



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:44 PM UTC

PDB ID : 1Z6R / pdb_00001z6r
Title : Crystal structure of Mlc from Escherichia coli
Authors : Schiefner, A.; Gerber, K.; Seitz, S.; Welte, W.; Diederichs, K.; Boos, W.
Deposited on : 2005-03-23
Resolution : 2.70 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

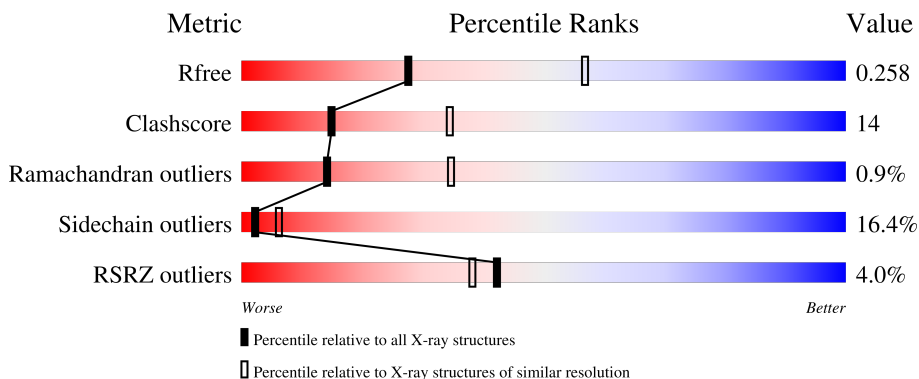
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	406	
1	B	406	
1	C	406	
1	D	406	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11728 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 Mlc protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	382	Total	C	N	O	S	Se	0	0	0
			2931	1855	514	549	4	9			
1	B	382	Total	C	N	O	S	Se	0	0	0
			2931	1855	514	549	4	9			
1	C	382	Total	C	N	O	S	Se	0	0	0
			2931	1855	514	549	4	9			
1	D	382	Total	C	N	O	S	Se	0	0	0
			2931	1855	514	549	4	9			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP P50456
A	52	HIS	ARG	engineered mutation	UNP P50456
A	54	MSE	MET	modified residue	UNP P50456
A	167	MSE	MET	modified residue	UNP P50456
A	176	MSE	MET	modified residue	UNP P50456
A	201	MSE	MET	modified residue	UNP P50456
A	286	MSE	MET	modified residue	UNP P50456
A	289	MSE	MET	modified residue	UNP P50456
A	329	MSE	MET	modified residue	UNP P50456
A	384	MSE	MET	modified residue	UNP P50456
A	394	MSE	MET	modified residue	UNP P50456
B	1	MSE	MET	modified residue	UNP P50456
B	52	HIS	ARG	engineered mutation	UNP P50456
B	54	MSE	MET	modified residue	UNP P50456
B	167	MSE	MET	modified residue	UNP P50456
B	176	MSE	MET	modified residue	UNP P50456
B	201	MSE	MET	modified residue	UNP P50456
B	286	MSE	MET	modified residue	UNP P50456
B	289	MSE	MET	modified residue	UNP P50456
B	329	MSE	MET	modified residue	UNP P50456
B	384	MSE	MET	modified residue	UNP P50456

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Chain	Residue	Modelled	Actual	Comment	Reference
B	394	MSE	MET	modified residue	UNP P50456
C	1	MSE	MET	modified residue	UNP P50456
C	52	HIS	ARG	engineered mutation	UNP P50456
C	54	MSE	MET	modified residue	UNP P50456
C	167	MSE	MET	modified residue	UNP P50456
C	176	MSE	MET	modified residue	UNP P50456
C	201	MSE	MET	modified residue	UNP P50456
C	286	MSE	MET	modified residue	UNP P50456
C	289	MSE	MET	modified residue	UNP P50456
C	329	MSE	MET	modified residue	UNP P50456
C	384	MSE	MET	modified residue	UNP P50456
C	394	MSE	MET	modified residue	UNP P50456
D	1	MSE	MET	modified residue	UNP P50456
D	52	HIS	ARG	engineered mutation	UNP P50456
D	54	MSE	MET	modified residue	UNP P50456
D	167	MSE	MET	modified residue	UNP P50456
D	176	MSE	MET	modified residue	UNP P50456
D	201	MSE	MET	modified residue	UNP P50456
D	286	MSE	MET	modified residue	UNP P50456
D	289	MSE	MET	modified residue	UNP P50456
D	329	MSE	MET	modified residue	UNP P50456
D	384	MSE	MET	modified residue	UNP P50456
D	394	MSE	MET	modified residue	UNP P50456

