



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 07:11 PM UTC

PDB ID : 1GO4 / pdb_00001go4
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

<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>.

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

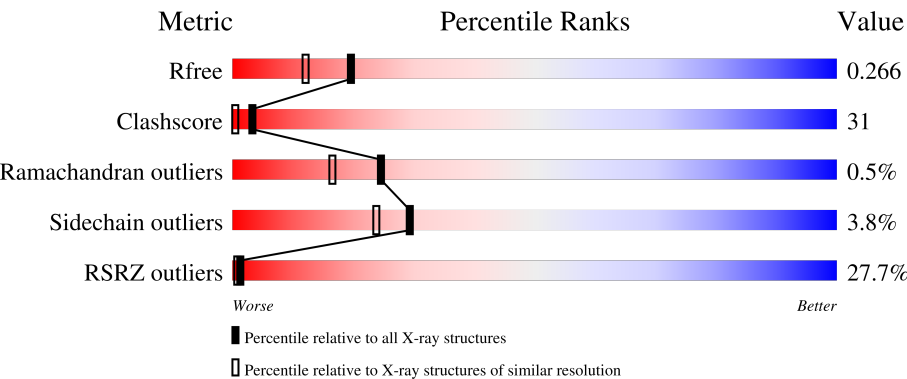
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.05 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}	180053	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (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 ≥ 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	12% 59% 33% ..
1	B	205	9% 68% 22% 5%
1	C	205	3% 70% 21% 5%
1	D	205	64% 28% 61% 5% 6%
2	E	100	26% 49% 35% .. 13%

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Mol	Chain	Length	Quality of chain
2	F	100	24% 57% 27% • 13%
2	G	100	40% 49% 43% 7% •
2	H	100	47% 40% 48% • • 7%

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 Mitotic spindle assembly checkpoint protein MAD1.

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			

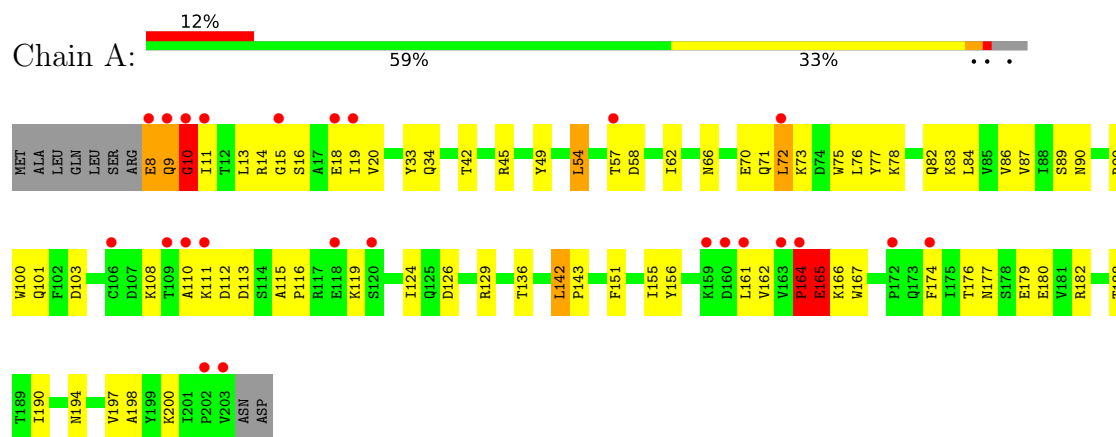
- Molecule 3 is water.

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

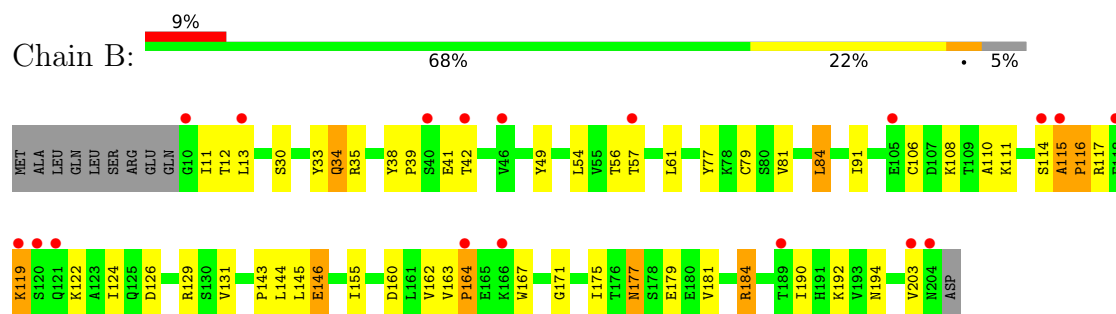
3 Residue-property plots [i](#)

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.

