



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 06:52 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 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/ValidationPDFNotes.html>

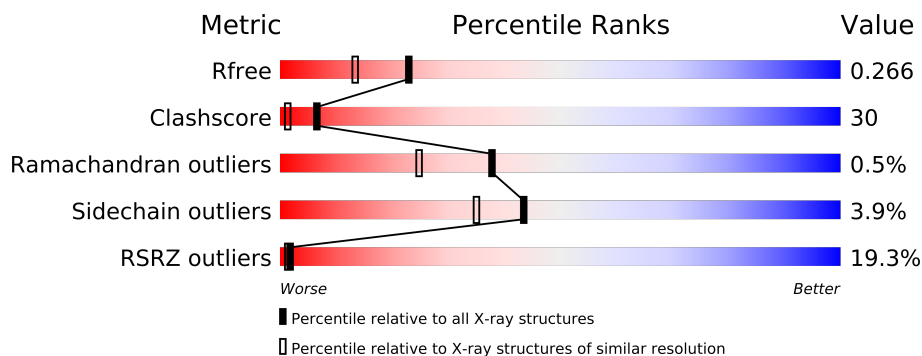
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	1380 (2.06-2.02)
Clashscore	79885	1577 (2.06-2.02)
Ramachandran outliers	78287	1565 (2.06-2.02)
Sidechain outliers	78261	1565 (2.06-2.02)
RSRZ outliers	66119	1381 (2.06-2.02)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	205	
1	B	205	
1	C	205	
1	D	205	
2	E	100	
2	F	100	
2	G	100	
2	H	100	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9928 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

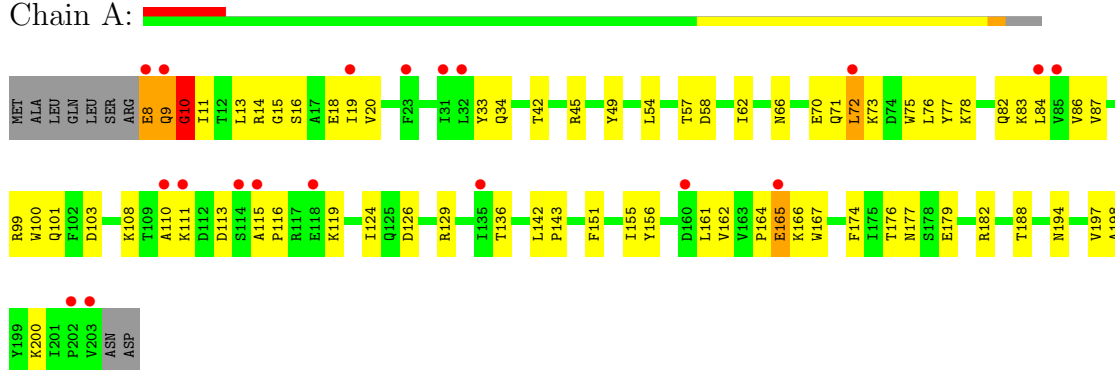
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	88	Total 88	O 88	0	0
3	B	124	Total 124	O 124	0	0
3	C	225	Total 225	O 225	0	0
3	D	45	Total 45	O 45	0	0
3	E	56	Total 56	O 56	0	0
3	F	35	Total 35	O 35	0	0
3	G	24	Total 24	O 24	0	0
3	H	31	Total 31	O 31	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

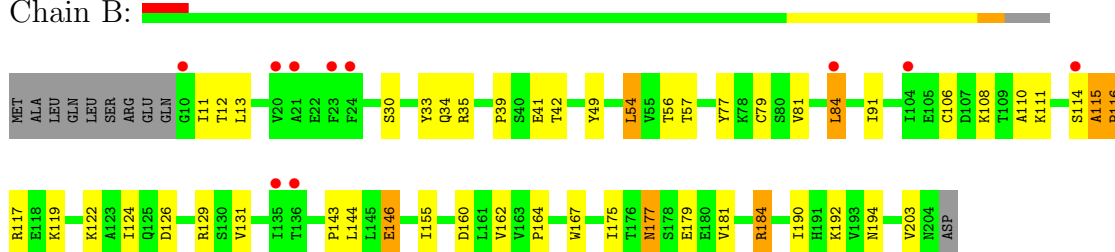
• Molecule 1: MITOTIC SPINDLE ASSEMBLY CHECKPOINT PROTEIN MAD2A

