



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:04 PM UTC

PDB ID : 1CK7 / pdb_00001ck7
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 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
Mogul : 2022.3.0, CSD as543be (2022)
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

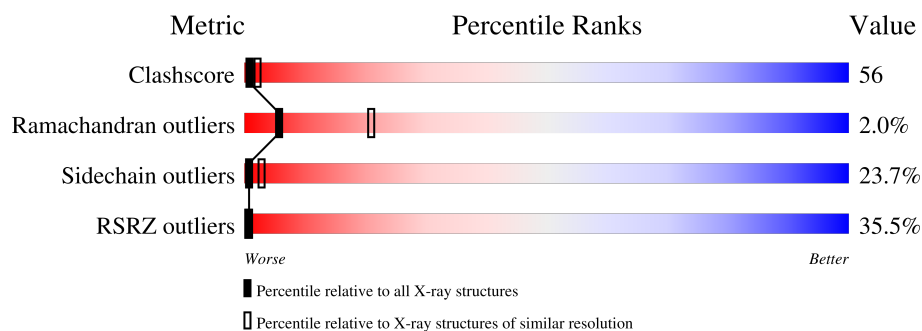
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

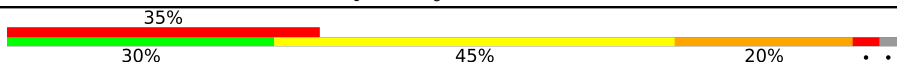
The reported resolution of this entry is 2.80 Å.

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	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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 (CCD ID: ZN) (formula: Zn).

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

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 6 is SULFATE ION (CCD ID: 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		

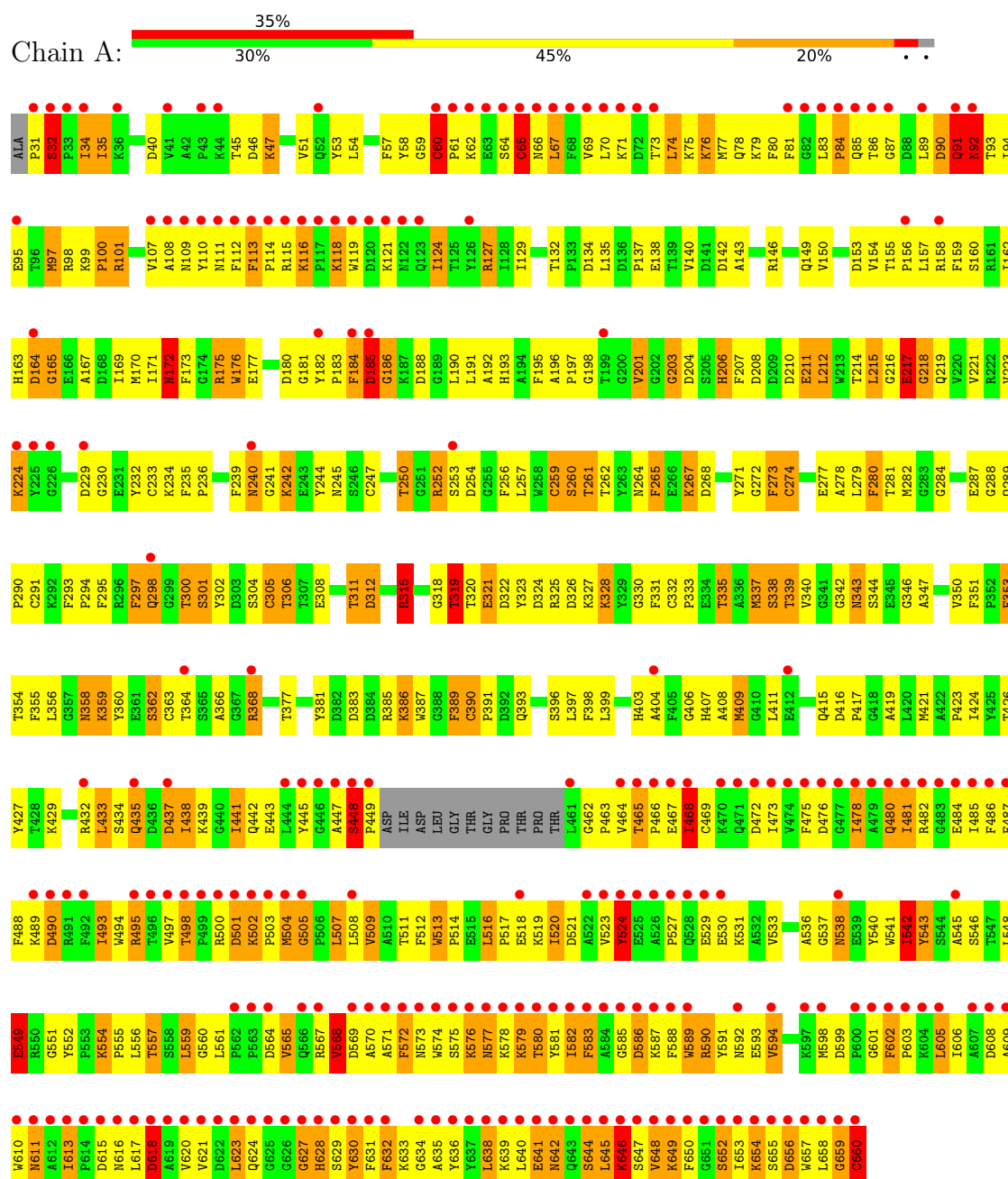
- Molecule 7 is water.

