



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 23, 2021 – 04:39 PM EDT

PDB ID : 1CK7
Title : GELATINASE A (FULL-LENGTH)
Authors : Morgunova, E.; Tuuttila, A.; Bergmann, U.; Isupov, M.; Lindqvist, Y.; Schneider, G.; Tryggvason, K.
Deposited on : 1999-04-28
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.2
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

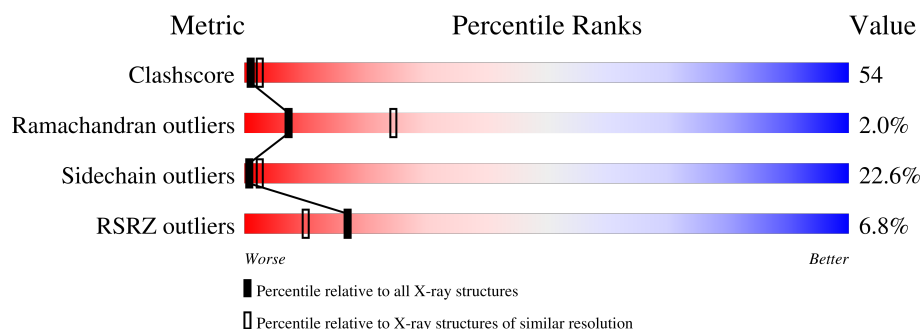
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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))
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	631	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 5051 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 PROTEIN (GELATINASE A).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	619	Total	C	N	O	S	0	0	0
			4930	3166	812	925	27			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	404	ALA	GLU	engineered mutation	UNP P08253

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	Ca	0	0
			3	3		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Na	0	0
			1	1		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	104	Total	O	0	0
			104	104		

4 Data and refinement statistics

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	121.32Å 121.32Å 345.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.00 – 2.80 34.89 – 2.66	Depositor EDS
% Data completeness (in resolution range)	99.7 (34.00-2.80) 88.5 (34.89-2.66)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.92 (at 2.65Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.286 , 0.327 0.283 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	52.4	Xtriage
Anisotropy	0.006	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 66.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	5051	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, SO4, ZN, CL, CA

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	1.32	2/5085 (0.0%)	1.36	40/6891 (0.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	660	CYS	C-OXT	82.38	2.79	1.23
1	A	220	VAL	CB-CG1	5.94	1.65	1.52

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	659	GLY	C-N-CA	10.63	148.28	121.70
1	A	524	TYR	CA-CB-CG	10.03	132.45	113.40
1	A	175	ARG	NE-CZ-NH2	-9.59	115.50	120.30
1	A	252	ARG	NE-CZ-NH2	-8.82	115.89	120.30
1	A	222	ARG	NE-CZ-NH1	8.70	124.65	120.30
1	A	60	CYS	CA-CB-SG	8.57	129.44	114.00
1	A	641	GLU	N-CA-CB	8.37	125.66	110.60
1	A	385	ARG	CD-NE-CZ	7.61	134.25	123.60
1	A	660	CYS	CA-CB-SG	7.27	127.09	114.00
1	A	185	ASP	CB-CG-OD1	7.18	124.76	118.30
1	A	186	GLY	O-C-N	-6.67	112.03	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	229	ASP	O-C-N	-6.62	111.94	123.20
1	A	182	TYR	N-CA-CB	-6.59	98.74	110.60
1	A	297	PHE	C-N-CA	-6.57	105.27	121.70
1	A	589	TRP	CA-CB-CG	6.47	126.00	113.70
1	A	193	HIS	CA-CB-CG	6.36	124.40	113.60
1	A	184	PHE	CB-CG-CD2	6.29	125.21	120.80
1	A	134	ASP	CB-CG-OD2	6.28	123.95	118.30
1	A	383	ASP	CB-CG-OD2	-6.23	112.69	118.30
1	A	222	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	A	252	ARG	NH1-CZ-NH2	6.12	126.13	119.40
1	A	240	ASN	C-N-CA	-6.11	109.47	122.30
1	A	315	ARG	CA-CB-CG	6.09	126.79	113.40
1	A	435	GLN	OE1-CD-NE2	-5.91	108.31	121.90
1	A	240	ASN	CA-C-N	5.84	127.88	116.20
1	A	188	ASP	CB-CG-OD1	5.75	123.47	118.30
1	A	435	GLN	CG-CD-NE2	5.70	130.37	116.70
1	A	182	TYR	CB-CG-CD1	-5.52	117.69	121.00
1	A	263	TYR	CB-CG-CD1	5.51	124.31	121.00
1	A	60	CYS	CB-CA-C	5.41	121.22	110.40
1	A	113	PHE	CA-CB-CG	-5.40	100.95	113.90
1	A	385	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	A	242	LYS	CA-CB-CG	5.32	125.11	113.40
1	A	218	GLY	O-C-N	-5.28	114.25	122.70
1	A	432	ARG	CD-NE-CZ	5.17	130.84	123.60
1	A	175	ARG	CA-CB-CG	-5.16	102.06	113.40
1	A	211	GLU	C-N-CA	-5.14	108.84	121.70
1	A	543	TYR	O-C-N	5.11	130.87	122.70
1	A	232	TYR	CB-CG-CD1	5.08	124.05	121.00
1	A	297	PHE	N-CA-CB	5.05	119.68	110.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	185	ASP	Mainchain

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	4930	0	4651	518	1
2	A	2	0	0	0	0
3	A	3	0	0	0	0
4	A	1	0	0	0	0
5	A	1	0	0	0	0
6	A	10	0	0	0	0
7	A	104	0	0	13	0
All	All	5051	0	4651	518	1

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 54.