Chain A:



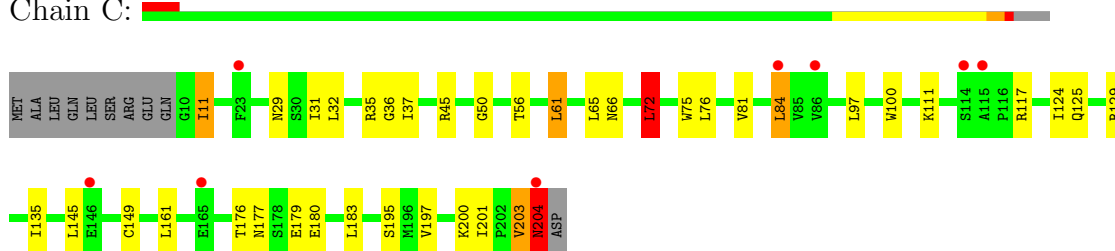
• Molecule 1: MITOTIC SPINDLE ASSEMBLY CHECKPOINT PROTEIN MAD2A

Chain B:



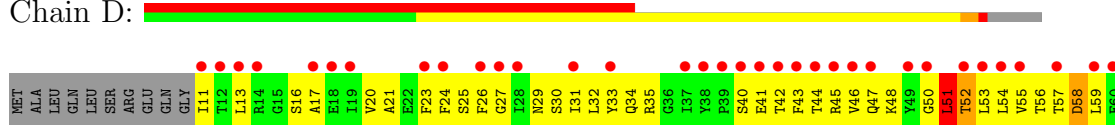
• Molecule 1: MITOTIC SPINDLE ASSEMBLY CHECKPOINT PROTEIN MAD2A

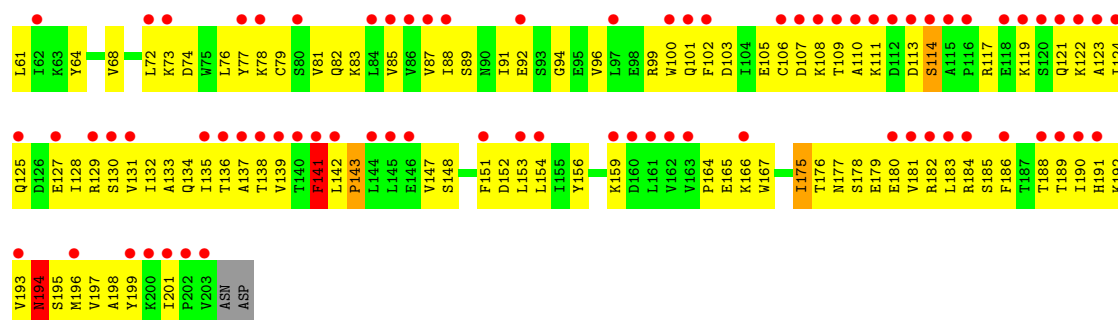
Chain C:



• Molecule 1: MITOTIC SPINDLE ASSEMBLY CHECKPOINT PROTEIN MAD2A

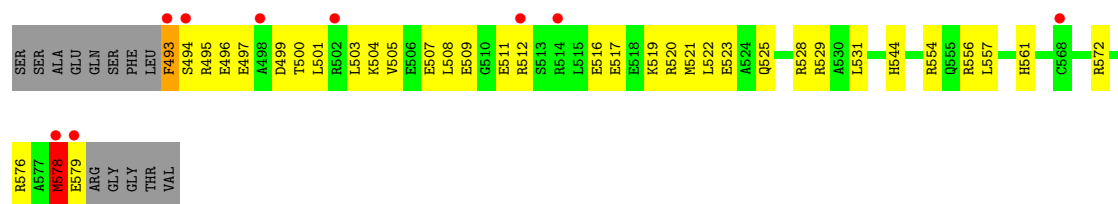
Chain D:





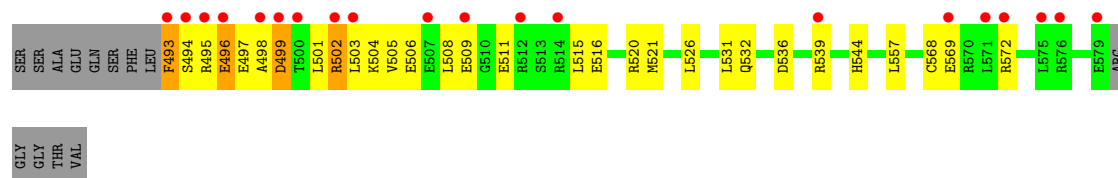
• Molecule 2: MAD1 (MITOTIC ARREST DEFICIENT)-LIKE 1

Chain E:



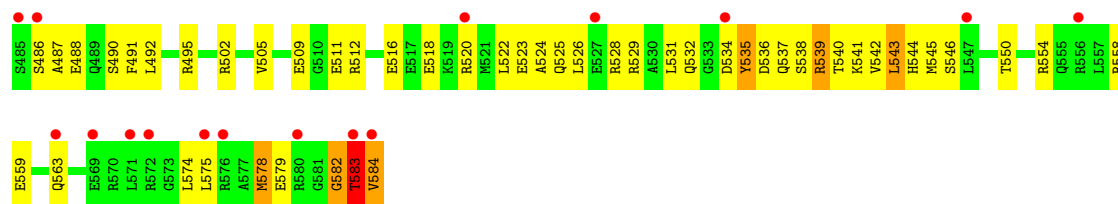
• Molecule 2: MAD1 (MITOTIC ARREST DEFICIENT)-LIKE 1

Chain F:



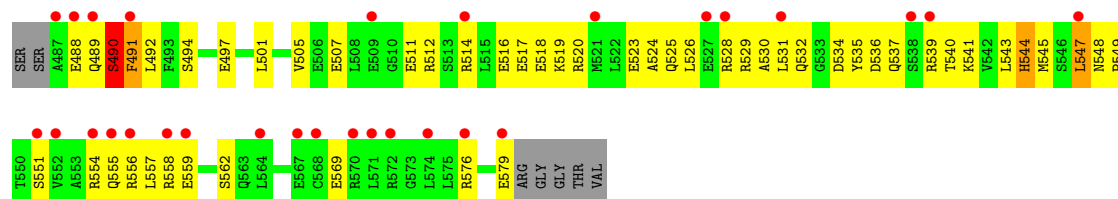
• Molecule 2: MAD1 (MITOTIC ARREST DEFICIENT)-LIKE 1

Chain G:



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

Chain H:



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)	0.36 , 54.8	EDS
Estimated twinning fraction	0.011 for h,-k,-h-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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.

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	770	0	766	79	0
3	A	88	0	0	12	0
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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 30.

All (553) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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	Distance(Å)	Clash(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
1:A:162:VAL:O	1:A:164:PRO:CD	2.29	0.81

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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

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	194/205 (95%)	185 (95%)	8 (4%)	1 (0%)	38	25
1	B	193/205 (94%)	187 (97%)	5 (3%)	1 (0%)	38	25
1	C	193/205 (94%)	190 (98%)	3 (2%)	0	100	100
1	D	191/205 (93%)	167 (87%)	22 (12%)	2 (1%)	22	9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	22	9
2	H	91/100 (91%)	84 (92%)	6 (7%)	1 (1%)	21	8
All	All	1130/1220 (93%)	1070 (95%)	54 (5%)	6 (0%)	38	25

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 ⓘ

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%)	73	71
1	B	180/189 (95%)	174 (97%)	6 (3%)	50	42
1	C	180/189 (95%)	174 (97%)	6 (3%)	50	42
1	D	179/189 (95%)	175 (98%)	4 (2%)	64	60
2	E	78/88 (89%)	72 (92%)	6 (8%)	18	9
2	F	78/88 (89%)	72 (92%)	6 (8%)	18	9
2	G	88/88 (100%)	82 (93%)	6 (7%)	22	13
2	H	83/88 (94%)	79 (95%)	4 (5%)	35	25
All	All	1047/1108 (94%)	1006 (96%)	41 (4%)	43	35