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

3 Residue-property plots

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: PROTEIN (GELATINASE A)



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 34.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (34.00-2.80) 98.8 (34.00-2.80)	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 (Not available) , (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)	0.31 , 69.1	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: ZN, CA, CL, NA, SO4

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	1.35	1/5085 (0.0%)	1.83	139/6891 (2.0%)

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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	660	CYS	C-OXT	78.16	2.79	1.23

All (139) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	659	GLY	CA-C-N	14.77	148.28	121.70
1	A	659	GLY	C-N-CA	14.77	148.28	121.70
1	A	435	GLN	OE1-CD-NE2	-14.29	108.31	122.60
1	A	113	PHE	CA-CB-CG	-12.85	100.95	113.80
1	A	218	GLY	O-C-N	-10.80	114.25	123.43
1	A	193	HIS	CA-CB-CG	10.60	124.40	113.80
1	A	524	TYR	CA-CB-CG	10.30	132.45	113.90
1	A	211	GLU	CA-C-N	-10.15	108.84	123.05
1	A	211	GLU	C-N-CA	-10.15	108.84	123.05
1	A	229	ASP	O-C-N	-9.60	111.94	122.12
1	A	641	GLU	N-CA-CB	9.35	125.66	110.41
1	A	435	GLN	CG-CD-NE2	9.31	130.37	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	273	PHE	CA-CB-CG	-8.93	104.87	113.80
1	A	280	PHE	CA-CB-CG	8.88	122.67	113.80
1	A	330	GLY	CA-C-O	-8.73	111.96	121.48
1	A	613	ILE	N-CA-C	8.63	116.48	107.76
1	A	297	PHE	CA-C-N	-8.52	105.27	121.54
1	A	297	PHE	C-N-CA	-8.52	105.27	121.54
1	A	182	TYR	N-CA-CB	-8.48	98.74	111.21
1	A	305	CYS	CA-C-O	-8.38	111.92	121.81
1	A	186	GLY	O-C-N	-8.20	112.03	122.70
1	A	107	VAL	N-CA-C	8.18	120.39	108.53
1	A	240	ASN	CA-C-N	-8.01	109.47	122.20
1	A	240	ASN	C-N-CA	-8.01	109.47	122.20
1	A	163	HIS	CA-CB-CG	-7.96	105.84	113.80
1	A	358	ASN	CA-CB-CG	7.83	120.44	112.60
1	A	353	PHE	CA-C-N	-7.82	112.22	123.00
1	A	353	PHE	C-N-CA	-7.82	112.22	123.00
1	A	92	ASN	CA-CB-CG	7.69	120.29	112.60
1	A	172	ASN	CA-CB-CG	-7.26	105.34	112.60
1	A	385	ARG	CD-NE-CZ	7.04	134.25	124.40
1	A	60	CYS	CB-CA-C	7.03	121.22	109.69
