOH:O	2.13	0.47
1:D:23:PHE:HB2	3:D:2007:HOH:O	2.14	0.47
1:A:42:THR:O	1:A:57:THR:HG22	2.14	0.47
1:D:13:LEU:HD22	1:D:111:LYS:HG2	1.95	0.47
1:D:176:THR:CG2	1:D:177:ASN:H	2.27	0.47
1:D:44:THR:HG23	1:D:44:THR:O	2.15	0.47
1:B:143:PRO:HD2	3:B:2017:HOH:O	2.15	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:D:129:ARG:CB	1:D:129:ARG:HH11	2.28	0.47
2:E:499:ASP:OD1	2:H:528:ARG:HD2	2.15	0.47
1:C:203:VAL:HG13	1:C:204:ASN:CG	2.34	0.47
2:H:490:SER:C	2:H:491:PHE:CD2	2.89	0.47
1:C:72:LEU:HD22	1:C:76:LEU:HG	1.97	0.47
1:D:185:SER:N	3:D:2040:HOH:O	2.48	0.47
1:D:20:VAL:HG12	1:D:24:PHE:HE1	1.80	0.47
1:A:99:ARG:HG3	3:A:2049:HOH:O	2.14	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:D:178:SER:CB	3:D:2045:HOH:O	2.62	0.46
1:B:110:ALA:HA	1:B:117:ARG:HH21	1.80	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
2:H:548:ASN:HB2	2:H:549:PRO:HD2	1.98	0.46
1:A:72:LEU:HD22	1:A:76:LEU:HG	1.97	0.46
2:F:568:CYS:O	2:F:572:ARG:HB2	2.15	0.46
1:A:34:GLN:NE2	1:A:136:THR:HA	2.31	0.46
1:A:161:LEU:HD23	1:A:162:VAL:O	2.16	0.46
2:G:543:LEU:N	2:G:543:LEU:CD1	2.77	0.46
2:G:520:ARG:HA	2:G:523:GLU:HG2	1.97	0.46
2:F:499:ASP:O	2:F:503:LEU:HG	2.16	0.46
1:D:16:SER:HA	3:D:2001:HOH:O	2.15	0.46
1:D:117:ARG:HB3	1:D:189:THR:HG21	1.98	0.46
1:D:26:PHE:HB3	1:D:53:LEU:HD13	1.98	0.46
1:A:86:VAL:HB	1:A:100:TRP:HB2	1.97	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
2:H:490:SER:O	2:H:491:PHE:HD2	1.99	0.45
1:A:71:GLN:NE2	1:A:75:TRP:NE1	2.63	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:33:TYR:CE1	1:D:40:SER:CB	3.00	0.45
1:D:26:PHE:CE2	1:D:48:LYS:HG2	2.51	0.45
1:D:175:ILE:HD13	3:D:2045:HOH:O	2.17	0.45
1:D:51:LEU:CD2	1:D:51:LEU:C	2.84	0.45
1:B:167:TRP:CB	3:B:2087:HOH:O	2.65	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:179:GLU:O	1:A:198:ALA:HA	2.17	0.45
2:H:528:ARG:C	3:H:2014:HOH:O	2.55	0.45
1:D:55:VAL:N	3:D:2009:HOH:O	2.49	0.45
1:A:176:THR:HG22	1:A:177:ASN:OD1	2.16	0.45
1:D:64:TYR:HE1	2:H:545:MET:HG3	1.82	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:B:91:ILE:HG22	2:F:557:LEU:CD1	2.47	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:49:TYR:O	1:B:129:ARG:HD2	2.16	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:D:88:ILE:HG12	3:D:2017:HOH:O	2.17	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:117:ARG:HD3	1:D:189:THR:CG2	2.42	0.44
1:B:192:LYS:HE2	1:B:194:ASN:OD1	2.18	0.44
1:A:66:ASN:O	1:A:70:GLU:HG2	2.17	0.44
2:F:493:PHE:HD1	2:F:494:SER:N	2.16	0.44
2:E:497:GLU:O	2:E:501:LEU:HG	2.18	0.44