All (518) 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:A:233:CYS:SG	1:A:259:CYS:SG	2.38	1.18
1:A:247:CYS:SG	1:A:274:CYS:SG	2.35	1.10
1:A:224:LYS:HE2	1:A:224:LYS:HA	1.33	1.09
1:A:65:CYS:HA	1:A:69:VAL:HG21	1.29	1.06
1:A:109:ASN:ND2	1:A:113:PHE:CE1	2.23	1.06
1:A:319:THR:HG22	1:A:328:LYS:HB3	1.36	1.06
1:A:172:ASN:HD22	1:A:173:PHE:N	1.55	1.02
1:A:602:PHE:HB3	1:A:603:PRO:HA	1.40	1.02
1:A:73:THR:HA	1:A:76:LYS:HD2	1.39	0.99
1:A:315:ARG:HG3	1:A:315:ARG:HH11	1.28	0.98
1:A:482:ARG:HG2	1:A:530:GLU:OE2	1.64	0.98
1:A:223:VAL:CG1	1:A:272:GLY:HA3	1.96	0.96
1:A:185:ASP:HB3	7:A:1017:HOH:O	1.67	0.95
1:A:172:ASN:ND2	1:A:173:PHE:H	1.64	0.95
1:A:640:LEU:HA	1:A:647:SER:O	1.66	0.95
1:A:320:THR:HG22	7:A:1030:HOH:O	1.67	0.94
1:A:91:GLN:HE21	1:A:91:GLN:N	1.63	0.94
1:A:108:ALA:HB1	1:A:110:TYR:CD1	2.02	0.94
1:A:489:LYS:HG3	1:A:490:ASP:H	1.32	0.94
1:A:570:ALA:HB3	1:A:583:PHE:HB2	1.51	0.93
1:A:172:ASN:HD22	1:A:173:PHE:H	1.03	0.92
1:A:617:LEU:HA	1:A:633:LYS:HD3	1.51	0.92
1:A:66:ASN:H	1:A:69:VAL:HG22	1.36	0.90
1:A:224:LYS:HA	1:A:224:LYS:CE	1.98	0.89
1:A:118:LYS:O	1:A:118:LYS:HG2	1.69	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:ASN:HD21	1:A:387:TRP:H	1.22	0.88
1:A:66:ASN:H	1:A:69:VAL:CG2	1.87	0.88
1:A:646:LYS:O	1:A:648:VAL:HG22	1.73	0.88
1:A:611:ASN:HB2	1:A:645:LEU:CD1	2.05	0.87
1:A:108:ALA:HB1	1:A:110:TYR:HD1	1.39	0.87
1:A:579:LYS:HG2	1:A:590:ARG:NE	1.89	0.87
1:A:639:LYS:NZ	1:A:649:LYS:HB2	1.89	0.86
1:A:640:LEU:HD11	1:A:645:LEU:HA	1.56	0.85
1:A:70:LEU:HG	1:A:74:LEU:HD12	1.58	0.85
1:A:57:PHE:CZ	1:A:101:ARG:HD2	2.12	0.85
1:A:91:GLN:HE21	1:A:91:GLN:H	1.21	0.85
1:A:320:THR:HG21	1:A:326:ASP:HB2	1.58	0.85
1:A:467:GLU:HA	7:A:1006:HOH:O	1.77	0.85
1:A:70:LEU:O	1:A:74:LEU:HB2	1.77	0.85
1:A:645:LEU:C	1:A:645:LEU:HD13	1.98	0.84
1:A:91:GLN:H	1:A:91:GLN:NE2	1.77	0.83
1:A:74:LEU:HD13	1:A:87:GLY:O	1.79	0.83
1:A:65:CYS:HA	1:A:69:VAL:CG2	2.08	0.82
1:A:648:VAL:O	1:A:649:LYS:HG3	1.79	0.82
1:A:162:ILE:HD11	1:A:167:ALA:HB2	1.63	0.81
1:A:611:ASN:HB2	1:A:645:LEU:HD11	1.62	0.81
1:A:53:TYR:CG	1:A:97:MET:HE2	2.15	0.81
1:A:224:LYS:HG3	1:A:280:PHE:CE2	2.16	0.80
1:A:260:SER:HB3	1:A:265:PHE:CD1	2.17	0.80
1:A:74:LEU:HD21	1:A:89:LEU:HD23	1.64	0.80
1:A:155:THR:HB	1:A:156:PRO:CD	2.11	0.79
1:A:114:PRO:HG2	1:A:198:GLY:CA	2.13	0.79
1:A:113:PHE:CB	1:A:196:ALA:HB3	2.13	0.79
1:A:319:THR:CG2	1:A:328:LYS:HB3	2.12	0.79
1:A:109:ASN:ND2	1:A:113:PHE:CZ	2.51	0.79
1:A:233:CYS:CB	1:A:259:CYS:SG	2.71	0.79
1:A:481:ILE:HG22	1:A:482:ARG:H	1.46	0.79
1:A:433:LEU:HD22	1:A:437:ASP:HB2	1.64	0.78
1:A:641:GLU:HG3	1:A:647:SER:OG	1.84	0.78
1:A:579:LYS:HG2	1:A:590:ARG:HE	1.48	0.77
1:A:260:SER:HB3	1:A:265:PHE:HD1	1.48	0.77
1:A:641:GLU:CG	1:A:647:SER:OG	2.32	0.77
1:A:475:PHE:HB2	1:A:478:ILE:HD11	1.66	0.77
1:A:502:LYS:HE2	1:A:503:PRO:HD2	1.66	0.77
1:A:531:LYS:NZ	1:A:549:GLU:OE2	2.15	0.77
1:A:549:GLU:HB3	1:A:552:TYR:CD2	2.18	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:641:GLU:CB	1:A:647:SER:OG	2.33	0.76
1:A:169:ILE:HG23	1:A:203:GLY:O	1.84	0.76
1:A:576:LYS:CE	1:A:642:ASN:HB3	2.16	0.76
1:A:646:LYS:C	1:A:646:LYS:HD3	2.06	0.76
1:A:542:ILE:O	1:A:549:GLU:HB2	1.86	0.76
1:A:339:THR:HG22	1:A:346:GLY:HA2	1.65	0.75
1:A:61:PRO:HD2	1:A:64:SER:OG	1.86	0.75
1:A:590:ARG:NH1	1:A:602:PHE:HZ	1.84	0.75
1:A:109:ASN:CG	1:A:113:PHE:CZ	2.59	0.75
1:A:639:LYS:HG2	1:A:649:LYS:O	1.87	0.75
1:A:645:LEU:O	1:A:645:LEU:HD22	1.87	0.74
1:A:154:VAL:HG11	1:A:438:ILE:HG23	1.69	0.74
1:A:481:ILE:HG22	1:A:482:ARG:N	2.01	0.74
1:A:311:THR:HB	7:A:1013:HOH:O	1.88	0.74
1:A:155:THR:HB	1:A:156:PRO:HD2	1.68	0.74
1:A:398:PHE:CE2	1:A:399:LEU:HD23	2.22	0.73
1:A:635:ALA:O	7:A:1094:HOH:O	2.06	0.73
1:A:112:PHE:CD1	1:A:112:PHE:O	2.41	0.73
1:A:201:VAL:O	1:A:204:ASP:HB2	1.89	0.72
1:A:646:LYS:O	1:A:648:VAL:CG2	2.36	0.72
1:A:195:PHE:CD2	1:A:201:VAL:HG13	2.25	0.72
1:A:480:GLN:HG3	1:A:485:ILE:HD13	1.72	0.72
1:A:158:ARG:NH2	1:A:449:PRO:HD2	2.05	0.72
1:A:611:ASN:CB	1:A:645:LEU:HD11	2.19	0.71
1:A:639:LYS:HE3	1:A:649:LYS:O	1.90	0.71
1:A:65:CYS:CA	1:A:69:VAL:HG21	2.15	0.71
1:A:113:PHE:CG	1:A:196:ALA:HB3	2.25	0.71
1:A:644:SER:O	1:A:647:SER:HB3	1.89	0.71
1:A:239:PHE:CE2	1:A:240:ASN:ND2	2.58	0.71
1:A:185:ASP:OD1	1:A:185:ASP:O	2.07	0.71
1:A:658:LEU:O	1:A:660:CYS:HB2	1.91	0.71
1:A:641:GLU:HB2	1:A:647:SER:CB	2.21	0.71
1:A:233:CYS:CB	1:A:259:CYS:HG	2.03	0.71
1:A:157:LEU:O	1:A:158:ARG:HD3	1.91	0.70
1:A:172:ASN:ND2	1:A:173:PHE:N	2.30	0.70
1:A:157:LEU:HD11	1:A:445:TYR:CD2	2.26	0.70
1:A:364:THR:HG23	1:A:366:ALA:H	1.56	0.70