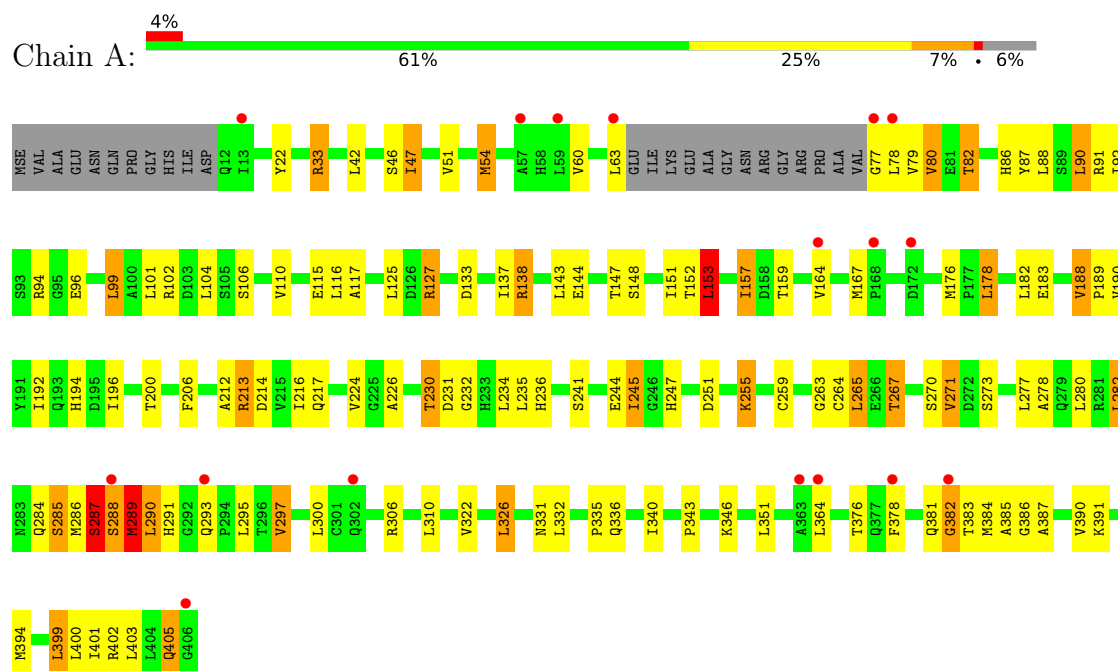
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0

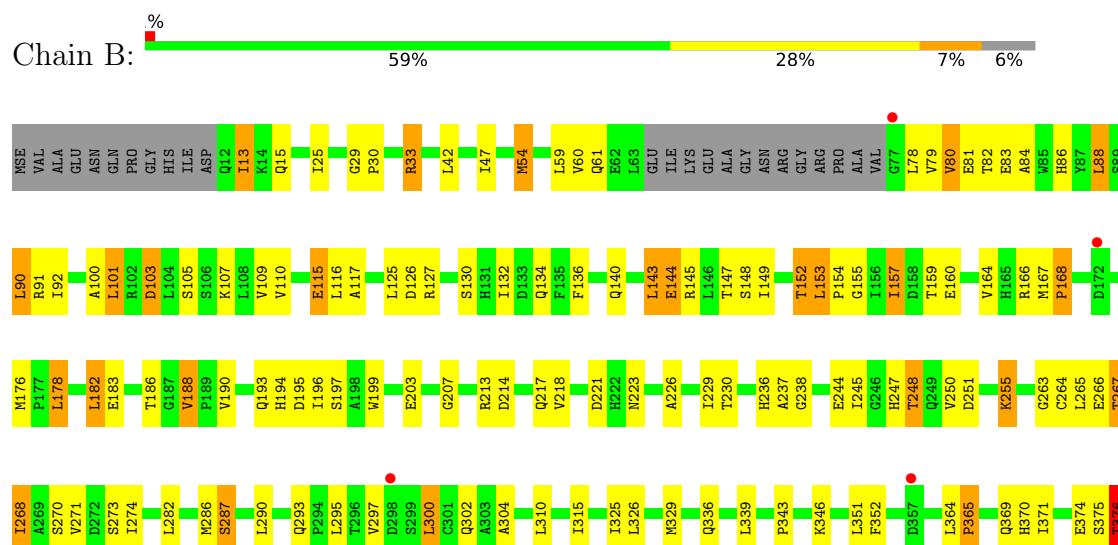
3 Residue-property plots [i](#)