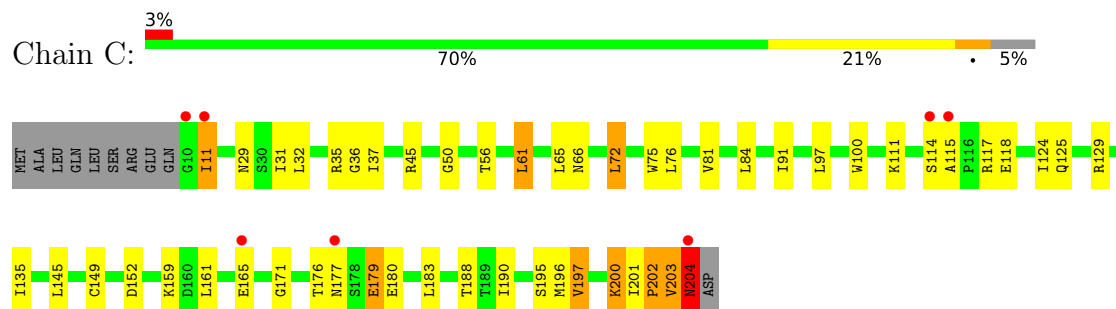
- Molecule 1: Mitotic spindle assembly checkpoint protein MAD2A



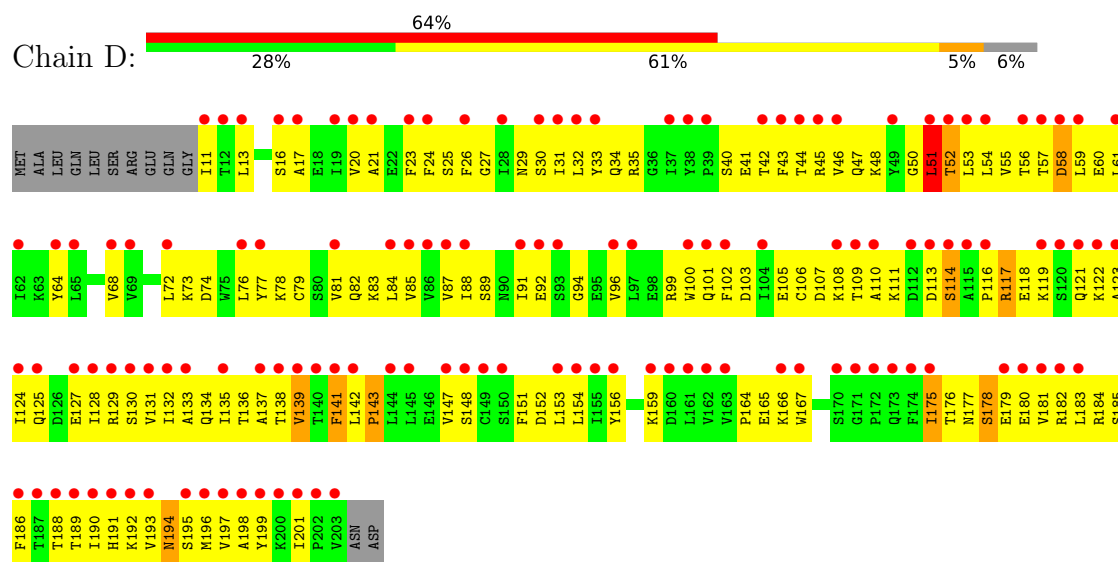
- Molecule 1: Mitotic spindle assembly checkpoint protein MAD2A



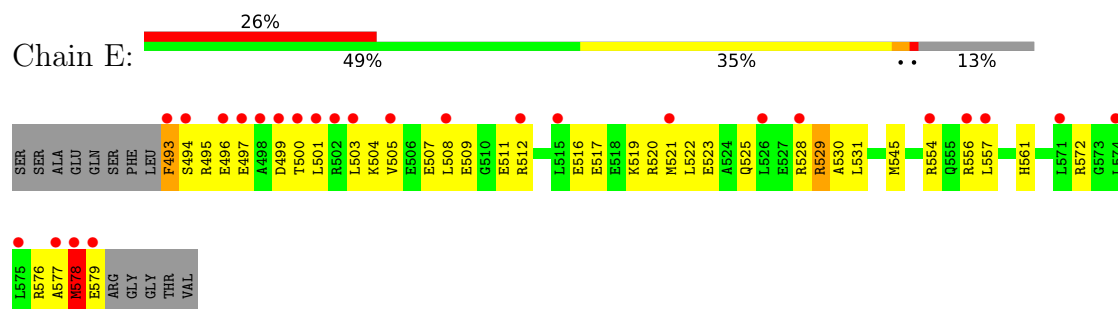
- Molecule 1: Mitotic spindle assembly checkpoint protein MAD2A