1:A:129:ILE:CD1	1:A:170:MET:HB3	2.23	0.69
1:A:549:GLU:HB3	1:A:552:TYR:HD2	1.58	0.69
1:A:40:ASP:OD2	1:A:368:ARG:NH2	2.25	0.68
1:A:114:PRO:HG2	1:A:198:GLY:HA3	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:574:TRP:HB3	1:A:577:ASN:OD1	1.94	0.68
1:A:513:TRP:HB3	1:A:516:LEU:HD22	1.75	0.68
1:A:524:TYR:CE1	1:A:580:THR:HG21	2.29	0.68
1:A:135:LEU:HB2	1:A:140:VAL:HG23	1.75	0.68
1:A:571:ALA:O	1:A:572:PHE:HB3	1.94	0.68
1:A:315:ARG:HH11	1:A:315:ARG:CG	2.04	0.67
1:A:31:PRO:O	1:A:32:SER:OG	2.12	0.67
1:A:119:TRP:N	1:A:445:TYR:OH	2.27	0.67
1:A:223:VAL:HG11	1:A:272:GLY:HA3	1.74	0.67
1:A:114:PRO:CG	1:A:198:GLY:HA3	2.25	0.67
1:A:247:CYS:CB	1:A:274:CYS:SG	2.83	0.67
1:A:579:LYS:HG2	1:A:590:ARG:CD	2.24	0.67
1:A:242:LYS:HZ1	1:A:351:PHE:HD2	1.43	0.67
1:A:639:LYS:HZ2	1:A:649:LYS:HB2	1.57	0.67
1:A:224:LYS:HG3	1:A:280:PHE:HE2	1.58	0.66
1:A:224:LYS:O	1:A:224:LYS:HD3	1.95	0.66
1:A:613:ILE:HD12	1:A:631:PHE:CD2	2.30	0.66
1:A:53:TYR:CB	1:A:97:MET:HE2	2.24	0.66
1:A:533:VAL:HG22	1:A:542:ILE:HG23	1.78	0.66
1:A:518:GLU:H	1:A:518:GLU:CD	2.00	0.66
1:A:615:ASP:O	1:A:616:ASN:HB2	1.96	0.66
1:A:119:TRP:CE2	1:A:197:PRO:HB3	2.31	0.66
1:A:606:ILE:HB	1:A:615:ASP:OD1	1.94	0.66
1:A:617:LEU:H	1:A:617:LEU:HD23	1.60	0.65
1:A:628:HIS:HA	1:A:640:LEU:O	1.95	0.65
1:A:489:LYS:HG3	1:A:490:ASP:N	2.09	0.65
1:A:618:ASP:OD1	1:A:633:LYS:HA	1.96	0.65
1:A:513:TRP:CB	1:A:516:LEU:HD22	2.27	0.64
1:A:219:GLN:HE22	1:A:337:MET:H	1.44	0.64
1:A:53:TYR:CD2	1:A:97:MET:HB2	2.33	0.64
1:A:113:PHE:HB2	1:A:196:ALA:HB3	1.78	0.64
1:A:57:PHE:HZ	1:A:190:LEU:HD22	1.62	0.64
1:A:552:TYR:CE1	1:A:554:LYS:HE3	2.32	0.64
1:A:247:CYS:HB3	1:A:274:CYS:SG	2.38	0.64
1:A:652:SER:O	1:A:656:ASP:HB2	1.97	0.64
1:A:129:ILE:HD12	1:A:170:MET:HB3	1.80	0.63
1:A:90:ASP:O	1:A:93:THR:N	2.31	0.63
1:A:493:ILE:O	1:A:493:ILE:HG13	1.98	0.63
1:A:164:ASP:OD1	1:A:165:GLY:N	2.32	0.63
1:A:627:GLY:HA2	1:A:642:ASN:ND2	2.13	0.63
1:A:71:LYS:HB3	1:A:87:GLY:HA3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:545:ALA:O	1:A:546:SER:HB3	1.98	0.62
1:A:114:PRO:HG2	1:A:198:GLY:HA2	1.81	0.62
1:A:542:ILE:HG13	1:A:552:TYR:CZ	2.34	0.62
1:A:572:PHE:CE1	1:A:620:VAL:HG11	2.34	0.62
1:A:119:TRP:CD2	1:A:197:PRO:HB3	2.35	0.62
1:A:433:LEU:HD22	1:A:437:ASP:CB	2.29	0.62
1:A:576:LYS:HE3	1:A:642:ASN:HB3	1.82	0.62
1:A:639:LYS:CG	1:A:649:LYS:O	2.48	0.61
1:A:592:ASN:OD1	1:A:594:VAL:HG23	2.00	0.61
1:A:628:HIS:HE1	1:A:639:LYS:HD2	1.65	0.61
1:A:224:LYS:HG3	1:A:280:PHE:CZ	2.35	0.61
1:A:233:CYS:HB3	1:A:259:CYS:SG	2.39	0.61
1:A:552:TYR:CZ	1:A:554:LYS:HE3	2.35	0.61
1:A:555:PRO:HB2	1:A:557:THR:HG23	1.82	0.61
1:A:590:ARG:NH1	1:A:602:PHE:CZ	2.68	0.61
1:A:611:ASN:HB2	1:A:645:LEU:CG	2.31	0.61
1:A:142:ASP:OD1	1:A:146:ARG:NH1	2.34	0.61
1:A:469:CYS:HA	1:A:660:CYS:SG	2.41	0.61
1:A:90:ASP:O	1:A:92:ASN:N	2.35	0.60
1:A:109:ASN:O	1:A:113:PHE:HZ	1.84	0.60
1:A:398:PHE:CD2	1:A:399:LEU:HD23	2.36	0.60
1:A:247:CYS:CB	1:A:274:CYS:HG	2.11	0.60
1:A:289:GLN:HB3	1:A:290:PRO:HD2	1.82	0.60
1:A:581:TYR:HA	1:A:589:TRP:O	2.02	0.60
1:A:108:ALA:CB	1:A:110:TYR:HD1	2.14	0.60
1:A:114:PRO:HG3	7:A:1007:HOH:O	2.02	0.60
1:A:639:LYS:NZ	1:A:649:LYS:CB	2.63	0.60
1:A:315:ARG:NH1	1:A:332:CYS:O	2.34	0.60
1:A:260:SER:CB	1:A:265:PHE:HD1	2.12	0.60
1:A:277:GLU:HB2	1:A:291:CYS:SG	2.42	0.59
1:A:520:ILE:HD13	1:A:520:ILE:H	1.66	0.59
1:A:617:LEU:H	1:A:617:LEU:CD2	2.14	0.59
1:A:233:CYS:HB3	1:A:259:CYS:HB2	1.84	0.59
1:A:565:VAL:HG23	1:A:567:ARG:H	1.67	0.59
1:A:66:ASN:OD1	1:A:69:VAL:HG13	2.03	0.59
1:A:221:VAL:O	1:A:232:TYR:HA	2.03	0.59
1:A:224:LYS:HG3	1:A:282:MET:HE1	1.84	0.59
1:A:475:PHE:HB2	1:A:478:ILE:CD1	2.32	0.59
1:A:574:TRP:CZ2	1:A:576:LYS:NZ	2.70	0.58
1:A:214:THR:HG22	1:A:219:GLN:HA	1.86	0.58
1:A:426:THR:OG1	1:A:511:THR:HG22	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:588:PHE:HE2	1:A:609:ALA:HB3	1.68	0.58
1:A:645:LEU:HD13	1:A:646:LYS:N	2.18	0.58
1:A:488:PHE:CB	1:A:520:ILE:HD11	2.32	0.58
1:A:623:LEU:HD13	1:A:623:LEU:H	1.67	0.58
1:A:653:ILE:O	1:A:657:TRP:HB2	2.04	0.58
1:A:100:PRO:HB3	1:A:191:LEU:HD21	1.84	0.58
1:A:153:ASP:HB2	7:A:1059:HOH:O	2.04	0.58
1:A:466:PRO:HB2	1:A:494:TRP:CH2	2.37	0.58
1:A:480:GLN:HG3	1:A:485:ILE:CD1	2.33	0.58
1:A:624:GLN:O	1:A:624:GLN:HG3	2.02	0.58
1:A:113:PHE:CD2	1:A:114:PRO:O	2.57	0.57
1:A:368:ARG:NH1	1:A:389:PHE:HZ	2.03	0.57
1:A:78:GLN:OE1	1:A:86:THR:O	2.23	0.57
1:A:404:ALA:O	1:A:407:HIS:HB2	2.05	0.57
1:A:576:LYS:NZ	1:A:642:ASN:HA	2.20	0.57
1:A:590:ARG:O	1:A:598:MET:SD	2.63	0.57
1:A:639:LYS:CE	1:A:649:LYS:HB2	2.34	0.57
1:A:67:LEU:O	1:A:71:LYS:HG2	2.03	0.57