1	A	180	ASP	CA-CB-CG	-7.02	105.58	112.60
1	A	611	ASN	CA-CB-CG	6.62	119.22	112.60
1	A	217	GLU	CA-C-N	-6.59	113.42	122.57
1	A	217	GLU	C-N-CA	-6.59	113.42	122.57
1	A	284	GLY	CA-C-O	-6.57	113.55	121.83
1	A	60	CYS	CA-CB-SG	6.54	129.44	114.40
1	A	589	TRP	CA-CB-CG	6.53	126.00	113.60
1	A	304	SER	CA-C-O	-6.46	114.37	121.28
1	A	549	GLU	CA-C-O	6.44	128.27	121.19
1	A	618	ASP	CA-C-N	-6.43	112.07	122.36
1	A	618	ASP	C-N-CA	-6.43	112.07	122.36
1	A	208	ASP	CA-CB-CG	-6.42	106.18	112.60
1	A	116	LYS	CA-C-O	6.36	123.42	119.29
1	A	315	ARG	CA-CB-CG	6.35	126.79	114.10
1	A	35	ILE	CA-C-O	-6.32	115.11	121.49
1	A	107	VAL	O-C-N	6.29	129.56	123.14
1	A	184	PHE	CA-C-N	-6.28	114.14	123.00
1	A	184	PHE	C-N-CA	-6.28	114.14	123.00
1	A	181	GLY	CA-C-O	6.27	126.01	118.86
1	A	284	GLY	N-CA-C	-6.24	101.36	112.22
1	A	175	ARG	CB-CA-C	-6.24	103.32	113.37
1	A	362	SER	CA-C-O	-6.20	114.64	121.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	642	ASN	CA-CB-CG	-6.13	106.47	112.60
1	A	541	TRP	CA-C-N	-6.11	115.61	123.19
1	A	541	TRP	C-N-CA	-6.11	115.61	123.19
1	A	513	TRP	CA-C-O	6.10	127.98	121.28
1	A	260	SER	CA-C-N	6.09	129.57	120.31
1	A	260	SER	C-N-CA	6.09	129.57	120.31
1	A	175	ARG	CA-CB-CG	-6.02	102.06	114.10
1	A	298	GLN	OE1-CD-NE2	6.02	128.62	122.60
1	A	319	THR	CA-C-O	6.00	126.54	119.28
1	A	278	ALA	N-CA-C	-5.96	105.50	112.89
1	A	383	ASP	O-C-N	-5.88	115.45	122.15
1	A	259	CYS	CA-C-O	-5.87	114.99	121.33
1	A	218	GLY	CA-C-N	-5.87	112.38	120.71
1	A	218	GLY	C-N-CA	-5.87	112.38	120.71
1	A	435	GLN	CA-C-N	5.83	128.36	120.38
1	A	435	GLN	C-N-CA	5.83	128.36	120.38
1	A	389	PHE	CA-C-O	-5.83	114.41	121.05
1	A	235	PHE	CA-CB-CG	5.80	119.60	113.80
1	A	437	ASP	CA-CB-CG	5.79	118.39	112.60
1	A	543	TYR	O-C-N	5.79	130.87	123.11
1	A	245	ASN	CA-CB-CG	-5.74	106.86	112.60
1	A	642	ASN	CB-CA-C	5.74	119.89	110.88
1	A	359	LYS	CA-C-O	-5.68	114.49	120.80
1	A	359	LYS	O-C-N	5.66	129.81	123.19
1	A	241	GLY	CA-C-O	-5.63	112.96	119.10
1	A	261	THR	CB-CA-C	-5.62	99.89	110.67
1	A	397	LEU	N-CA-C	-5.60	105.32	111.82
1	A	468	ILE	N-CA-C	5.59	115.79	110.53
1	A	521	ASP	N-CA-C	-5.57	106.84	113.97
1	A	300	THR	CA-C-N	-5.56	115.38	122.77
1	A	300	THR	C-N-CA	-5.56	115.38	122.77
1	A	312	ASP	CA-CB-CG	5.55	118.15	112.60