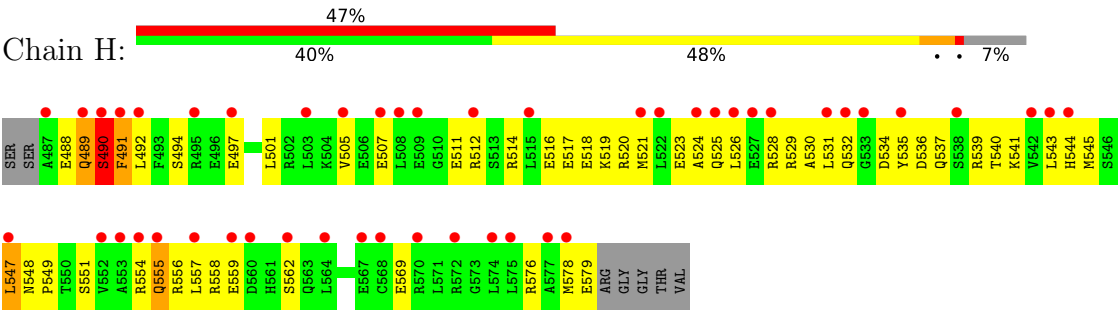


- Molecule 1: Mitotic spindle assembly checkpoint protein MAD2A



• Molecule 2: Mitotic spindle assembly checkpoint protein MAD1





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) 99.7 (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%)	wwPDB-VP
Wilson B-factor (Å ²)	41.5	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 51.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.011 for h,-k,-h-l	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, 0.333 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	0.90	3/1606 (0.2%)	1.17	15/2179 (0.7%)
1	B	0.80	1/1596 (0.1%)	1.14	9/2166 (0.4%)
1	C	1.03	1/1596 (0.1%)	1.27	18/2166 (0.8%)
1	D	0.54	1/1584 (0.1%)	1.38	14/2150 (0.7%)
2	E	0.82	4/726 (0.6%)	1.22	9/966 (0.9%)
2	F	0.56	0/726	0.85	0/966
2	G	0.60	0/821	1.34	9/1092 (0.8%)
2	H	0.48	0/775	1.17	7/1032 (0.7%)
All	All	0.78	10/9430 (0.1%)	1.22	81/12717 (0.6%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	10	GLY	N-CA	23.12	1.78	1.45
2	E	578	MET	CA-C	-7.31	1.43	1.52
1	D	194	ASN	N-CA	6.73	1.54	1.46
2	E	545	MET	SD-CE	6.68	1.96	1.79
1	A	9	GLN	CG-CD	-6.29	1.36	1.52
1	C	91	ILE	CA-CB	6.11	1.61	1.54
2	E	578	MET	N-CA	5.82	1.53	1.46
2	E	577	ALA	CA-C	5.52	1.59	1.53
1	A	8	GLU	CG-CD	-5.31	1.38	1.52
1	B	163	VAL	C-N	5.28	1.40	1.33