1:A:176:TRP:HA	1:A:184:PHE:O	2.04	0.57
1:A:214:THR:HB	1:A:218:GLY:O	2.05	0.56
1:A:233:CYS:HB3	1:A:259:CYS:CB	2.35	0.56
1:A:363:CYS:CB	1:A:390:CYS:SG	2.93	0.56
1:A:114:PRO:HD2	1:A:197:PRO:O	2.06	0.56
1:A:355:PHE:HB3	1:A:360:TYR:CE1	2.40	0.56
1:A:297:PHE:HB3	1:A:302:TYR:HE2	1.70	0.56
1:A:343:ASN:ND2	1:A:343:ASN:H	2.02	0.56
1:A:265:PHE:HE1	1:A:271:TYR:HB3	1.71	0.56
1:A:223:VAL:CG1	1:A:272:GLY:CA	2.80	0.56
1:A:545:ALA:O	1:A:546:SER:CB	2.51	0.56
1:A:576:LYS:HZ2	1:A:642:ASN:CB	2.19	0.56
1:A:113:PHE:CD2	1:A:113:PHE:C	2.79	0.56
1:A:480:GLN:CG	1:A:485:ILE:HD13	2.34	0.56
1:A:623:LEU:HD21	1:A:630:TYR:HE1	1.71	0.56
1:A:124:ILE:O	1:A:159:PHE:HA	2.07	0.55
1:A:252:ARG:NH2	1:A:254:ASP:OD2	2.39	0.55
1:A:590:ARG:HH11	1:A:602:PHE:HZ	1.54	0.55
1:A:360:TYR:CE2	1:A:364:THR:HG21	2.42	0.55
1:A:256:PHE:HA	1:A:279:LEU:HD13	1.88	0.55
1:A:621:VAL:HG12	1:A:632:PHE:CE1	2.41	0.55
1:A:644:SER:OG	1:A:647:SER:HB2	2.06	0.55
1:A:576:LYS:NZ	1:A:642:ASN:HB3	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:SER:O	1:A:438:ILE:HG12	2.07	0.54
1:A:611:ASN:HB2	1:A:645:LEU:HG	1.89	0.54
1:A:158:ARG:HH21	1:A:449:PRO:HD2	1.72	0.54
1:A:484:GLU:HB2	1:A:486:PHE:HE1	1.72	0.54
1:A:478:ILE:HG12	1:A:487:PHE:CD2	2.42	0.54
1:A:223:VAL:HG13	1:A:272:GLY:HA3	1.88	0.54
1:A:641:GLU:H	1:A:647:SER:CB	2.21	0.54
1:A:533:VAL:HG22	1:A:542:ILE:HD13	1.89	0.54
1:A:653:ILE:N	7:A:1094:HOH:O	2.39	0.54
1:A:53:TYR:HB3	1:A:97:MET:HE2	1.89	0.54
1:A:132:THR:HG23	1:A:132:THR:O	2.07	0.54
1:A:464:VAL:HG22	1:A:465:THR:N	2.22	0.54
1:A:623:LEU:N	1:A:623:LEU:HD22	2.23	0.54
1:A:127:ARG:HH21	1:A:311:THR:HG22	1.73	0.54
1:A:342:GLY:HA2	1:A:387:TRP:CZ2	2.43	0.54
1:A:473:ILE:HD12	1:A:489:LYS:HD3	1.89	0.53
1:A:214:THR:O	1:A:396:SER:HA	2.09	0.53
1:A:605:LEU:CB	1:A:608:ASP:HB2	2.37	0.53
1:A:638:LEU:HD21	1:A:650:PHE:CE1	2.43	0.53
1:A:158:ARG:HH21	1:A:449:PRO:CD	2.20	0.53
1:A:574:TRP:NE1	1:A:576:LYS:NZ	2.57	0.53
1:A:621:VAL:HG12	1:A:632:PHE:CZ	2.44	0.53
1:A:192:ALA:HB1	1:A:206:HIS:O	2.08	0.53
1:A:339:THR:HG22	1:A:346:GLY:CA	2.37	0.53
1:A:339:THR:HB	1:A:347:ALA:O	2.08	0.53
1:A:468:ILE:HD13	1:A:503:PRO:HG2	1.90	0.53
1:A:466:PRO:HB2	1:A:494:TRP:HH2	1.73	0.52
1:A:617:LEU:HD23	1:A:617:LEU:N	2.24	0.52
1:A:630:TYR:CD2	1:A:639:LYS:HB3	2.44	0.52
1:A:118:LYS:O	1:A:119:TRP:C	2.48	0.52
1:A:281:THR:HG23	1:A:289:GLN:O	2.10	0.52
1:A:175:ARG:O	1:A:176:TRP:C	2.46	0.52
1:A:236:PRO:HA	1:A:244:TYR:O	2.09	0.52
1:A:579:LYS:HB3	1:A:590:ARG:HD2	1.90	0.52
1:A:129:ILE:HD11	1:A:170:MET:HB3	1.91	0.52
1:A:435:GLN:HA	1:A:438:ILE:HG13	1.92	0.52
1:A:475:PHE:CB	1:A:478:ILE:HD11	2.37	0.52
1:A:628:HIS:HB3	1:A:630:TYR:CZ	2.45	0.52
1:A:498:THR:O	1:A:501:ASP:OD1	2.26	0.52
1:A:640:LEU:CD1	1:A:645:LEU:HA	2.34	0.52
1:A:588:PHE:CE2	1:A:609:ALA:HB3	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:529:GLU:HB2	1:A:531:LYS:HG3	1.92	0.52
1:A:641:GLU:N	1:A:647:SER:OG	2.43	0.52
1:A:119:TRP:HB2	1:A:445:TYR:OH	2.10	0.52
1:A:57:PHE:CZ	1:A:190:LEU:HD22	2.45	0.51
1:A:252:ARG:HH21	1:A:254:ASP:CG	2.11	0.51
1:A:576:LYS:HZ1	1:A:642:ASN:HA	1.74	0.51
1:A:64:SER:O	1:A:69:VAL:HG11	2.11	0.51
1:A:78:GLN:HG2	1:A:83:LEU:HD12	1.92	0.51
1:A:576:LYS:NZ	1:A:642:ASN:CB	2.73	0.51
1:A:66:ASN:OD1	1:A:69:VAL:HG22	2.11	0.51
1:A:551:GLY:O	1:A:554:LYS:HE2	2.11	0.51
1:A:630:TYR:HD2	1:A:639:LYS:HB3	1.76	0.51
1:A:119:TRP:NE1	1:A:408:ALA:O	2.43	0.51
1:A:576:LYS:NZ	1:A:642:ASN:CA	2.73	0.51
1:A:127:ARG:NH2	1:A:311:THR:HG22	2.25	0.51
1:A:137:PRO:O	1:A:138:GLU:C	2.49	0.51
1:A:472:ASP:OD1	1:A:654:LYS:NZ	2.43	0.51
1:A:623:LEU:HD21	1:A:630:TYR:CE1	2.45	0.51
1:A:224:LYS:CG	1:A:282:MET:HE1	2.41	0.50
1:A:433:LEU:HD13	1:A:438:ILE:HD13	1.93	0.50
1:A:573:ASN:HD21	1:A:578:LYS:HA	1.77	0.50
1:A:628:HIS:CE1	1:A:639:LYS:HD2	2.45	0.50
1:A:641:GLU:HB2	1:A:647:SER:OG	2.09	0.50
1:A:113:PHE:HD2	1:A:114:PRO:O	1.93	0.50
1:A:536:ALA:O	1:A:537:GLY:C	2.47	0.50
1:A:80:PHE:HA	1:A:415:GLN:NE2	2.26	0.50
1:A:632:PHE:CD1	1:A:632:PHE:N	2.79	0.50
1:A:66:ASN:N	1:A:69:VAL:CG2	2.68	0.50
1:A:363:CYS:HB3	1:A:390:CYS:SG	2.51	0.50
1:A:176:TRP:CE3	1:A:185:ASP:HA	2.46	0.50
1:A:513:TRP:HD1	1:A:543:TYR:CE2	2.30	0.50
1:A:114:PRO:HG2	1:A:197:PRO:O	2.12	0.50
1:A:212:LEU:O	1:A:212:LEU:HG	2.12	0.50
1:A:47:LYS:O	1:A:51:VAL:HG23	2.12	0.50
1:A:66:ASN:N	1:A:69:VAL:HG22	2.17	0.50
1:A:265:PHE:CE1	1:A:271:TYR:HB3	2.47	0.49
1:A:468:ILE:CD1	1:A:503:PRO:HG2	2.42	0.49
1:A:639:LYS:O	1:A:648:VAL:CG1	2.60	0.49
1:A:108:ALA:CB	1:A:110:TYR:CD1	2.88	0.49
1:A:108:ALA:O	1:A:110:TYR:N	2.45	0.49