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: Mlc protein

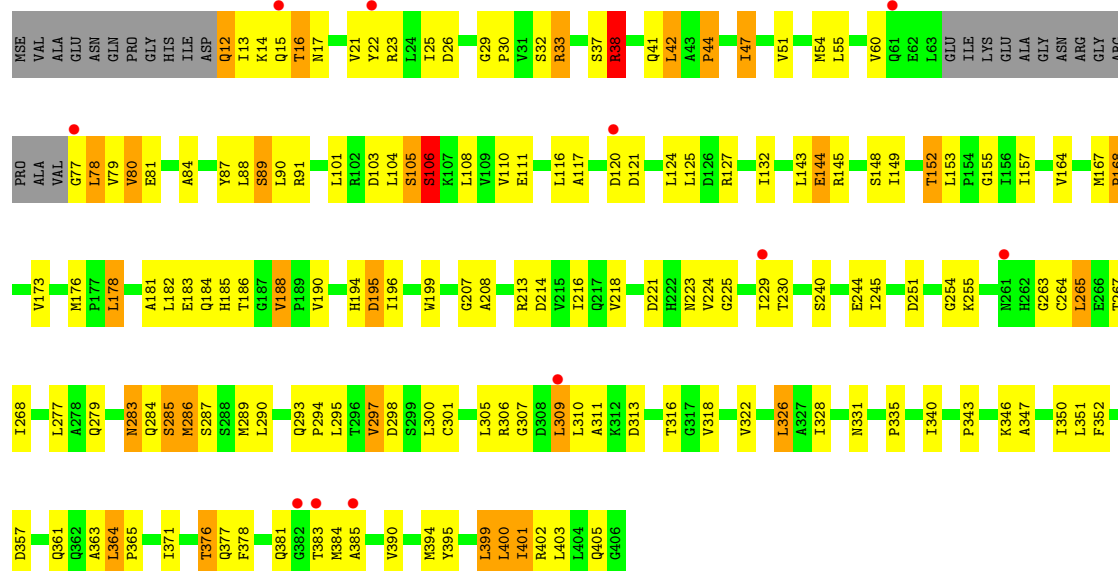


• Molecule 1: Mlc protein

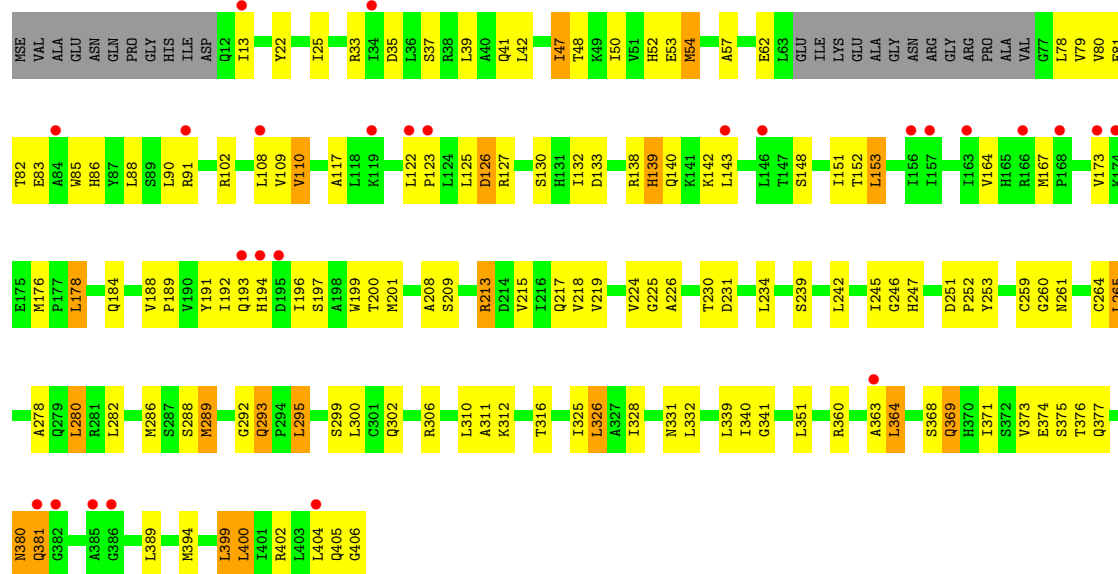




• Molecule 1: Mlc protein



• Molecule 1: Mlc protein



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	235.95Å 74.71Å 154.95Å 90.00° 129.15° 90.00°	Depositor
Resolution (Å)	19.94 – 2.70 19.94 – 2.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.94-2.70) 98.7 (19.94-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 2.71Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.203 , 0.263 0.201 , 0.258	Depositor DCC
R_{free} test set	2856 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	67.0	Xtriage
Anisotropy	0.084	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 77.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.025 for -h-2*1,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11728	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.84	6/2969 (0.2%)	1.02	7/4010 (0.2%)
1	B	0.94	3/2969 (0.1%)	1.08	9/4010 (0.2%)
1	C	1.09	14/2969 (0.5%)	1.02	7/4010 (0.2%)
1	D	1.05	13/2969 (0.4%)	0.98	5/4010 (0.1%)
All	All	0.99	36/11876 (0.3%)	1.02	28/16040 (0.2%)

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	C	0	3