3:A:2075:HOH:O	2:G:545:MET:CA	2.53	0.44
1:A:13:LEU:HD23	1:A:77:TYR:CE1	2.52	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:D:182:ARG:HH21	2:H:531:LEU:HD21	1.82	0.43
1:D:92:GLU:OE2	1:D:92:GLU:N	2.50	0.43
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: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
2:G:502:ARG:NH2	2:H:497:GLU:OE2	2.51	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:H:524:ALA:HB2	3:H:2008:HOH:O	2.17	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:535:TYR:CD1	2:H:540:THR:HB	2.54	0.43
1:B:181:VAL:HG21	2:G:492:LEU:HD13	1.99	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:H:528:ARG:O	2:H:528:ARG:CG	2.67	0.43
2:G:575:LEU:HA	2:G:575:LEU:HD23	1.88	0.43
2:H:535:TYR:HD1	2:H:540:THR:HB	1.83	0.43
1:D:74:ASP:OD1	1:D:78:LYS:HE3	2.18	0.43
1:D:196:MET:CE	2:H:531:LEU:HD22	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:66:ASN:CB	3:C:2081:HOH:O	2.62	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
1:B:162:VAL:HG23	3:B:2084:HOH:O	2.19	0.43
2:G:502:ARG:HB2	2:G:502:ARG:HE	1.54	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
1:D:30:SER:C	1:D:34:GLN:HG2	2.38	0.42
2:F:504:LYS:O	2:F:508:LEU:HD23	2.19	0.42
1:D:134:GLN:HB3	1:D:183:LEU:HD13	2.01	0.42
1:C:100:TRP:CD2	1:C:197:VAL:HG22	2.54	0.42
2:H:554:ARG:NH1	2:H:554:ARG:HG3	2.32	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
1:B:35:ARG:HD2	1:B:35:ARG:HA	1.81	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: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:D:128:ILE:HG21	3:D:2007:HOH:O	2.19	0.42
1:D:117:ARG:CG	1:D:189:THR:HG21	2.48	0.42
1:B:146:GLU:HG2	1:B:146:GLU:H	1.63	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:136:THR:O	1:D:139:VAL:CG2	2.61	0.42
2:E:579:GLU:OE1	2:E:579:GLU:HA	2.20	0.42
1:D:13:LEU:HG	1:D:77:TYR:CD1	2.55	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
2:E:505:VAL:HG23	2:F:505:VAL:CG2	2.48	0.41
1:D:117:ARG:HD2	1:D:189:THR:HG22	1.92	0.41
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:C:145:LEU:HA	1:C:145:LEU:HD23	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:D:53:LEU:C	1:D:54:LEU:HD12	2.40	0.41
1:A:115:ALA:HB1	1:A:116:PRO:HD2	2.02	0.41
1:D:193:VAL:C	1:D:194:ASN:HD22	2.24	0.41
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:517:GLU:CA	2:E:520:ARG:HH21	2.33	0.41
1:B:84:LEU:HD22	1:B:155:ILE:HD13	2.01	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:HB3	2:E:578:MET:HE2	1.81	0.41
1:D:50:GLY:C	1:D:51:LEU:HD13	2.40	0.41
2:H:489:GLN:O	2:H:491:PHE:N	2.54	0.41