1:A:475:PHE:CE1	1:A:487:PHE:HB3	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:GLU:HG2	1:A:427:TYR:OH	2.12	0.49
1:A:538:ASN:OD1	1:A:538:ASN:N	2.45	0.49
1:A:221:VAL:HB	1:A:233:CYS:SG	2.53	0.49
1:A:415:GLN:O	1:A:417:PRO:HD3	2.12	0.49
1:A:529:GLU:OE1	1:A:531:LYS:HE3	2.12	0.49
1:A:368:ARG:NH1	1:A:389:PHE:CZ	2.80	0.49
1:A:486:PHE:HB3	1:A:488:PHE:CE1	2.48	0.49
1:A:567:ARG:CB	1:A:567:ARG:CZ	2.91	0.49
1:A:53:TYR:CD1	1:A:97:MET:HE2	2.47	0.49
1:A:261:THR:HB	1:A:262:THR:HG23	1.94	0.49
1:A:57:PHE:CZ	1:A:101:ARG:CD	2.92	0.49
1:A:142:ASP:OD1	1:A:146:ARG:HG3	2.13	0.49
1:A:321:GLU:HG2	7:A:1078:HOH:O	2.13	0.49
1:A:339:THR:CG2	1:A:346:GLY:HA2	2.38	0.49
1:A:561:LEU:HD21	1:A:582:ILE:HD12	1.95	0.49
1:A:78:GLN:CG	1:A:83:LEU:HD12	2.42	0.49
1:A:586:ASP:HB3	1:A:615:ASP:OD2	2.13	0.49
1:A:533:VAL:HG22	1:A:542:ILE:CD1	2.43	0.48
1:A:247:CYS:HG	1:A:274:CYS:HG	0.51	0.48
1:A:442:GLN:O	1:A:445:TYR:O	2.30	0.48
1:A:513:TRP:O	1:A:516:LEU:HB2	2.13	0.48
1:A:554:LYS:CB	1:A:555:PRO:HD2	2.43	0.48
1:A:322:ASP:HB3	1:A:325:ARG:HB3	1.96	0.48
1:A:493:ILE:CG2	1:A:509:VAL:HB	2.44	0.48
1:A:583:PHE:CD1	1:A:583:PHE:N	2.81	0.48
1:A:618:ASP:OD1	1:A:633:LYS:HD2	2.13	0.48
1:A:639:LYS:HZ1	1:A:649:LYS:CB	2.26	0.48
1:A:90:ASP:O	1:A:91:GLN:C	2.52	0.48
1:A:623:LEU:H	1:A:623:LEU:HD22	1.76	0.48
1:A:54:LEU:HD12	1:A:70:LEU:HD12	1.96	0.48
1:A:60:CYS:HB2	1:A:73:THR:HG21	1.96	0.48
1:A:91:GLN:N	1:A:91:GLN:NE2	2.39	0.48
1:A:469:CYS:CB	1:A:660:CYS:HG	2.23	0.48
1:A:565:VAL:HG23	1:A:567:ARG:O	2.14	0.48
1:A:71:LYS:HA	1:A:87:GLY:CA	2.44	0.48
1:A:605:LEU:HB3	1:A:608:ASP:HB2	1.94	0.48
1:A:218:GLY:O	1:A:219:GLN:C	2.50	0.48
1:A:579:LYS:HG2	1:A:590:ARG:CG	2.44	0.48
1:A:280:PHE:HE2	1:A:282:MET:HE1	1.78	0.47
1:A:580:THR:O	1:A:591:TYR:N	2.47	0.47
1:A:320:THR:HG21	1:A:326:ASP:CB	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:602:PHE:HB3	1:A:603:PRO:CA	2.26	0.47
1:A:197:PRO:HG3	1:A:408:ALA:O	2.14	0.47
1:A:294:PRO:HA	1:A:302:TYR:O	2.14	0.47
1:A:176:TRP:O	1:A:183:PRO:HA	2.14	0.47
1:A:297:PHE:O	1:A:298:GLN:HG2	2.13	0.47
1:A:64:SER:O	1:A:69:VAL:HG21	2.14	0.47
1:A:108:ALA:C	1:A:110:TYR:HD1	2.18	0.47
1:A:134:ASP:OD2	1:A:212:LEU:HA	2.15	0.47
1:A:244:TYR:OH	1:A:250:THR:HG21	2.14	0.47
1:A:289:GLN:HB3	1:A:290:PRO:CD	2.45	0.47
1:A:524:TYR:CE2	1:A:533:VAL:HG11	2.50	0.47
1:A:577:ASN:OD1	1:A:577:ASN:N	2.48	0.47
1:A:646:LYS:O	1:A:646:LYS:HD3	2.14	0.47
1:A:343:ASN:ND2	1:A:386:LYS:HZ2	2.13	0.47
1:A:484:GLU:HG2	1:A:497:VAL:HG12	1.96	0.47
1:A:567:ARG:HB2	1:A:567:ARG:NH1	2.30	0.47
1:A:618:ASP:OD1	1:A:618:ASP:N	2.38	0.47
1:A:315:ARG:NH2	1:A:335:THR:OG1	2.48	0.47
1:A:654:LYS:HG3	1:A:660:CYS:SG	2.55	0.47
1:A:305:CYS:HB2	1:A:315:ARG:HD2	1.98	0.46
1:A:398:PHE:CE2	1:A:399:LEU:CD2	2.96	0.46
1:A:475:PHE:CD2	1:A:478:ILE:HD11	2.50	0.46
1:A:493:ILE:HG23	1:A:509:VAL:HB	1.98	0.46
1:A:488:PHE:HB3	1:A:520:ILE:HD11	1.96	0.46
1:A:78:GLN:HG2	1:A:83:LEU:HB2	1.97	0.46
1:A:281:THR:O	1:A:288:GLY:HA2	2.16	0.46
1:A:71:LYS:CB	1:A:87:GLY:HA3	2.44	0.46
1:A:343:ASN:HD22	1:A:344:SER:N	2.13	0.46
1:A:478:ILE:HG12	1:A:487:PHE:HD2	1.81	0.46
1:A:540:TYR:CZ	1:A:559:LEU:HD22	2.51	0.46
1:A:543:TYR:CD2	1:A:548:LEU:HA	2.50	0.46
1:A:83:LEU:HD13	1:A:93:THR:HA	1.96	0.46
1:A:484:GLU:OE1	1:A:495:ARG:NH1	2.36	0.46
1:A:176:TRP:O	1:A:184:PHE:N	2.38	0.46
1:A:502:LYS:HE2	1:A:503:PRO:CD	2.42	0.46
1:A:646:LYS:HD3	1:A:647:SER:N	2.30	0.46
1:A:224:LYS:HE2	1:A:224:LYS:CA	2.24	0.45
1:A:297:PHE:O	1:A:324:ASP:OD2	2.33	0.45
1:A:129:ILE:HD11	1:A:170:MET:CE	2.46	0.45
1:A:438:ILE:HG12	1:A:438:ILE:H	1.51	0.45
1:A:574:TRP:CE2	1:A:576:LYS:NZ	2.76	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:576:LYS:HZ1	1:A:642:ASN:CA	2.29	0.45
1:A:60:CYS:HA	1:A:61:PRO:HD3	1.80	0.45
1:A:538:ASN:O	1:A:556:LEU:HG	2.17	0.45
1:A:574:TRP:O	1:A:578:LYS:N	2.49	0.45
1:A:591:TYR:OH	7:A:1016:HOH:O	1.99	0.45
1:A:295:PHE:CE2	1:A:302:TYR:HB2	2.52	0.45
1:A:527:PRO:HG3	1:A:573:ASN:ND2	2.31	0.45
1:A:81:PHE:HZ	1:A:101:ARG:NH2	2.15	0.45
1:A:215:LEU:HD23	1:A:215:LEU:HA	1.65	0.45
1:A:481:ILE:CG2	1:A:482:ARG:N	2.73	0.45
1:A:79:LYS:HD2	1:A:85:GLN:NE2	2.32	0.45
1:A:403:HIS:O	1:A:403:HIS:CD2	2.69	0.45
1:A:46:ASP:CG	1:A:94:ILE:HD13	2.37	0.45
1:A:306:THR:HB	1:A:308:GLU:H	1.82	0.45
1:A:611:ASN:CB	1:A:645:LEU:CD1	2.82	0.45
1:A:118:LYS:O	1:A:118:LYS:CG	2.51	0.45
1:A:464:VAL:HG22	1:A:465:THR:H	1.80	0.45
1:A:513:TRP:N	1:A:514:PRO:HD3	2.32	0.45
1:A:280:PHE:CE2	1:A:282:MET:HE1	2.52	0.45
1:A:315:ARG:CG	1:A:315:ARG:NH1	2.74	0.44
1:A:524:TYR:CZ	1:A:580:THR:HG21	2.52	0.44
1:A:93:THR:O	1:A:97:MET:HG2	2.17	0.44