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	139	HIS	CE1-NE2	22.08	1.54	1.32
1	C	38	ARG	CZ-NH1	21.54	1.62	1.32
1	C	285	SER	CB-OG	16.96	1.76	1.42
1	D	133	ASP	CG-OD1	14.96	1.53	1.25
1	D	139	HIS	CG-ND1	13.96	1.53	1.38
1	B	406	GLY	C-O	13.06	1.49	1.23
1	C	77	GLY	N-CA	12.72	1.66	1.45
1	C	44	PRO	C-N	11.65	1.50	1.33
1	C	286	MSE	C-O	-10.65	1.09	1.24
1	D	126	ASP	CG-OD2	10.25	1.44	1.25
1	D	260	GLY	C-O	9.37	1.36	1.23
1	D	126	ASP	CG-OD1	9.29	1.43	1.25
1	A	138	ARG	CZ-NH1	9.29	1.45	1.32
1	C	41	GLN	C-O	-8.97	1.11	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	286	MSE	C-N	8.95	1.46	1.33
1	C	283	ASN	CG-OD1	8.19	1.39	1.23
1	C	38	ARG	CG-CD	7.96	1.76	1.52
1	D	260	GLY	C-N	7.84	1.46	1.33
1	A	77	GLY	N-CA	7.83	1.58	1.45
1	D	139	HIS	CG-CD2	7.52	1.44	1.35
1	D	406	GLY	C-O	7.50	1.38	1.23
1	D	133	ASP	C-O	7.12	1.32	1.24
1	B	384	MSE	SE-CE	7.06	2.16	1.95
1	D	130	SER	CB-OG	6.84	1.55	1.42
1	D	289	MSE	SE-CE	6.83	2.15	1.95
1	A	138	ARG	CD-NE	6.31	1.55	1.46
1	A	289	MSE	SE-CE	6.08	2.13	1.95
1	C	289	MSE	SE-CE	6.04	2.13	1.95
1	A	306	ARG	CZ-NH1	5.92	1.41	1.32
1	A	138	ARG	CZ-NH2	5.86	1.41	1.33
1	D	261	ASN	C-O	5.85	1.29	1.23
1	C	32	SER	C-N	5.66	1.41	1.33
1	C	307	GLY	C-O	5.61	1.31	1.23
1	C	405	GLN	CA-C	5.43	1.55	1.52
1	C	306	ARG	CZ-NH1	5.33	1.40	1.32
1	B	100	ALA	CA-CB	-5.14	1.45	1.53