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
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 chains 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	196/205 (95%)	0.59	19 (9%) 8 7	34, 53, 80, 95	0
1	B	195/205 (95%)	0.45	10 (5%) 27 25	29, 45, 69, 86	0
1	C	195/205 (95%)	0.26	8 (4%) 35 34	21, 33, 61, 87	0
1	D	193/205 (94%)	2.87	110 (56%) 0 0	80, 98, 103, 105	0
2	E	87/100 (87%)	0.80	9 (10%) 7 6	27, 68, 94, 100	0
2	F	87/100 (87%)	0.96	20 (22%) 1 1	30, 69, 100, 104	0
2	G	100/100 (100%)	1.15	16 (16%) 3 2	49, 78, 92, 95	0
2	H	93/100 (93%)	1.47	29 (31%) 1 0	52, 82, 95, 101	0
All	All	1146/1220 (93%)	1.06	221 (19%) 2 1	21, 62, 100, 105	0

All (221) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	114	SER	14.5
1	D	190	ILE	12.3
1	D	120	SER	8.4
1	D	123	ALA	8.4
1	D	203	VAL	8.3
1	D	124	ILE	8.0
2	G	485	SER	7.8
1	D	144	LEU	7.6
2	G	584	VAL	7.4
1	D	45	ARG	7.3
2	H	531	LEU	7.2
1	D	44	THR	7.2
1	D	119	LYS	7.2
1	D	13	LEU	7.1
1	D	11	ILE	7.0
1	D	86	VAL	6.6

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Mol	Chain	Res	Type	RSRZ
1	D	112	ASP	6.5
1	D	202	PRO	6.5
1	D	141	PHE	6.5
1	D	115	ALA	6.4
1	D	113	ASP	6.3
1	D	57	THR	6.1
1	D	52	THR	6.1
1	D	53	LEU	6.0
1	D	118	GLU	5.7
1	D	183	LEU	5.6
2	E	493	PHE	5.5
1	D	38	TYR	5.5
1	D	125	GLN	5.5
2	F	503	LEU	5.5
2	H	487	ALA	5.4
2	F	493	PHE	5.3
1	D	116	PRO	5.3
2	H	547	LEU	5.3
1	D	47	GLN	5.2
2	E	494	SER	5.2
1	D	129	ARG	5.2
1	D	189	THR	5.1
1	D	59	LEU	5.1
1	D	85	VAL	5.1
1	D	138	THR	5.0
2	H	488	GLU	5.0
2	G	534	ASP	4.9
1	D	121	GLN	4.8
2	F	495	ARG	4.8
1	D	140	THR	4.8
2	G	580	ARG	4.8
1	D	139	VAL	4.8
1	D	26	PHE	4.7
1	D	14	ARG	4.7
1	D	142	LEU	4.7
1	D	87	VAL	4.7
1	A	202	PRO	4.6
1	D	184	ARG	4.6
1	D	154	LEU	4.5
2	G	576	ARG	4.5
1	A	203	VAL	4.5
1	D	131	VAL	4.5