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	195	SER	N-CA-CB	-28.46	67.16	110.42
2	G	583	THR	N-CA-C	-20.69	88.28	114.56
1	D	59	LEU	N-CA-CB	-16.75	84.80	110.44
1	D	195	SER	N-CA-C	15.47	133.02	110.59
1	C	203	VAL	O-C-N	14.35	140.51	122.57
1	A	9	GLN	CA-C-N	-13.73	94.50	121.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	9	GLN	C-N-CA	-13.73	94.50	121.41
1	D	194	ASN	CB-CA-C	-12.99	91.00	110.62
1	C	203	VAL	CA-C-O	12.27	136.12	120.78
2	E	493	PHE	CA-CB-CG	11.97	125.77	113.80
1	C	203	VAL	CA-C-N	11.36	142.14	121.70
1	C	203	VAL	C-N-CA	11.36	142.14	121.70
1	D	51	LEU	N-CA-C	-11.07	91.32	108.14
1	D	52	THR	N-CA-CB	-10.91	92.51	110.52
2	H	555	GLN	OE1-CD-NE2	-9.99	112.61	122.60
1	A	10	GLY	N-CA-C	9.98	136.84	113.18
2	H	492	LEU	N-CA-C	-9.91	100.02	114.39
2	G	584	VAL	N-CA-C	-9.44	84.58	111.00
1	B	179	GLU	N-CA-C	-9.02	96.15	110.14
2	G	537	GLN	OE1-CD-NE2	-9.02	113.58	122.60
2	E	578	MET	O-C-N	8.75	134.23	122.59
1	D	175	ILE	N-CA-C	-8.53	95.44	107.80
1	C	118	GLU	N-CA-C	8.38	121.35	111.71
2	E	578	MET	CA-C-O	8.36	132.47	120.51
2	E	578	MET	N-CA-C	-8.12	93.50	110.80
1	D	116	PRO	CB-CA-C	7.85	121.61	111.64
1	D	118	GLU	N-CA-C	7.76	120.72	111.33
1	D	58	ASP	N-CA-C	-7.73	96.97	109.96
2	H	491	PHE	CA-C-N	7.47	133.41	121.98
2	H	491	PHE	C-N-CA	7.47	133.41	121.98
2	E	530	ALA	N-CA-C	7.38	119.41	111.36
1	B	171	GLY	N-CA-C	-7.08	103.40	112.10
1	C	165	GLU	N-CA-C	7.02	122.96	111.37
2	E	493	PHE	CB-CA-C	6.87	123.15	110.10
2	G	577	ALA	N-CA-C	-6.82	105.59	114.04
1	A	9	GLN	CB-CG-CD	-6.80	101.03	112.60
2	G	537	GLN	CG-CD-NE2	6.76	126.54	116.40
1	B	175	ILE	N-CA-C	-6.71	96.05	106.72
2	H	489	GLN	N-CA-C	-6.66	104.02	111.28
2	G	583	THR	CA-C-N	6.57	133.52	121.70
2	G	583	THR	C-N-CA	6.57	133.52	121.70
1	C	171	GLY	N-CA-C	-6.36	104.28	112.10
2	H	555	GLN	CG-CD-NE2	6.32	125.88	116.40
1	D	117	ARG	N-CA-C	6.30	119.60	110.28
1	B	38	TYR	CA-C-N	6.29	126.32	119.90
1	B	38	TYR	C-N-CA	6.29	126.32	119.90
1	A	142	LEU	CA-C-N	6.12	126.03	119.85
1	A	142	LEU	C-N-CA	6.12	126.03	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	165	GLU	CA-C-N	-6.06	115.73	126.45
1	A	165	GLU	C-N-CA	-6.06	115.73	126.45
1	A	190	ILE	N-CA-CB	6.02	121.16	111.23
1	C	204	ASN	CB-CA-C	5.89	121.30	110.10
1	A	112	ASP	N-CA-C	-5.86	106.37	112.93
2	G	583	THR	CA-C-O	5.81	125.18	118.55
1	C	202	PRO	CB-CA-C	5.78	121.09	111.56
1	A	164	PRO	CB-CA-C	5.76	118.77	111.39
1	D	139	VAL	N-CA-C	-5.75	107.90	113.53
2	E	529	ARG	N-CA-C	5.73	117.93	110.53
1	C	197	VAL	CB-CA-C	-5.68	102.03	110.33
1	C	159	LYS	N-CA-C	5.68	118.25	111.71
2	E	578	MET	CA-C-N	5.66	131.90	121.70
2	E	578	MET	C-N-CA	5.66	131.90	121.70
2	H	491	PHE	O-C-N	5.64	128.93	122.55
1	B	164	PRO	CA-N-CD	-5.59	104.17	112.00
1	B	145	LEU	N-CA-C	-5.51	100.20	108.96
1	B	34	GLN	N-CA-C	5.40	119.12	112.54
1	A	90	ASN	N-CA-C	-5.38	101.69	109.59
1	C	190	ILE	N-CA-C	-5.37	107.55	111.90
1	D	60	GLU	N-CA-C	-5.34	106.83	113.55
1	A	89	SER	N-CA-C	5.29	117.72	109.52
1	D	178	SER	N-CA-C	5.28	117.43	109.41
1	C	188	THR	N-CA-C	-5.22	106.95	113.38
1	C	152	ASP	N-CA-C	-5.19	100.84	108.99
1	A	190	ILE	N-CA-C	-5.17	98.58	109.34
1	A	9	GLN	CA-CB-CG	-5.11	103.89	114.10
1	B	164	PRO	N-CA-C	5.11	119.25	111.34
2	G	535	TYR	CA-CB-CG	5.11	123.09	113.90
1	C	115	ALA	CA-C-N	5.09	125.09	119.90
1	C	115	ALA	C-N-CA	5.09	125.09	119.90
1	C	114	SER	N-CA-C	-5.07	107.49	113.97
1	C	179	GLU	N-CA-C	-5.06	102.29	110.14

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	74	0
1	B	1568	0	1588	48	0
1	C	1568	0	1588	40	0
1	D	1556	0	1579	206	0
2	E	722	0	720	58	0
2	F	722	0	722	42	0
2	G	816	0	811	66	0
2	H	770	0	766	83	0
3	A	88	0	0	13	0
3	B	124	0	0	18	0
3	C	225	0	0	18	0
3	D	45	0	0	71	0
3	E	56	0	0	13	0
3	F	35	0	0	4	0
3	G	24	0	0	8	0
3	H	31	0	0	24	0
All	All	9928	0	9370	572	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 31.