1	A	318	GLY	CA-C-O	5.54	126.74	121.64
1	A	35	ILE	O-C-N	5.54	129.23	122.58
1	A	660	CYS	CA-CB-SG	5.52	127.09	114.40
1	A	229	ASP	CA-C-O	5.51	126.58	120.63
1	A	242	LYS	CA-CB-CG	5.50	125.11	114.10
1	A	301	SER	CA-C-O	-5.50	114.47	120.36
1	A	274	CYS	CA-C-O	5.50	124.81	120.19
1	A	164	ASP	CA-CB-CG	-5.49	107.11	112.60
1	A	293	PHE	CA-C-O	-5.49	112.86	119.67
1	A	177	GLU	CA-C-O	-5.49	115.21	120.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	649	LYS	O-C-N	-5.44	115.35	122.59
1	A	297	PHE	N-CA-CB	5.44	119.68	110.49
1	A	60	CYS	CA-C-N	5.44	125.38	119.78
1	A	60	CYS	C-N-CA	5.44	125.38	119.78
1	A	92	ASN	N-CA-CB	5.43	118.41	110.47
1	A	127	ARG	CA-C-N	-5.43	115.59	122.43
1	A	127	ARG	C-N-CA	-5.43	115.59	122.43
1	A	91	GLN	OE1-CD-NE2	-5.42	117.18	122.60
1	A	287	GLU	CA-C-N	5.40	131.82	122.05
1	A	287	GLU	C-N-CA	5.40	131.82	122.05
1	A	177	GLU	N-CA-CB	-5.37	102.35	110.35
1	A	505	GLY	CA-C-O	-5.36	113.85	121.52
1	A	335	THR	CA-C-O	-5.31	113.56	120.25
1	A	65	CYS	CA-C-N	5.30	130.91	122.10
1	A	65	CYS	C-N-CA	5.30	130.91	122.10
1	A	216	GLY	N-CA-C	-5.30	107.91	113.58
1	A	646	LYS	N-CA-C	-5.27	105.96	112.38
1	A	568	VAL	CA-C-O	-5.26	114.69	120.43
1	A	252	ARG	NH1-CZ-NH2	5.26	126.13	119.30
1	A	84	PRO	CA-C-N	-5.23	115.47	122.42
1	A	84	PRO	C-N-CA	-5.23	115.47	122.42
1	A	517	PRO	CA-C-N	5.22	127.53	120.38
1	A	517	PRO	C-N-CA	5.22	127.53	120.38
1	A	542	ILE	CA-C-N	-5.18	114.10	122.81
1	A	542	ILE	C-N-CA	-5.18	114.10	122.81
1	A	206	HIS	CA-CB-CG	-5.16	108.64	113.80
1	A	656	ASP	CA-CB-CG	5.16	117.76	112.60
1	A	100	PRO	O-C-N	5.16	129.54	122.99
1	A	319	THR	N-CA-CB	-5.15	102.56	110.44
1	A	203	GLY	CA-C-O	5.14	124.71	119.10
1	A	216	GLY	CA-C-O	5.14	124.20	119.83
1	A	368	ARG	CA-CB-CG	5.14	124.39	114.10
1	A	602	PHE	CA-C-O	-5.12	113.14	120.16
1	A	301	SER	O-C-N	5.11	129.04	123.22
1	A	435	GLN	CB-CG-CD	5.10	121.26	112.60
1	A	359	LYS	CA-C-N	5.05	130.12	122.99
1	A	359	LYS	C-N-CA	5.05	130.12	122.99
1	A	185	ASP	CA-C-O	-5.04	114.90	120.30
1	A	240	ASN	O-C-N	-5.03	115.81	122.40
1	A	265	PHE	CA-CB-CG	-5.02	108.78	113.80
1	A	513	TRP	CA-C-N	5.02	124.68	119.56
1	A	513	TRP	C-N-CA	5.02	124.68	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	230	GLY	N-CA-C	5.01	120.88	114.66