1:A:447:ALA:O	1:A:448:SER:OG	2.30	0.44
1:A:513:TRP:HD1	1:A:543:TYR:CD2	2.34	0.44
1:A:188:ASP:N	1:A:211:GLU:OE2	2.50	0.44
1:A:568:VAL:HG21	1:A:582:ILE:HG22	2.00	0.44
1:A:81:PHE:CE1	1:A:423:PRO:HG2	2.53	0.44
1:A:344:SER:HB3	1:A:347:ALA:HB3	2.00	0.44
1:A:406:GLY:O	1:A:411:LEU:HB2	2.17	0.44
1:A:512:PHE:HB2	1:A:513:TRP:CE3	2.53	0.44
1:A:633:LYS:HA	1:A:633:LYS:HD2	1.86	0.44
1:A:581:TYR:CE2	1:A:590:ARG:HD3	2.52	0.44
1:A:633:LYS:O	1:A:634:GLY:C	2.56	0.44
1:A:195:PHE:O	1:A:203:GLY:N	2.48	0.44
1:A:344:SER:CB	1:A:377:THR:HG21	2.48	0.44
1:A:83:LEU:CD1	1:A:93:THR:HA	2.47	0.44
1:A:331:PHE:C	1:A:333:PRO:HD3	2.38	0.44
1:A:641:GLU:H	1:A:647:SER:HB3	1.83	0.44
1:A:53:TYR:HB3	1:A:97:MET:CE	2.48	0.43
1:A:233:CYS:SG	1:A:259:CYS:CB	3.07	0.43
1:A:579:LYS:HE3	1:A:599:ASP:OD2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:654:LYS:HB3	1:A:654:LYS:HE3	1.52	0.43
1:A:224:LYS:HB2	1:A:273:PHE:O	2.18	0.43
1:A:605:LEU:HB2	1:A:608:ASP:HB2	2.00	0.43
1:A:639:LYS:HE3	1:A:649:LYS:C	2.38	0.43
1:A:34:ILE:HG22	1:A:34:ILE:O	2.17	0.43
1:A:300:THR:HG22	1:A:301:SER:N	2.33	0.43
1:A:641:GLU:CA	1:A:647:SER:OG	2.65	0.43
1:A:69:VAL:HG23	1:A:70:LEU:N	2.34	0.43
1:A:239:PHE:HB3	1:A:244:TYR:CE1	2.53	0.43
1:A:411:LEU:HD11	1:A:441:ILE:HD12	1.99	0.43
1:A:574:TRP:HE3	1:A:581:TYR:HE1	1.66	0.43
1:A:79:LYS:HB2	1:A:85:GLN:NE2	2.33	0.43
1:A:113:PHE:HB2	1:A:114:PRO:HD2	2.00	0.43
1:A:354:THR:HG21	7:A:1042:HOH:O	2.18	0.43
1:A:403:HIS:CD2	1:A:403:HIS:C	2.92	0.43
1:A:586:ASP:O	1:A:605:LEU:HD22	2.18	0.43
1:A:108:ALA:C	1:A:110:TYR:CD1	2.92	0.43
1:A:159:PHE:CE2	1:A:409:MET:HE1	2.54	0.43
1:A:267:LYS:HG3	1:A:268:ASP:N	2.34	0.43
1:A:70:LEU:HG	1:A:74:LEU:CD1	2.38	0.43
1:A:127:ARG:HH11	1:A:127:ARG:HD3	1.70	0.43
1:A:338:SER:O	1:A:391:PRO:HD3	2.19	0.43
1:A:416:ASP:HB3	1:A:419:ALA:HB2	2.01	0.43
1:A:557:THR:O	1:A:560:GLY:N	2.47	0.43
1:A:572:PHE:CD1	1:A:620:VAL:HG11	2.54	0.43
1:A:576:LYS:H	1:A:576:LYS:HG2	1.43	0.43
1:A:113:PHE:CD1	1:A:113:PHE:N	2.84	0.42
1:A:416:ASP:OD1	1:A:465:THR:HG21	2.18	0.42
1:A:488:PHE:CD2	1:A:493:ILE:HG22	2.54	0.42
1:A:644:SER:OG	1:A:647:SER:CB	2.67	0.42
1:A:638:LEU:CD2	1:A:650:PHE:CE1	3.02	0.42
1:A:340:VAL:O	1:A:389:PHE:HB2	2.20	0.42
1:A:355:PHE:CZ	1:A:356:LEU:HG	2.54	0.42
1:A:433:LEU:HB3	1:A:438:ILE:HD13	2.01	0.42
1:A:196:ALA:HB1	1:A:197:PRO:HD2	2.00	0.42
1:A:211:GLU:HA	1:A:211:GLU:OE1	2.18	0.42
1:A:480:GLN:OE1	1:A:623:LEU:HA	2.19	0.42
1:A:585:GLY:HA2	1:A:616:ASN:OD1	2.19	0.42
1:A:75:LYS:HA	1:A:78:GLN:OE1	2.20	0.42
1:A:154:VAL:HG11	1:A:438:ILE:CG2	2.43	0.42
1:A:323:TYR:HA	7:A:1030:HOH:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:PHE:HB2	1:A:114:PRO:CD	2.50	0.42
1:A:568:VAL:HG21	1:A:582:ILE:CG2	2.50	0.42
1:A:66:ASN:O	1:A:69:VAL:HG22	2.19	0.42
1:A:112:PHE:O	1:A:112:PHE:CG	2.71	0.42
1:A:462:GLY:HA2	1:A:463:PRO:HD3	1.80	0.42
1:A:567:ARG:CZ	1:A:567:ARG:HB3	2.50	0.42
1:A:556:LEU:O	1:A:557:THR:C	2.58	0.42
1:A:57:PHE:CE2	1:A:101:ARG:HD2	2.53	0.41
1:A:279:LEU:HD12	7:A:1067:HOH:O	2.20	0.41
1:A:343:ASN:ND2	1:A:343:ASN:N	2.64	0.41
1:A:513:TRP:HB2	1:A:516:LEU:HD22	2.01	0.41
1:A:564:ASP:OD1	1:A:565:VAL:N	2.52	0.41
1:A:617:LEU:HA	1:A:633:LYS:CD	2.36	0.41
1:A:59:GLY:O	1:A:60:CYS:C	2.57	0.41
1:A:438:ILE:O	1:A:442:GLN:HG3	2.20	0.41
1:A:73:THR:HA	1:A:76:LYS:CD	2.29	0.41
1:A:223:VAL:HG13	1:A:272:GLY:CA	2.48	0.41
1:A:350:VAL:O	1:A:353:PHE:HB3	2.19	0.41
1:A:155:THR:OG1	1:A:157:LEU:HD12	2.21	0.41
1:A:613:ILE:HG23	1:A:617:LEU:HD13	2.03	0.41
1:A:654:LYS:O	1:A:660:CYS:HB2	2.20	0.41
1:A:58:TYR:CZ	1:A:77:MET:HA	2.55	0.41
1:A:109:ASN:HD22	1:A:109:ASN:HA	1.62	0.41
1:A:239:PHE:HB3	1:A:244:TYR:HE1	1.85	0.41
1:A:613:ILE:CG2	1:A:617:LEU:HD13	2.51	0.41
1:A:81:PHE:HE1	1:A:423:PRO:HG2	1.86	0.41
1:A:171:ILE:HG23	1:A:207:PHE:HE1	1.85	0.41
1:A:207:PHE:CD1	1:A:207:PHE:N	2.89	0.41
1:A:524:TYR:CD2	1:A:533:VAL:HB	2.56	0.41
1:A:583:PHE:N	1:A:583:PHE:HD1	2.19	0.41
1:A:652:SER:H	1:A:656:ASP:CG	2.24	0.41
1:A:588:PHE:CE2	1:A:610:TRP:NE1	2.88	0.41
1:A:47:LYS:HE3	1:A:89:LEU:CD1	2.50	0.40
1:A:47:LYS:HE3	1:A:70:LEU:HD21	2.02	0.40
1:A:83:LEU:HB3	1:A:84:PRO:CD	2.51	0.40
1:A:109:ASN:O	1:A:113:PHE:CZ	2.71	0.40
1:A:297:PHE:HB3	1:A:302:TYR:CE2	2.54	0.40
1:A:623:LEU:CD2	1:A:630:TYR:HE1	2.34	0.40
1:A:574:TRP:CD1	1:A:576:LYS:HG2	2.57	0.40
1:A:645:LEU:CD1	1:A:645:LEU:C	2.72	0.40
1:A:162:ILE:HD12	1:A:164:ASP:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:646:LYS:C	1:A:646:LYS:CD	2.80	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:ASN:ND2	1:A:240:ASN:ND2[10_675]	1.61	0.59