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	44	PRO	O-C-N	9.19	135.05	122.64
1	B	88	LEU	CA-C-N	-7.31	112.91	123.00
1	B	88	LEU	C-N-CA	-7.31	112.91	123.00
1	A	287	SER	N-CA-C	-6.96	105.72	114.56
1	D	153	LEU	N-CA-C	6.33	113.82	108.13
1	A	381	GLN	N-CA-C	-6.26	102.09	110.55
1	C	38	ARG	NE-CZ-NH1	-6.25	115.25	121.50
1	C	381	GLN	N-CA-C	-6.13	100.57	110.32
1	B	168	PRO	CA-C-N	-5.93	112.39	122.11
1	B	168	PRO	C-N-CA	-5.93	112.39	122.11
1	C	297	VAL	CB-CA-C	-5.87	104.36	112.04
1	D	280	LEU	N-CA-C	-5.83	104.85	111.14
1	C	286	MSE	CA-C-O	5.78	126.47	119.31
1	B	406	GLY	CA-C-O	-5.68	108.88	120.80
1	D	139	HIS	ND1-CG-CD2	5.60	111.70	106.10
1	D	381	GLN	N-CA-C	-5.52	106.71	113.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	153	LEU	N-CA-C	5.46	113.14	108.22
1	B	376	THR	N-CA-CB	-5.45	102.32	110.17
1	A	157	ILE	N-CA-C	5.39	115.74	107.77
1	B	103	ASP	CB-CA-C	-5.33	99.82	110.42
1	A	245	ILE	N-CA-CB	5.29	119.70	110.65
1	C	285	SER	CA-CB-OG	-5.27	100.57	111.10
1	A	102	ARG	N-CA-C	5.25	117.36	109.23
1	D	260	GLY	CA-C-O	5.20	129.62	120.57
1	C	44	PRO	CA-C-O	-5.14	111.25	120.60
1	A	245	ILE	CB-CG1-CD1	-5.10	103.08	113.80
1	B	352	PHE	CA-C-N	-5.05	113.73	119.28
1	B	352	PHE	C-N-CA	-5.05	113.73	119.28

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	286	MSE	Mainchain
1	C	38	ARG	Sidechain
1	C	44	PRO	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	2931	0	2988	76	0
1	B	2931	0	2988	93	0
1	C	2931	0	2988	93	0
1	D	2931	0	2988	78	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
All	All	11728	0	11952	326	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 14.