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 [i](#)

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	534	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	534	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 56.

All (534) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:645:LEU:C	1:A:645:LEU:HD13	1.98	0.89
1:A:118:LYS:O	1:A:118:LYS:HG2	1.69	0.89
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: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:646:LYS:C	1:A:646:LYS:HD3	2.06	0.80
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:LEU:HD21	1:A:89:LEU:HD23	1.64	0.80
1:A:109:ASN:CG	1:A:113:PHE:CZ	2.59	0.79
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:53:TYR:CG	1:A:97:MET:HE2	2.18	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
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: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:280:PHE:CE2	1:A:282:MET:HE1	2.20	0.75
1:A:242:LYS:HZ1	1:A:351:PHE:HD2	1.32	0.75
1:A:639:LYS:HG2	1:A:649:LYS:O	1.87	0.75
1:A:129:ILE:HD11	1:A:170:MET:HE3	1.66	0.74
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:53:TYR:CB	1:A:97:MET:HE2	2.17	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:280:PHE:HE2	1:A:282:MET:HE1	1.54	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:518:GLU:H	1:A:518:GLU:CD	2.00	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
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: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: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:533:VAL:HG22	1:A:542:ILE:HG23	1.78	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:53:TYR:HB3	1:A:97:MET:HE2	1.78	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:504:MET:HE1	1:A:507:LEU:HD22	1.81	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
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:489:LYS:HG3	1:A:490:ASP:N	2.09	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:31:PRO:O	1:A:32:SER:OG	2.12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:113:PHE:C	1:A:113:PHE:CD2	2.79	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: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
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:118:LYS:O	1:A:119:TRP:C	2.48	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:175:ARG:O	1:A:176:TRP:C	2.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:LEU:O	1:A:71:LYS:HG2	2.03	0.57
1:A:176:TRP:H	1:A:176:TRP:CD1	2.21	0.57
1:A:576:LYS:HZ2	1:A:642:ASN:CB	2.18	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:252:ARG:HH21	1:A:254:ASP:CG	2.11	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: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:536:ALA:O	1:A:537:GLY:C	2.47	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:90:ASP:O	1:A:91:GLN:C	2.52	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:574:TRP:NE1	1:A:576:LYS:HZ3	2.06	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:281:THR:HG23	1:A:289:GLN:O	2.10	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:504:MET:HE2	1:A:505:GLY:N	2.24	0.52
1:A:218:GLY:O	1:A:219:GLN:C	2.50	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:469:CYS:HG	1:A:660:CYS:HG	1.08	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
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:108:ALA:C	1:A:110:TYR:HD1	2.18	0.51
1:A:57:PHE:CZ	1:A:190:LEU:HD22	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:ARG:NH2	1:A:311:THR:HG22	2.25	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:137:PRO:O	1:A:138:GLU:C	2.49	0.51
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: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:576:LYS:HZ1	1:A:642:ASN:HA	1.75	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
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:46:ASP:CG	1:A:94:ILE:HD13	2.37	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:633:LYS:O	1:A:634:GLY:C	2.56	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:331:PHE:C	1:A:333:PRO:HD3	2.38	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:639:LYS:HE3	1:A:649:LYS:C	2.38	0.48
1:A:504:MET:HE1	1:A:507:LEU:CD2	2.44	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: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:403:HIS:C	1:A:403:HIS:CD2	2.92	0.48
1:A:579:LYS:HG2	1:A:590:ARG:CG	2.44	0.48
1:A:108:ALA:C	1:A:110:TYR:CD1	2.92	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:556:LEU:O	1:A:557:THR:C	2.58	0.46
1:A:78:GLN:HG2	1:A:83:LEU:HB2	1.97	0.46
1:A:159:PHE:CZ	1:A:409:MET:HE3	2.51	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:59:GLY:O	1:A:60:CYS:C	2.57	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:421:MET:HE3	1:A:421:MET:HB3	1.78	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
1:A:652:SER:H	1:A:656:ASP:CG	2.24	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:646:LYS:HD3	1:A:647:SER:N	2.30	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:HIS:CD2	1:A:403:HIS:O	2.69	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:646:LYS:C	1:A:646:LYS:CD	2.80	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:169:ILE:HD11	1:A:409:MET:HE1	1.98	0.44
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: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:149:GLN:O	1:A:150:VAL:C	2.60	0.44
1:A:188:ASP:H	1:A:211:GLU:CD	2.26	0.44
1:A:344:SER:HB3	1:A:347:ALA:HB3	2.00	0.44
1:A:447:ALA:O	1:A:448:SER:OG	2.30	0.44
1:A:343:ASN:HD22	1:A:343:ASN:C	2.25	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:576:LYS:HZ1	1:A:642:ASN:CA	2.30	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:641:GLU:H	1:A:647:SER:HB3	1.83	0.44
1:A:645:LEU:C	1:A:645:LEU:CD1	2.72	0.44
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
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:34:ILE:HG22	1:A:34:ILE:O	2.17	0.43
1:A:277:GLU:H	1:A:277:GLU:CD	2.25	0.43
1:A:641:GLU:CA	1:A:647:SER:OG	2.65	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:648:VAL:C	1:A:649:LYS:HG3	2.41	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:586:ASP:O	1:A:605:LEU:HD22	2.18	0.43
1:A:267:LYS:HG3	1:A:268:ASP:N	2.34	0.43
1:A:300:THR:HG22	1:A:301:SER:N	2.33	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:109:ASN:C	1:A:113:PHE:HZ	2.26	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:53:TYR:CD1	1:A:97:MET:HE2	2.53	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:381:TYR:CD1	1:A:381:TYR:C	2.97	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
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:69:VAL:HG23	1:A:70:LEU:N	2.34	0.42
1:A:111:ASN:O	1:A:111:ASN:CG	2.62	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:57:PHE:CE2	1:A:101:ARG:HD2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:ILE:CD1	1:A:409:MET:HE1	2.50	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:438:ILE:O	1:A:442:GLN:HG3	2.20	0.41
1:A:175:ARG:HH21	1:A:210:ASP:CG	2.28	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:142:ASP:O	1:A:143:ALA:C	2.62	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: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:109:ASN:C	1:A:113:PHE:CZ	3.00	0.40
1:A:574:TRP:CD1	1:A:576:LYS:HG2	2.57	0.40
1:A:162:ILE:HD12	1:A:164:ASP:O	2.21	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