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	615/631 (98%)	565 (92%)	38 (6%)	12 (2%)	7	24

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	186	GLY
1	A	448	SER
1	A	490	ASP
1	A	572	PHE
1	A	601	GLY
1	A	627	GLY
1	A	91	GLN
1	A	176	TRP
1	A	481	ILE
1	A	659	GLY
1	A	165	GLY
1	A	32	SER

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	518/527 (98%)	401 (77%)	117 (23%)	1 2

All (117) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	SER
1	A	34	ILE
1	A	35	ILE
1	A	47	LYS
1	A	60	CYS
1	A	62	LYS
1	A	65	CYS
1	A	67	LEU
1	A	74	LEU
1	A	91	GLN
1	A	92	ASN
1	A	95	GLU
1	A	97	MET
1	A	101	ARG
1	A	109	ASN
1	A	115	ARG
1	A	116	LYS
1	A	118	LYS
1	A	121	LYS
1	A	124	ILE
1	A	160	SER
1	A	161	ARG
1	A	166	GLU
1	A	172	ASN
1	A	201	VAL
1	A	212	LEU
1	A	217	GLU
1	A	224	LYS
1	A	234	LYS
1	A	253	SER

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Mol	Chain	Res	Type
1	A	257	LEU
1	A	264	ASN
1	A	267	LYS
1	A	296	ARG
1	A	298	GLN
1	A	306	THR
1	A	311	THR
1	A	312	ASP
1	A	315	ARG
1	A	319	THR
1	A	321	GLU
1	A	327	LYS
1	A	328	LYS
1	A	337	MET
1	A	338	SER
1	A	339	THR
1	A	343	ASN
1	A	358	ASN
1	A	359	LYS
1	A	362	SER
1	A	390	CYS
1	A	393	GLN
1	A	409	MET
1	A	424	ILE
1	A	429	LYS
1	A	432	ARG
1	A	433	LEU
1	A	438	ILE
1	A	439	LYS
1	A	443	GLU
1	A	448	SER
1	A	465	THR
1	A	468	ILE
1	A	476	ASP
1	A	480	GLN
1	A	493	ILE
1	A	495	ARG
1	A	498	THR
1	A	501	ASP
1	A	502	LYS
1	A	504	MET
1	A	507	LEU