All (572) 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:9:GLN:C	1:A:10:GLY:CA	2.30	1.03
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:56:THR:OG1	3:B:2031:HOH:O	1.69	0.95
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
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
1:D:196:MET:HE1	2:H:531:LEU:HD22	1.53	0.90
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
1:D:30:SER:O	1:D:34:GLN:HG2	1.74	0.86
1:C:36:GLY:C	3:C:2035:HOH:O	2.06	0.86
2:F:521:MET:HE3	3:F:2006:HOH:O	1.75	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:H:557:LEU:C	2:H:557:LEU:HD23	2.16	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:141:PHE:C	1:D:141:PHE:CD2	2.70	0.69
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:G:578:MET:HE2	2:G:583:THR:HG21	1.77	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
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
2:G:536:ASP:HA	2:H:521:MET:HE2	1.78	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
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:H:489:GLN:C	2:H:491:PHE:H	2.04	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:180:GLU:CD	2:H:532:GLN:HG2	2.24	0.62
1:D:117:ARG:CB	1:D:189:THR:HG21	2.28	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:179:GLU:CD	3:C:2194:HOH:O	2.42	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
1:D:51:LEU:C	1:D:51:LEU:HD22	2.25	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
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
2:G:578:MET:C	2:G:584:VAL:OXT	2.44	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:A:9:GLN:O	1:A:10:GLY:C	2.45	0.59
1:C:11:ILE:HD12	1:C:11:ILE:H	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:H:557:LEU:C	2:H:557:LEU:CD2	2.75	0.59
2:G:524:ALA:C	3:G:2010:HOH:O	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:G:542:VAL:C	2:G:543:LEU:HD12	2.29	0.58
1:D:68:VAL:HG11	1:D:153:LEU:CD1	2.33	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
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:G:502:ARG:NH2	2:H:497:GLU:CD	2.62	0.57
2:H:545:MET:HE3	3:H:2023: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
2:G:540:THR:N	3:G:2014:HOH:O	2.19	0.57
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: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:E:557:LEU:C	2:E:557:LEU:HD23	2.31	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
2:F:496:GLU:C	2:F:498:ALA:H	2.14	0.55
1:D:101:GLN:HB3	3:D:2044:HOH:O	2.05	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:D:136:THR:HB	3:D:2024:HOH:O	2.06	0.55
2:F:503:LEU:O	2:F:506:GLU:HG2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:489:GLN:C	2:H:491:PHE:N	2.65	0.54
1:D:43:PHE:HD2	3:D:2009:HOH:O	1.91	0.54
1:D:176:THR:CG2	1:D:177:ASN:N	2.70	0.54
2:F:495:ARG:O	2:F:495:ARG:HG2	2.05	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
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
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:574:LEU:HD11	2:G:578:MET:HE1	1.91	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:G:511:GLU:CD	2:H:512:ARG:HH21	2.18	0.51
1:C:203:VAL:HG13	1:C:204:ASN:CG	2.34	0.51
1:B:144:LEU:HB3	3:B:2076:HOH:O	2.11	0.51
1:D:199:TYR:C	3:D:2045:HOH:O	2.53	0.51
2:E:554:ARG:NH1	3:E:2040:HOH:O	2.43	0.51
1:B:39:PRO:HB3	1:B:41:GLU:CD	2.36	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:H:490:SER:C	2:H:491:PHE:CD2	2.89	0.51
2:H:501:LEU:O	2:H:505:VAL:HG23	2.10	0.51
1:D:34:GLN:OE1	1:D:136:THR:HA	2.12	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:G:531:LEU:HD23	2:G:531:LEU:C	2.37	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:D:51:LEU:C	1:D:51:LEU:CD2	2.84	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
2:H:528:ARG:C	3:H:2014:HOH:O	2.55	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:40:SER:C	1:D:42:THR:H	2.20	0.49
2:E:493:PHE:HD2	2:E:496:GLU:CB	2.25	0.49
2:G:579:GLU:HA	2:G:584:VAL:C	2.32	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:A:161:LEU:HD23	1:A:161:LEU:C	2.38	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:30:SER:C	1:D:34:GLN:HG2	2.38	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:D:53:LEU:C	1:D:54:LEU:HD12	2.40	0.47
1:D:129:ARG:HH11	1:D:129:ARG:CB	2.28	0.47
1:D:184:ARG:C	3:D:2040:HOH:O	2.57	0.47
2:E:499:ASP:OD1	2:H:528:ARG:HD2	2.15	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
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
2:G:488:GLU:CD	2:G:488:GLU:N	2.74	0.46
2:G:487:ALA:O	2:G:490:SER:HB2	2.15	0.46
2:F:496:GLU:C	2:F:498:ALA:N	2.74	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
1:D:193:VAL:C	1:D:194:ASN:HD22	2.24	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
1:D:50:GLY:C	1:D:51:LEU:HD13	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:G:536:ASP:C	3:G:2014:HOH:O	2.55	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: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:G:488:GLU:CD	2:G:488:GLU:H	2.23	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: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: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
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
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:B:167:TRP:CG	3:B:2087:HOH:O	2.70	0.45
1:D:96:VAL:CG1	1:D:175:ILE:HG12	2.47	0.45
3:D:2031:HOH:O	2:H:540:THR:C	2.59	0.45
2:E:578:MET:HE2	2:E:578:MET:HB3	1.76	0.45
1:B:167:TRP:HB2	3:B:2087:HOH:O	2.16	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:201:ILE:O	1:C:202:PRO:C	2.60	0.44
1:D:84:LEU:HD13	1:D:84:LEU:C	2.43	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:490:SER:C	2:H:491:PHE:HD2	2.26	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
2:F:536:ASP:C	2:F:536:ASP:OD1	2.62	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:141:PHE:C	1:D:141:PHE:HD2	2.26	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
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
2:H:578:MET:O	2:H:579:GLU:C	2.62	0.42
1:D:184:ARG:CA	3:D:2038:HOH:O	2.67	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
1:D:183:LEU:C	3:D:2038:HOH:O	2.61	0.41
1:C:180:GLU:HG2	1:C:196:MET:HE1	2.01	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:B:84:LEU:HD22	1:B:155:ILE:HD13	2.01	0.41
2:E:517:GLU:CA	2:E:520:ARG:HH21	2.33	0.41
2:F:498:ALA:O	2:F:502:ARG:HG3	2.20	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
1:A:180:GLU:CD	3:A:2077:HOH:O	2.63	0.41
1:B:84:LEU:CD1	1:B:84:LEU:C	2.94	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:489:GLN:O	2:H:491:PHE:N	2.54	0.41
1:D:73:LYS:NZ	3:D:2013:HOH:O	2.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:194:ASN:HB3	3:B:2115:HOH:O	2.21	0.41
2:G:544:HIS:CD2	2:G:544:HIS:C	2.99	0.41
2:G:564:LEU:C	2:G:564:LEU:HD13	2.46	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:F:564:LEU:C	2:F:564:LEU:HD13	2.46	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
2:H:544:HIS:CD2	2:H:544:HIS:C	2.99	0.40
1:B:11:ILE:CG2	1:B:190:ILE:HD12	2.45	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%)	24 16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	193/205 (94%)	187 (97%)	5 (3%)	1 (0%)	24	16
1	C	193/205 (94%)	190 (98%)	3 (2%)	0	100	100
1	D	191/205 (93%)	167 (87%)	22 (12%)	2 (1%)	12	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%)	12	6
2	H	91/100 (91%)	84 (92%)	6 (7%)	1 (1%)	11	5
All	All	1130/1220 (93%)	1070 (95%)	54 (5%)	6 (0%)	24	16