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	615/631 (98%)	565 (92%)	38 (6%)	12 (2%)	6	21

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%)	395 (76%)	123 (24%)	1	3

All (123) 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	45	THR
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	76	LYS
1	A	90	ASP
1	A	91	GLN
1	A	92	ASN
1	A	95	GLU
1	A	97	MET
1	A	98	ARG
1	A	99	LYS
1	A	101	ARG
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	172	ASN
1	A	201	VAL
1	A	212	LEU
1	A	215	LEU
1	A	217	GLU
1	A	224	LYS
1	A	234	LYS
1	A	250	THR
1	A	253	SER
1	A	257	LEU
1	A	264	ASN
1	A	267	LYS
1	A	306	THR
1	A	311	THR
1	A	312	ASP
1	A	315	ARG
1	A	319	THR
1	A	321	GLU

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Mol	Chain	Res	Type
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	386	LYS
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	441	ILE
1	A	443	GLU
1	A	448	SER
1	A	465	THR
1	A	468	ILE
1	A	476	ASP
1	A	478	ILE
1	A	480	GLN
1	A	493	ILE
1	A	495	ARG
1	A	498	THR
1	A	500	ARG
1	A	501	ASP
1	A	502	LYS
1	A	504	MET
1	A	507	LEU
1	A	508	LEU
1	A	509	VAL
1	A	516	LEU
1	A	519	LYS
1	A	520	ILE
1	A	523	VAL
1	A	524	TYR

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Mol	Chain	Res	Type
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	579	LYS
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	593	GLU
1	A	594	VAL
1	A	605	LEU
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	644	SER
1	A	645	LEU
1	A	646	LYS
1	A	648	VAL
1	A	652	SER
1	A	654	LYS
1	A	655	SER
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 oligosaccharides 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	0.99	0	6,6,6	1.16	0
6	SO4	A	777	-	4,4,4	0.68	0	6,6,6	0.21	0

There are no bond length outliers.

There are no bond angle outliers.