1:C:11:ILE:HG12	1:C:124:ILE:HD11	2.03	0.41
1:D:102:PHE:N	1:D:102:PHE:CD1	2.89	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:B:194:ASN:HB3	3:B:2115:HOH:O	2.21	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
2:G:578:MET:HG3	2:G:583:THR:CG2	2.51	0.41
1:D:179:GLU:HG3	1:D:201:ILE:HG12	2.02	0.40
1:D:82:GLN:O	1:D:83:LYS:HG3	2.21	0.40
2:E:517:GLU:HA	2:E:520:ARG:NH2	2.36	0.40
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
2:G:488:GLU:N	2:G:488:GLU:CD	2.74	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:D:21:ALA:HB2	1:D:76:LEU:HD12	2.04	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:121:GLN:O	1:D:125:GLN:HG2	2.21	0.40
1:D:117:ARG:HH11	1:D:189:THR:HG22	1.87	0.40
1:C:129:ARG:HD2	3:C:2133:HOH:O	2.20	0.40
2:E:519:LYS:O	2:E:523:GLU:HG3	2.21	0.40
1:D:107:ASP:OD1	1:D:109:THR:HG23	2.20	0.40
2:H:532:GLN:HG3	3:H:2014:HOH:O	2.21	0.40
3:D:2031:HOH:O	2:H:540:THR:C	2.59	0.40
2:H:551:SER:O	2:H:555:GLN:HG3	2.21	0.40
1:B:11:ILE:CG2	1:B:190:ILE:HD12	2.45	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%)	34	22
1	B	193/205 (94%)	187 (97%)	5 (3%)	1 (0%)	34	22
1	C	193/205 (94%)	190 (98%)	3 (2%)	0	100	100
1	D	191/205 (93%)	167 (87%)	22 (12%)	2 (1%)	19	8
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%)	19	8
2	H	91/100 (91%)	84 (92%)	6 (7%)	1 (1%)	17	7
All	All	1130/1220 (93%)	1070 (95%)	54 (5%)	6 (0%)	34	22

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%)	68	65
1	B	180/189 (95%)	174 (97%)	6 (3%)	45	37
1	C	180/189 (95%)	174 (97%)	6 (3%)	45	37
1	D	179/189 (95%)	175 (98%)	4 (2%)	60	53
2	E	78/88 (89%)	72 (92%)	6 (8%)	16	7
2	F	78/88 (89%)	72 (92%)	6 (8%)	16	7
2	G	88/88 (100%)	82 (93%)	6 (7%)	20	11
2	H	83/88 (94%)	79 (95%)	4 (5%)	31	22
All	All	1047/1108 (94%)	1006 (96%)	41 (4%)	39	30

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

Some 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 ⓘ

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	196/205 (95%)	0.73	27 (13%) 4 4	34, 53, 80, 95	0
1	B	195/205 (95%)	0.62	20 (10%) 9 9	29, 45, 69, 86	0
1	C	195/205 (95%)	0.48	20 (10%) 9 9	21, 33, 61, 87	0
1	D	193/205 (94%)	3.35	124 (64%) 0 0	80, 98, 103, 105	0
2	E	87/100 (87%)	1.00	16 (18%) 2 2	27, 68, 94, 100	0
2	F	87/100 (87%)	1.17	22 (25%) 1 0	30, 69, 100, 104	0
2	G	100/100 (100%)	1.34	21 (21%) 1 1	49, 78, 92, 95	0
2	H	93/100 (93%)	1.68	31 (33%) 0 0	52, 82, 95, 101	0
All	All	1146/1220 (93%)	1.29	281 (24%) 1 1	21, 62, 100, 105	0