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%)	176 (97%)	5 (3%)	38	34
1	B	180/189 (95%)	172 (96%)	8 (4%)	25	19
1	C	180/189 (95%)	173 (96%)	7 (4%)	28	23
1	D	179/189 (95%)	176 (98%)	3 (2%)	53	53
2	E	78/88 (89%)	73 (94%)	5 (6%)	16	9
2	F	78/88 (89%)	74 (95%)	4 (5%)	21	14
2	G	88/88 (100%)	83 (94%)	5 (6%)	18	11
2	H	83/88 (94%)	80 (96%)	3 (4%)	31	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1047/1108 (94%)	1007 (96%)	40 (4%)	29	24

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	LEU
1	A	72	LEU
1	A	84	LEU
1	A	164	PRO
1	A	165	GLU
1	B	61	LEU
1	B	84	LEU
1	B	116	PRO
1	B	119	LYS
1	B	146	GLU
1	B	164	PRO
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	200	LYS
1	C	204	ASN
1	D	51	LEU
1	D	141	PHE
1	D	143	PRO
2	E	509	GLU
2	E	531	LEU
2	E	561	HIS
2	E	572	ARG
2	E	578	MET
2	F	496	GLU
2	F	499	ASP
2	F	502	ARG
2	F	531	LEU
2	G	535	TYR
2	G	539	ARG
2	G	543	LEU
2	G	578	MET
2	G	583	THR

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Mol	Chain	Res	Type
2	H	490	SER
2	H	547	LEU
2	H	556	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	66	ASN
1	A	101	GLN
1	B	34	GLN
1	B	47	GLN
1	B	177	ASN
1	B	204	ASN
1	C	29	ASN
1	C	47	GLN
1	C	177	ASN
1	D	47	GLN
1	D	66	ASN
1	D	134	GLN
1	D	177	ASN
1	D	194	ASN
2	E	525	GLN
2	E	563	GLN
2	F	565	GLN
2	G	525	GLN
2	G	561	HIS
2	H	525	GLN
2	H	537	GLN
2	H	555	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 ⓘ

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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%)	0.83	24 (12%) 8 7	34, 53, 80, 95	0
1	B	195/205 (95%)	0.59	18 (9%) 14 14	29, 45, 69, 86	0
1	C	195/205 (95%)	-0.00	7 (3%) 46 46	21, 33, 61, 87	0
1	D	193/205 (94%)	2.67	131 (67%) 0 0	80, 98, 103, 105	0
2	E	87/100 (87%)	1.37	26 (29%) 1 0	27, 68, 94, 100	0
2	F	87/100 (87%)	1.13	24 (27%) 1 1	30, 69, 100, 104	0
2	G	100/100 (100%)	1.98	40 (40%) 1 0	49, 78, 92, 95	0
2	H	93/100 (93%)	2.08	47 (50%) 0 0	52, 82, 95, 101	0
All	All	1146/1220 (93%)	1.22	317 (27%) 1 1	21, 62, 100, 105	0

All (317) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	493	PHE	8.7
2	G	584	VAL	8.3
1	D	190	ILE	7.2
1	D	181	VAL	6.4
1	D	124	ILE	6.3
2	H	547	LEU	5.9
2	G	534	ASP	5.9
1	D	193	VAL	5.8
2	E	494	SER	5.5
2	G	485	SER	5.4
1	D	53	LEU	5.4
1	C	204	ASN	5.3
1	D	115	ALA	5.3
1	D	114	SER	5.3
2	H	531	LEU	5.0
1	D	123	ALA	5.0