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%)	1.78	220 (35%) 1 0	9, 43, 150, 274	0

All (220) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	111	ASN	12.3
1	A	109	ASN	9.9
1	A	113	PHE	9.9
1	A	650	PHE	9.4
1	A	110	TYR	8.3
1	A	648	VAL	8.1
1	A	67	LEU	8.1
1	A	108	ALA	7.9
1	A	499	PRO	7.8
1	A	651	GLY	7.7
1	A	638	LEU	7.4
1	A	637	TYR	7.2
1	A	118	LYS	6.9
1	A	643	GLN	6.9
1	A	68	PHE	6.8
1	A	115	ARG	6.6
1	A	645	LEU	6.6
1	A	117	PRO	6.6
1	A	639	LYS	6.5
1	A	116	LYS	6.5
1	A	528	GLN	6.4
1	A	646	LYS	6.3
1	A	652	SER	6.2
1	A	624	GLN	6.2
1	A	636	TYR	6.2
1	A	69	VAL	6.1
1	A	657	TRP	6.1

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Mol	Chain	Res	Type	RSRZ
1	A	107	VAL	6.1
1	A	604	LYS	6.1
1	A	66	ASN	6.0
1	A	114	PRO	6.0
1	A	461	LEU	6.0
1	A	112	PHE	5.9
1	A	659	GLY	5.7
1	A	603	PRO	5.7
1	A	62	LYS	5.7
1	A	617	LEU	5.7
1	A	449	PRO	5.6
1	A	497	VAL	5.6
1	A	581	TYR	5.5
1	A	445	TYR	5.5
1	A	71	LYS	5.3
1	A	649	LYS	5.3
1	A	87	GLY	5.2
1	A	91	GLN	5.1
1	A	504	MET	5.0
1	A	120	ASP	5.0
1	A	621	VAL	5.0
1	A	572	PHE	4.9
1	A	471	GLN	4.9
1	A	65	CYS	4.9
1	A	70	LEU	4.8
1	A	226	GLY	4.8
1	A	484	GLU	4.8
1	A	629	SER	4.7
1	A	491	ARG	4.7
1	A	618	ASP	4.6
1	A	72	ASP	4.6
1	A	579	LYS	4.6
1	A	447	ALA	4.5
1	A	473	ILE	4.5
1	A	612	ALA	4.5
1	A	634	GLY	4.5
1	A	575	SER	4.4
1	A	31	PRO	4.4
1	A	85	GLN	4.4
1	A	158	ARG	4.4
1	A	526	ALA	4.4
1	A	483	GLY	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	614	PRO	4.3
1	A	588	PHE	4.2
1	A	597	LYS	4.2
1	A	527	PRO	4.2
1	A	607	ALA	4.2
1	A	628	HIS	4.2
1	A	656	ASP	4.1
1	A	640	LEU	4.1
1	A	503	PRO	4.1
1	A	653	ILE	4.1
1	A	654	LYS	4.0
1	A	446	GLY	4.0
1	A	481	ILE	4.0
1	A	435	GLN	4.0
1	A	658	LEU	3.9
1	A	478	ILE	3.9
1	A	615	ASP	3.9
1	A	605	LEU	3.9
1	A	482	ARG	3.9
1	A	625	GLY	3.8
1	A	608	ASP	3.8
1	A	468	ILE	3.8
1	A	613	ILE	3.8
1	A	620	VAL	3.8
1	A	616	ASN	3.8
1	A	83	LEU	3.8
1	A	602	PHE	3.8
1	A	610	TRP	3.8
1	A	655	SER	3.7
1	A	464	VAL	3.7
1	A	33	PRO	3.7
1	A	601	GLY	3.7
1	A	44	LYS	3.6
1	A	485	ILE	3.6
1	A	185	ASP	3.6
1	A	477	GLY	3.6
1	A	626	GLY	3.6
1	A	529	GLU	3.6
1	A	642	ASN	3.6
1	A	619	ALA	3.6
1	A	500	ARG	3.6
1	A	594	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	84	PRO	3.6
1	A	573	ASN	3.5
1	A	502	LYS	3.5
1	A	630	TYR	3.5
1	A	495	ARG	3.5
1	A	489	LYS	3.4
1	A	622	ASP	3.4
1	A	545	ALA	3.4
1	A	164	ASP	3.4
1	A	64	SER	3.4