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Mol	Chain	Res	Type	RSRZ
1	D	111	LYS	4.5
2	G	527	GLU	4.4
1	D	100	TRP	4.4
1	D	137	ALA	4.4
2	H	489	GLN	4.3
1	C	204	ASN	4.3
2	H	555	GLN	4.2
1	D	43	PHE	4.2
1	D	49	TYR	4.2
1	D	122	LYS	4.0
1	D	33	TYR	4.0
1	D	92	GLU	4.0
2	F	496	GLU	4.0
2	H	568	CYS	4.0
2	H	527	GLU	4.0
1	A	8	GLU	3.9
1	D	62	ILE	3.8
1	D	153	LEU	3.8
2	F	502	ARG	3.8
2	F	499	ASP	3.8
2	H	556	ARG	3.8
1	D	73	LYS	3.8
1	C	114	SER	3.8
1	D	182	ARG	3.8
1	D	41	GLU	3.7
1	A	114	SER	3.7
1	D	77	TYR	3.7
1	D	46	VAL	3.6
2	H	491	PHE	3.6
1	A	31	ILE	3.6
2	F	512	ARG	3.6
2	E	498	ALA	3.6
1	B	84	LEU	3.6
1	D	180	GLU	3.5
1	D	12	THR	3.5
2	F	579	GLU	3.4
2	H	554	ARG	3.4
2	F	498	ALA	3.4
1	D	109	THR	3.3
1	D	188	THR	3.3
2	H	570	ARG	3.3
1	D	181	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	9	GLN	3.3
2	H	564	LEU	3.3
1	A	118	GLU	3.3
1	D	23	PHE	3.3
2	G	572	ARG	3.2
1	D	193	VAL	3.2
1	D	110	ALA	3.2
2	G	575	LEU	3.2
1	D	84	LEU	3.2
1	D	163	VAL	3.2
1	D	42	THR	3.2
1	D	135	ILE	3.1
2	F	500	THR	3.1
2	H	558	ARG	3.1
2	H	572	ARG	3.1
1	D	24	PHE	3.1
1	D	145	LEU	3.1
1	D	50	GLY	3.1
1	A	19	ILE	3.1
1	A	111	LYS	3.1
2	H	567	GLU	3.0
1	D	196	MET	3.0
2	H	514	ARG	3.0
1	D	166	LYS	2.9
1	C	86	VAL	2.9
2	H	509	GLU	2.9
1	A	160	ASP	2.9
1	D	31	ILE	2.9
1	D	159	LYS	2.9
1	D	199	TYR	2.9
1	D	28	ILE	2.8
1	D	107	ASP	2.8
1	A	115	ALA	2.8
1	D	39	PRO	2.8
1	D	72	LEU	2.8
2	E	514	ARG	2.8
1	D	146	GLU	2.8
2	E	502	ARG	2.8
1	D	54	LEU	2.8
1	D	136	THR	2.8
2	H	528	ARG	2.8
2	G	569	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
2	G	571	LEU	2.8
1	B	104	ILE	2.8
2	F	494	SER	2.7
2	F	576	ARG	2.7
1	B	10	GLY	2.7
2	F	539	ARG	2.7
2	G	520	ARG	2.7
2	F	571	LEU	2.7
1	D	102	PHE	2.7
1	A	84	LEU	2.7
1	D	18	GLU	2.7
1	A	110	ALA	2.7
2	H	579	GLU	2.7
1	A	32	LEU	2.6
1	D	19	ILE	2.6
2	H	539	ARG	2.6
1	A	135	ILE	2.6
1	A	165	GLU	2.6
2	H	552	VAL	2.6
1	A	72	LEU	2.5
1	D	108	LYS	2.5
1	D	191	HIS	2.5
2	F	507	GLU	2.5
1	D	127	GLU	2.5
1	D	162	VAL	2.5
1	D	97	LEU	2.4
2	E	578	MET	2.4
1	C	165	GLU	2.4
2	F	514	ARG	2.4
1	D	17	ALA	2.4
1	D	37	ILE	2.4
1	D	160	ASP	2.4
2	F	509	GLU	2.4
1	D	40	SER	2.4
1	D	201	ILE	2.4
2	G	547	LEU	2.3
1	B	23	PHE	2.3
1	D	101	GLN	2.3
1	D	60	GLU	2.3
1	A	23	PHE	2.3
2	F	572	ARG	2.3
1	D	130	SER	2.3

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Mol	Chain	Res	Type	RSRZ
2	H	538	SER	2.3
2	E	568	CYS	2.3
1	B	20	VAL	2.3
2	H	521	MET	2.3
2	G	556	ARG	2.3
2	H	559	GLU	2.3
1	D	80	SER	2.2
1	C	115	ALA	2.2
1	D	88	ILE	2.2
1	D	78	LYS	2.2
1	B	24	PHE	2.2
1	B	21	ALA	2.2
1	D	27	GLY	2.2
1	D	200	LYS	2.2
2	E	512	ARG	2.2
2	H	576	ARG	2.2
1	B	114	SER	2.2
2	H	551	SER	2.2
2	H	571	LEU	2.2
2	H	574	LEU	2.1
2	G	583	THR	2.1
1	D	161	LEU	2.1
1	C	23	PHE	2.1
2	G	563	GLN	2.1
1	D	55	VAL	2.1
2	F	569	GLU	2.1
1	B	136	THR	2.1
1	D	186	PHE	2.1
2	G	486	SER	2.1
1	C	84	LEU	2.1
1	C	146	GLU	2.0
1	B	135	ILE	2.0
1	D	106	CYS	2.0
1	A	85	VAL	2.0
1	D	151	PHE	2.0
2	E	579	GLU	2.0
2	F	575	LEU	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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.