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Mol	Chain	Res	Type	RSRZ
1	D	171	GLY	4.9
1	D	135	ILE	4.8
1	A	203	VAL	4.8
1	B	10	GLY	4.8
1	D	11	ILE	4.7
2	E	498	ALA	4.5
1	D	65	LEU	4.5
1	D	141	PHE	4.5
1	D	175	ILE	4.4
2	H	492	LEU	4.4
1	A	111	LYS	4.3
2	G	581	GLY	4.3
1	A	19	ILE	4.2
1	D	86	VAL	4.2
1	D	57	THR	4.2
1	D	116	PRO	4.2
1	A	110	ALA	4.2
1	D	13	LEU	4.2
2	G	583	THR	4.1
1	D	52	THR	4.1
1	A	8	GLU	4.1
1	D	186	PHE	4.0
2	G	582	GLY	4.0
2	H	527	GLU	4.0
1	D	154	LEU	4.0
2	G	576	ARG	4.0
2	H	557	LEU	3.9
1	D	188	THR	3.9
1	D	189	THR	3.9
1	D	45	ARG	3.9
1	D	87	VAL	3.8
1	D	100	TRP	3.8
1	D	46	VAL	3.8
1	D	26	PHE	3.8
2	H	528	ARG	3.7
2	H	521	MET	3.7
1	D	120	SER	3.7
1	D	119	LYS	3.7
1	D	96	VAL	3.7
1	D	62	ILE	3.7
1	B	118	GLU	3.7
1	D	92	GLU	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	204	ASN	3.6
1	D	162	VAL	3.6
2	G	527	GLU	3.6
2	F	493	PHE	3.6
1	D	187	THR	3.6
1	D	33	TYR	3.6
1	D	37	ILE	3.6
1	D	142	LEU	3.6
2	F	500	THR	3.6
1	D	172	PRO	3.6
1	C	165	GLU	3.6
1	D	32	LEU	3.5
2	E	574	LEU	3.5
2	G	569	GLU	3.5
1	D	54	LEU	3.5
1	D	131	VAL	3.5
1	D	174	PHE	3.5
2	E	578	MET	3.5
1	D	85	VAL	3.5
1	A	202	PRO	3.4
2	E	577	ALA	3.4
2	H	491	PHE	3.4
1	D	84	LEU	3.4
2	F	501	LEU	3.4
1	D	44	THR	3.4
2	E	505	VAL	3.4
2	F	505	VAL	3.4
1	D	19	ILE	3.4
1	D	129	ARG	3.4
1	D	102	PHE	3.4
2	H	567	GLU	3.4
1	D	31	ILE	3.4
1	D	72	LEU	3.4
2	H	564	LEU	3.4
1	D	166	LYS	3.3
1	D	68	VAL	3.3
1	D	69	VAL	3.3
1	D	97	LEU	3.3
1	D	153	LEU	3.3
2	E	500	THR	3.3
1	D	38	TYR	3.3
1	D	203	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	17	ALA	3.3
2	G	577	ALA	3.3
1	D	59	LEU	3.3
1	D	61	LEU	3.3
2	G	575	LEU	3.3
1	D	12	THR	3.3
1	D	77	TYR	3.2
1	D	196	MET	3.2
1	D	155	ILE	3.2
2	E	501	LEU	3.2
2	G	526	LEU	3.2
1	D	195	SER	3.2
2	F	578	MET	3.2
1	D	201	ILE	3.2
2	G	522	LEU	3.2
1	D	130	SER	3.2
1	D	202	PRO	3.2
1	D	197	VAL	3.1
2	G	505	VAL	3.1
1	D	28	ILE	3.1
2	E	515	LEU	3.1
2	F	515	LEU	3.1
1	B	114	SER	3.1
1	B	166	LYS	3.1
2	H	489	GLN	3.1
1	D	180	GLU	3.1
2	E	526	LEU	3.1
1	A	9	GLN	3.1
1	D	23	PHE	3.1
2	H	553	ALA	3.1
1	A	163	VAL	3.1
1	D	147	VAL	3.1
1	D	161	LEU	3.1
2	F	508	LEU	3.1
2	G	531	LEU	3.1
1	D	81	VAL	3.0
2	H	509	GLU	3.0
1	D	133	ALA	3.0
2	E	556	ARG	3.0
2	G	501	LEU	3.0
2	G	571	LEU	3.0
1	D	128	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
2	G	533	GLY	3.0
1	D	113	ASP	3.0
1	D	191	HIS	3.0
2	G	535	TYR	3.0
1	D	24	PHE	3.0
1	D	145	LEU	2.9
2	F	503	LEU	2.9
2	H	542	VAL	2.9
1	D	159	LYS	2.9
1	D	198	ALA	2.9
1	D	138	THR	2.9
2	E	521	MET	2.9
2	G	521	MET	2.9
2	H	524	ALA	2.9
1	D	139	VAL	2.8
1	D	49	TYR	2.8
2	E	502	ARG	2.8
2	F	571	LEU	2.8
2	F	496	GLU	2.8
1	D	199	TYR	2.8
1	D	137	ALA	2.8
2	E	496	GLU	2.8
2	E	579	GLU	2.8
2	G	515	LEU	2.8
1	C	11	ILE	2.8
1	D	93	SER	2.8
1	D	125	GLN	2.8