All (281) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	114	SER	17.0
1	D	190	ILE	13.4
1	D	120	SER	9.8
1	D	123	ALA	9.7
1	D	203	VAL	9.2
1	D	44	THR	9.0
1	D	141	PHE	8.9
1	D	124	ILE	8.8
2	H	531	LEU	8.7
2	G	584	VAL	8.3
1	D	144	LEU	8.2
1	D	86	VAL	8.1
1	D	11	ILE	8.0
2	G	485	SER	7.9
1	D	112	ASP	7.5
1	D	115	ALA	7.5

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Mol	Chain	Res	Type	RSRZ
1	D	113	ASP	7.2
1	D	202	PRO	7.1
1	D	45	ARG	7.0
1	D	119	LYS	6.7
2	F	503	LEU	6.6
1	D	52	THR	6.6
2	E	493	PHE	6.6
2	H	487	ALA	6.6
1	D	38	TYR	6.4
1	D	142	LEU	6.4
1	D	183	LEU	6.4
1	D	189	THR	6.3
1	D	129	ARG	6.3
1	D	125	GLN	6.2
1	D	184	ARG	6.1
2	F	493	PHE	6.0
1	D	47	GLN	6.0
1	D	154	LEU	5.9
1	D	137	ALA	5.9
1	D	139	VAL	5.9
1	D	59	LEU	5.8
1	D	111	LYS	5.8
1	A	202	PRO	5.8
1	D	138	THR	5.8
2	F	495	ARG	5.8
1	D	85	VAL	5.7
1	D	87	VAL	5.7
2	H	488	GLU	5.7
2	E	494	SER	5.7
1	D	116	PRO	5.6
1	D	14	ARG	5.6
2	G	580	ARG	5.6
1	D	131	VAL	5.6
1	D	57	THR	5.5
1	D	118	GLU	5.5
1	A	203	VAL	5.5
1	D	100	TRP	5.4
1	D	13	LEU	5.3
1	D	49	TYR	5.3
1	D	140	THR	5.2
2	H	489	GLN	5.2
1	D	53	LEU	5.2

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Mol	Chain	Res	Type	RSRZ
2	H	547	LEU	5.2
2	G	534	ASP	5.2
2	H	527	GLU	5.1
2	F	502	ARG	5.1
2	H	555	GLN	5.0
1	D	26	PHE	4.9
2	G	576	ARG	4.9
1	D	121	GLN	4.9
2	G	527	GLU	4.9
1	D	122	LYS	4.8
1	D	181	VAL	4.8
2	F	499	ASP	4.8
1	C	204	ASN	4.7
1	A	8	GLU	4.7
1	D	43	PHE	4.7
2	F	496	GLU	4.6
1	D	153	LEU	4.6
2	F	498	ALA	4.6
2	H	568	CYS	4.6
2	F	500	THR	4.6
1	D	109	THR	4.5
1	D	77	TYR	4.5
1	D	41	GLU	4.5
1	D	110	ALA	4.5
1	C	114	SER	4.4
1	D	62	ILE	4.4
1	D	145	LEU	4.3
2	H	491	PHE	4.3
2	H	556	ARG	4.3
1	D	188	THR	4.2
1	D	73	LYS	4.2
1	D	33	TYR	4.2
1	D	28	ILE	4.2
2	E	498	ALA	4.1
2	F	579	GLU	4.1
1	D	135	ILE	4.1
1	D	193	VAL	4.1
1	D	46	VAL	4.1
1	D	182	ARG	4.0
1	A	31	ILE	4.0
1	D	84	LEU	3.9
1	D	92	GLU	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	50	GLY	3.9
1	B	84	LEU	3.9
2	G	575	LEU	3.9
1	A	114	SER	3.8
1	D	72	LEU	3.8
1	D	102	PHE	3.8
1	D	23	PHE	3.8
1	D	18	GLU	3.7
2	H	564	LEU	3.7
1	A	111	LYS	3.7
2	H	509	GLU	3.7
1	D	146	GLU	3.7
1	C	86	VAL	3.6
1	D	163	VAL	3.6
1	D	31	ILE	3.6
1	D	180	GLU	3.6
2	H	554	ARG	3.6
1	A	9	GLN	3.6
1	A	160	ASP	3.6
1	D	24	PHE	3.5
1	D	19	ILE	3.5
1	D	127	GLU	3.5
2	H	552	VAL	3.5
1	D	199	TYR	3.5
2	E	502	ARG	3.5
2	E	514	ARG	3.5
2	H	570	ARG	3.5
1	D	17	ALA	3.4
2	H	528	ARG	3.4
2	H	558	ARG	3.4
1	A	118	GLU	3.4
2	G	569	GLU	3.4
1	A	32	LEU	3.3
1	B	104	ILE	3.3
2	F	571	LEU	3.3
1	D	40	SER	3.3
2	G	571	LEU	3.3
2	E	500	THR	3.3
1	A	72	LEU	3.3
2	E	578	MET	3.3