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Mol	Chain	Res	Type
1	A	508	LEU
1	A	509	VAL
1	A	516	LEU
1	A	519	LYS
1	A	520	ILE
1	A	524	TYR
1	A	538	ASN
1	A	542	ILE
1	A	549	GLU
1	A	554	LYS
1	A	557	THR
1	A	559	LEU
1	A	565	VAL
1	A	568	VAL
1	A	569	ASP
1	A	575	SER
1	A	576	LYS
1	A	577	ASN
1	A	580	THR
1	A	582	ILE
1	A	583	PHE
1	A	586	ASP
1	A	587	LYS
1	A	590	ARG
1	A	594	VAL
1	A	605	LEU
1	A	608	ASP
1	A	618	ASP
1	A	623	LEU
1	A	628	HIS
1	A	629	SER
1	A	630	TYR
1	A	632	PHE
1	A	636	TYR
1	A	638	LEU
1	A	639	LYS
1	A	644	SER
1	A	645	LEU
1	A	646	LYS
1	A	648	VAL
1	A	652	SER
1	A	654	LYS

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Mol	Chain	Res	Type
1	A	655	SER
1	A	656	ASP
1	A	660	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	ASN
1	A	85	GLN
1	A	91	GLN
1	A	104	ASN
1	A	109	ASN
1	A	172	ASN
1	A	219	GLN
1	A	240	ASN
1	A	264	ASN
1	A	343	ASN
1	A	415	GLN
1	A	573	ASN
1	A	628	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 7 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	SO4	A	778	-	4,4,4	0.95	0	6,6,6	1.25	1 (16%)
6	SO4	A	777	-	4,4,4	0.60	0	6,6,6	0.28	0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	778	SO4	O4-S-O3	2.12	118.10	109.06

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	619/631 (98%)	0.28	42 (6%) 17 10	9, 43, 150, 274	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	113	PHE	24.4
1	A	109	ASN	17.0
1	A	114	PRO	13.4
1	A	111	ASN	12.1
1	A	112	PHE	10.3
1	A	110	TYR	10.1
1	A	646	LYS	6.9
1	A	116	LYS	6.6
1	A	625	GLY	4.6
1	A	31	PRO	4.5
1	A	650	PHE	4.5
1	A	500	ARG	4.2
1	A	659	GLY	4.0
1	A	639	LYS	3.9
1	A	651	GLY	3.7
1	A	449	PRO	3.7
1	A	70	LEU	3.5
1	A	638	LEU	3.4
1	A	581	TYR	3.3
1	A	32	SER	3.3
1	A	108	ALA	3.1
1	A	621	VAL	3.0
1	A	620	VAL	2.7
1	A	648	VAL	2.7
1	A	118	LYS	2.5
1	A	619	ALA	2.5
1	A	435	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	610	TRP	2.5
1	A	445	TYR	2.3
1	A	588	PHE	2.3
1	A	637	TYR	2.3
1	A	647	SER	2.3
1	A	89	LEU	2.3
1	A	87	GLY	2.2
1	A	657	TRP	2.2
1	A	461	LEU	2.2
1	A	574	TRP	2.1
1	A	572	PHE	2.1
1	A	618	ASP	2.1
1	A	71	LYS	2.1
1	A	628	HIS	2.1
1	A	491	ARG	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 monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	NA	A	996	1/1	0.67	0.34	61,61,61,61	0
3	CA	A	994	1/1	0.82	0.19	63,63,63,63	0
3	CA	A	993	1/1	0.84	0.12	108,108,108,108	0
4	CL	A	995	1/1	0.89	0.41	58,58,58,58	0
6	SO4	A	777	5/5	0.89	0.23	81,82,82,83	0
3	CA	A	992	1/1	0.92	0.19	23,23,23,23	0
6	SO4	A	778	5/5	0.94	0.19	34,41,45,45	0
2	ZN	A	991	1/1	0.97	0.09	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	ZN	A	990	1/1	0.99	0.14	35,35,35,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.