2	F	579	GLU	2.8
2	F	575	LEU	2.8
1	D	109	THR	2.8
1	D	91	ILE	2.8
1	D	132	ILE	2.8
2	H	487	ALA	2.7
1	D	51	LEU	2.7
1	D	76	LEU	2.7
1	D	183	LEU	2.7
2	H	554	ARG	2.7
2	H	570	ARG	2.7
1	D	121	GLN	2.7
2	G	574	LEU	2.7
1	D	39	PRO	2.7
1	D	101	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
2	H	535	TYR	2.7
2	H	578	MET	2.7
2	G	519	LYS	2.7
2	H	515	LEU	2.7
1	C	177	ASN	2.6
2	F	574	LEU	2.6
2	H	560	ASP	2.6
2	H	574	LEU	2.6
1	D	192	LYS	2.6
1	D	20	VAL	2.6
1	D	127	GLU	2.6
1	D	167	TRP	2.6
1	A	120	SER	2.6
1	A	174	PHE	2.6
1	B	120	SER	2.6
2	G	486	SER	2.6
2	H	555	GLN	2.6
1	A	18	GLU	2.6
1	D	122	LYS	2.6
1	B	164	PRO	2.6
1	A	10	GLY	2.5
1	A	57	THR	2.5
1	A	109	THR	2.5
1	D	56	THR	2.5
1	D	144	LEU	2.5
2	E	508	LEU	2.5
2	G	578	MET	2.5
1	A	159	LYS	2.5
1	A	160	ASP	2.5
1	B	42	THR	2.5
1	D	42	THR	2.5
1	D	150	SER	2.5
1	D	110	ALA	2.5
2	H	507	GLU	2.4
1	A	106	CYS	2.4
1	D	156	TYR	2.4
1	B	40	SER	2.4
1	B	57	THR	2.4
1	D	148	SER	2.4
1	D	21	ALA	2.4
1	A	164	PRO	2.4
1	D	88	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
2	H	552	VAL	2.4
2	H	568	CYS	2.4
2	G	579	GLU	2.4
1	A	15	GLY	2.4
1	D	43	PHE	2.4
2	F	539	ARG	2.4
2	G	542	VAL	2.4
2	F	494	SER	2.4
2	H	562	SER	2.4
2	F	497	GLU	2.3
2	E	557	LEU	2.3
1	B	105	GLU	2.3
1	D	112	ASP	2.3
2	E	528	ARG	2.3
2	E	554	ARG	2.3
1	D	179	GLU	2.3
2	G	532	GLN	2.3
1	D	149	CYS	2.3
1	D	182	ARG	2.3
2	E	575	LEU	2.3
1	D	104	ILE	2.3
1	D	173	GLN	2.3
1	B	46	VAL	2.3
1	B	115	ALA	2.3
2	G	530	ALA	2.3
1	A	161	LEU	2.3
2	H	526	LEU	2.3
2	E	512	ARG	2.2
2	G	520	ARG	2.2
2	H	572	ARG	2.2
1	D	108	LYS	2.2
1	C	115	ALA	2.2
2	G	487	ALA	2.2
2	H	533	GLY	2.2
2	E	503	LEU	2.2
2	E	571	LEU	2.2
2	G	557	LEU	2.2
2	H	543	LEU	2.2
1	D	64	TYR	2.2
2	G	516	GLU	2.2
1	D	170	SER	2.2
2	F	572	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	11	ILE	2.2
1	D	140	THR	2.2
2	G	540	THR	2.2
1	D	160	ASP	2.2
2	G	517	GLU	2.2
1	A	72	LEU	2.2
1	B	13	LEU	2.2
2	G	547	LEU	2.2
1	C	114	SER	2.2
1	D	30	SER	2.2
2	E	497	GLU	2.2
2	H	559	GLU	2.2
2	H	525	GLN	2.2
2	G	503	LEU	2.2
1	A	172	PRO	2.1
2	H	497	GLU	2.1
2	H	505	VAL	2.1
1	C	10	GLY	2.1
2	G	573	GLY	2.1
2	H	532	GLN	2.1
2	F	577	ALA	2.1
2	H	495	ARG	2.1
2	H	522	LEU	2.1
1	D	16	SER	2.1
1	D	200	LYS	2.1
1	A	118	GLU	2.1
1	B	189	THR	2.1
2	G	555	GLN	2.1
2	F	502	ARG	2.1
2	F	512	ARG	2.1
2	F	498	ALA	2.1
2	H	490	SER	2.1
2	F	567	GLU	2.1
2	E	499	ASP	2.1
1	B	119	LYS	2.1
1	D	163	VAL	2.1
2	H	577	ALA	2.1
2	F	564	LEU	2.0
2	H	508	LEU	2.0
2	H	575	LEU	2.0
1	D	58	ASP	2.0
2	F	568	CYS	2.0

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Mol	Chain	Res	Type	RSRZ
2	G	580	ARG	2.0
2	H	512	ARG	2.0
2	H	544	HIS	2.0
1	B	203	VAL	2.0
2	H	538	SER	2.0
1	B	121	GLN	2.0
2	H	503	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.