1	A	474	VAL	3.3
1	A	587	LYS	3.3
1	A	123	GLN	3.3
1	A	583	PHE	3.3
1	A	570	ALA	3.3
1	A	567	ARG	3.3
1	A	89	LEU	3.3
1	A	563	PRO	3.2
1	A	571	ALA	3.2
1	A	564	ASP	3.2
1	A	498	THR	3.2
1	A	466	PRO	3.2
1	A	465	THR	3.1
1	A	229	ASP	3.1
1	A	580	THR	3.1
1	A	623	LEU	3.1
1	A	574	TRP	3.1
1	A	32	SER	3.1
1	A	566	GLN	3.1
1	A	470	LYS	3.1
1	A	480	GLN	3.0
1	A	86	THR	3.0
1	A	611	ASN	3.0
1	A	122	ASN	3.0
1	A	43	PRO	3.0
1	A	224	LYS	3.0
1	A	121	LYS	2.9
1	A	631	PHE	2.9
1	A	432	ARG	2.9
1	A	472	ASP	2.9
1	A	578	LYS	2.9
1	A	298	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	644	SER	2.9
1	A	635	ALA	2.9
1	A	660	CYS	2.8
1	A	518	GLU	2.8
1	A	569	ASP	2.8
1	A	586	ASP	2.8
1	A	585	GLY	2.8
1	A	490	ASP	2.8
1	A	600	PRO	2.8
1	A	34	ILE	2.8
1	A	364	THR	2.8
1	A	63	GLU	2.7
1	A	52	GLN	2.7
1	A	501	ASP	2.7
1	A	525	GLU	2.7
1	A	609	ALA	2.7
1	A	156	PRO	2.6
1	A	584	ALA	2.6
1	A	577	ASN	2.6
1	A	476	ASP	2.6
1	A	505	GLY	2.6
1	A	444	LEU	2.6
1	A	95	GLU	2.6
1	A	81	PHE	2.6
1	A	119	TRP	2.5
1	A	182	TYR	2.5
1	A	641	GLU	2.5
1	A	253	SER	2.5
1	A	61	PRO	2.5
1	A	582	ILE	2.5
1	A	92	ASN	2.5
1	A	448	SER	2.5
1	A	496	THR	2.5
1	A	524	TYR	2.4
1	A	60	CYS	2.4
1	A	562	PRO	2.4
1	A	82	GLY	2.4
1	A	523	VAL	2.4
1	A	508	LEU	2.4
1	A	404	ALA	2.4
1	A	576	LYS	2.4
1	A	475	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	199	THR	2.4
1	A	647	SER	2.3
1	A	36	LYS	2.3
1	A	627	GLY	2.3
1	A	184	PHE	2.3
1	A	632	PHE	2.3
1	A	240	ASN	2.3
1	A	538	ASN	2.3
1	A	486	PHE	2.3
1	A	437	ASP	2.3
1	A	126	TYR	2.3
1	A	225	TYR	2.3
1	A	412	GLU	2.2
1	A	492	PHE	2.2
1	A	467	GLU	2.2
1	A	522	ALA	2.2
1	A	73	THR	2.2
1	A	368	ARG	2.1
1	A	41	VAL	2.1
1	A	589	TRP	2.1
1	A	487	PHE	2.1
1	A	598	MET	2.0
1	A	479	ALA	2.0
1	A	530	GLU	2.0
1	A	592	ASN	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 oligosaccharides in this entry.

6.4 Ligands ⓘ

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($\text{\AA}^2$)	Q<0.9
3	CA	A	994	1/1	0.77	0.11	63,63,63,63	0
5	NA	A	996	1/1	0.79	0.17	61,61,61,61	0
6	SO4	A	777	5/5	0.85	0.23	81,82,82,83	0
4	CL	A	995	1/1	0.88	0.18	58,58,58,58	0
3	CA	A	993	1/1	0.91	0.13	108,108,108,108	0
6	SO4	A	778	5/5	0.91	0.14	34,41,45,45	0
3	CA	A	992	1/1	0.94	0.05	23,23,23,23	0
2	ZN	A	991	1/1	0.98	0.03	28,28,28,28	0
2	ZN	A	990	1/1	0.99	0.03	35,35,35,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.