1	D	39	PRO	3.2
1	D	42	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	196	MET	3.2
1	D	54	LEU	3.2
1	C	115	ALA	3.2
1	D	105	GLU	3.2
2	G	520	ARG	3.2
2	H	538	SER	3.1
2	G	572	ARG	3.1
2	F	512	ARG	3.1
2	F	576	ARG	3.1
1	B	20	VAL	3.1
1	D	107	ASP	3.1
1	D	185	SER	3.0
1	A	19	ILE	3.0
1	B	23	PHE	3.0
2	F	494	SER	3.0
1	A	84	LEU	3.0
2	E	568	CYS	3.0
1	B	10	GLY	3.0
2	H	539	ARG	2.9
1	D	186	PHE	2.9
2	H	572	ARG	2.9
1	A	135	ILE	2.9
2	F	539	ARG	2.9
2	E	512	ARG	2.9
2	H	514	ARG	2.9
1	D	37	ILE	2.9
2	G	547	LEU	2.9
1	D	106	CYS	2.8
1	A	112	ASP	2.8
1	D	159	LYS	2.8
1	D	136	THR	2.8
2	H	579	GLU	2.8
1	A	115	ALA	2.8
1	D	108	LYS	2.8
2	H	567	GLU	2.8
1	C	23	PHE	2.8
2	G	486	SER	2.7
1	D	51	LEU	2.7
2	F	514	ARG	2.7
1	D	162	VAL	2.7
1	D	88	ILE	2.7
1	B	135	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	110	ALA	2.6
2	G	556	ARG	2.6
1	C	31	ILE	2.6
1	C	154	LEU	2.6
1	D	200	LYS	2.6
2	G	514	ARG	2.6
1	A	23	PHE	2.6
1	C	28	ILE	2.6
1	C	165	GLU	2.6
1	D	166	LYS	2.5
1	D	27	GLY	2.5
1	B	21	ALA	2.5
1	C	76	LEU	2.5
1	D	104	ILE	2.5
1	B	28	ILE	2.5
1	C	81	VAL	2.5
1	D	101	GLN	2.5
2	H	571	LEU	2.5
1	D	60	GLU	2.5
1	B	136	THR	2.5
2	F	507	GLU	2.5
2	F	509	GLU	2.5
1	D	55	VAL	2.5
2	E	579	GLU	2.5
1	C	153	LEU	2.5
1	A	86	VAL	2.5
1	D	147	VAL	2.5
1	D	160	ASP	2.4
2	H	574	LEU	2.4
1	C	20	VAL	2.4
2	G	583	THR	2.4
1	D	80	SER	2.4
1	D	191	HIS	2.4
1	B	24	PHE	2.4
1	D	12	THR	2.4
1	D	56	THR	2.4
1	A	28	ILE	2.4
1	B	31	ILE	2.4
1	D	130	SER	2.4
2	E	564	LEU	2.4
1	B	85	VAL	2.4
1	C	84	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
2	H	576	ARG	2.3
1	D	78	LYS	2.3
2	G	578	MET	2.3
2	H	521	MET	2.3
1	C	146	GLU	2.3
2	H	551	SER	2.3
2	F	547	LEU	2.3
1	A	132	ILE	2.3
2	G	563	GLN	2.3
1	D	201	ILE	2.3
1	D	97	LEU	2.3
1	A	24	PHE	2.3
1	B	155	ILE	2.3
2	E	571	LEU	2.3
1	B	81	VAL	2.2
1	A	27	GLY	2.2
2	H	559	GLU	2.2
1	B	32	LEU	2.2
1	D	143	PRO	2.2
1	B	102	PHE	2.2
2	H	542	VAL	2.2
1	C	88	ILE	2.2
1	B	153	LEU	2.2
1	B	100	TRP	2.2
1	B	114	SER	2.2
2	E	499	ASP	2.2
1	A	85	VAL	2.2
1	C	87	VAL	2.2
2	F	572	ARG	2.1
2	F	575	LEU	2.1
2	G	517	GLU	2.1
1	A	100	TRP	2.1
1	C	102	PHE	2.1
1	D	151	PHE	2.1
1	A	165	GLU	2.1
2	H	492	LEU	2.1
2	G	537	GLN	2.1
1	D	171	GLY	2.1
1	D	83	LYS	2.1
1	D	164	PRO	2.1
2	E	505	VAL	2.1
1	D	179	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
2	E	496	GLU	2.1
2	F	569	GLU	2.1
1	C	24	PHE	2.1
1	C	118	GLU	2.0
2	E	517	GLU	2.0
1	D	99	ARG	2.0
2	G	581	GLY	2.0
1	A	30	SER	2.0
1	D	126	ASP	2.0
1	D	192	LYS	2.0
1	B	57	THR	2.0
1	D	176	THR	2.0
2	F	563	GLN	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.