All (326) 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:C:38:ARG:CG	1:C:38:ARG:CD	1.76	1.57
1:B:384:MSE:CE	1:B:384:MSE:SE	2.16	1.44
1:D:289:MSE:SE	1:D:289:MSE:CE	2.15	1.43
1:C:285:SER:OG	1:C:285:SER:CB	1.76	1.33
1:D:91:ARG:CZ	1:D:380:ASN:HD21	1.59	1.13
1:B:164:VAL:HG11	1:B:167:MSE:HE2	1.26	1.13
1:C:164:VAL:HG11	1:C:167:MSE:HE2	1.34	1.09
1:D:91:ARG:NH2	1:D:380:ASN:HD21	1.52	1.07
1:B:13:ILE:HD12	1:B:13:ILE:H	1.26	1.01
1:A:148:SER:HA	1:A:188:VAL:HG13	1.43	0.97
1:C:132:ILE:HD13	1:C:182:LEU:HD21	1.50	0.93
1:B:176:MSE:HE3	1:B:178:LEU:HG	1.52	0.91
1:A:264:CYS:O	1:A:267:THR:HB	1.70	0.90
1:C:176:MSE:HE3	1:C:178:LEU:HG	1.55	0.88
1:B:54:MSE:HE3	1:B:60:VAL:HG21	1.55	0.88
1:C:178:LEU:HD22	1:C:182:LEU:HD12	1.55	0.87
1:C:148:SER:HA	1:C:188:VAL:HG13	1.57	0.85
1:B:376:THR:CG2	1:B:378:PHE:O	2.25	0.84
1:B:148:SER:HA	1:B:188:VAL:HG13	1.59	0.84
1:D:91:ARG:CZ	1:D:380:ASN:ND2	2.41	0.83
1:A:402:ARG:O	1:A:405:GLN:HB2	1.79	0.82
1:A:164:VAL:HG11	1:A:167:MSE:HE2	1.58	0.82
1:B:245:ILE:O	1:B:248:THR:HG23	1.80	0.81
1:D:218:VAL:HG21	1:D:326:LEU:HD11	1.60	0.81
1:B:132:ILE:HD12	1:B:182:LEU:HD21	1.64	0.80
1:C:164:VAL:HG11	1:C:167:MSE:CE	2.11	0.79
1:D:91:ARG:NH2	1:D:380:ASN:ND2	2.30	0.79
1:C:264:CYS:O	1:C:267:THR:HB	1.83	0.78
1:C:38:ARG:CD	1:C:38:ARG:CB	2.60	0.77
1:C:89:SER:OG	1:C:383:THR:HB	1.84	0.77
1:C:216:ILE:HD12	1:C:335:PRO:HG3	1.67	0.77
1:B:194:HIS:HD2	1:B:196:ILE:H	1.33	0.77
1:C:194:HIS:HD2	1:C:196:ILE:H	1.33	0.76
1:A:183:GLU:HG3	1:A:190:VAL:HG23	1.69	0.74
1:D:148:SER:HA	1:D:188:VAL:HG13	1.70	0.74
1:D:167:MSE:HG2	1:D:173:VAL:HG21	1.69	0.74
1:B:178:LEU:HD22	1:B:182:LEU:CD1	2.18	0.73
1:C:343:PRO:O	1:C:346:LYS:HG2	1.87	0.73
1:B:166:ARG:HG3	1:B:166:ARG:HH11	1.54	0.72
1:A:51:VAL:HA	1:A:54:MSE:HE2	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:167:MSE:HE3	1:D:173:VAL:HG11	1.71	0.72
1:B:194:HIS:CD2	1:B:196:ILE:H	2.09	0.71
1:A:54:MSE:HE3	1:A:60:VAL:HG21	1.72	0.71
1:A:277:LEU:CD2	1:D:286:MSE:HE2	2.20	0.71
1:A:206:PHE:HZ	1:A:391:LYS:HG3	1.55	0.71
1:B:84:ALA:HA	1:B:144:GLU:HG2	1.73	0.70
1:D:176:MSE:HE3	1:D:178:LEU:HG	1.72	0.70
1:B:117:ALA:O	1:B:127:ARG:NH2	2.24	0.70
1:A:216:ILE:HD12	1:A:335:PRO:HG3	1.73	0.69
1:C:214:ASP:HA	1:C:229:ILE:O	1.91	0.69
1:D:218:VAL:CG2	1:D:326:LEU:HD11	2.22	0.69
1:B:221:ASP:HB3	1:B:223:ASN:H	1.57	0.69
1:D:200:THR:HA	1:D:217:GLN:OE1	1.93	0.69
1:A:148:SER:HA	1:A:188:VAL:CG1	2.22	0.67
1:B:130:SER:O	1:B:134:GLN:HG3	1.94	0.67
1:C:155:GLY:O	1:C:157:ILE:HD12	1.95	0.67
1:D:139:HIS:HB3	1:D:142:LYS:HD2	1.76	0.66
1:B:13:ILE:H	1:B:13:ILE:CD1	1.99	0.66
1:B:86:HIS:CD2	1:B:144:GLU:H	2.14	0.66
1:B:178:LEU:HD22	1:B:182:LEU:HD12	1.76	0.66
1:B:132:ILE:CD1	1:B:182:LEU:HD21	2.26	0.65
1:B:264:CYS:O	1:B:267:THR:HB	1.95	0.65
1:B:199:TRP:HZ2	1:B:376:THR:HG21	1.62	0.65
1:D:164:VAL:HG11	1:D:167:MSE:HE2	1.78	0.65
1:B:143:LEU:HD22	1:B:144:GLU:O	1.97	0.65
1:A:280:LEU:HD22	1:D:292:GLY:HA2	1.79	0.64
1:C:167:MSE:HE3	1:C:173:VAL:HG11	1.79	0.64
1:B:80:VAL:HG12	1:B:82:THR:HG23	1.79	0.64
1:C:105:SER:O	1:C:106:SER:HB3	1.97	0.63
1:C:12:GLN:HG3	1:C:13:ILE:HD12	1.81	0.63
1:C:183:GLU:HG2	1:C:188:VAL:O	1.99	0.63
1:B:376:THR:HG23	1:B:378:PHE:O	1.97	0.63
1:C:255:LYS:HD2	1:C:267:THR:HG23	1.82	0.62
1:C:117:ALA:O	1:C:127:ARG:NH2	2.32	0.62
1:B:244:GLU:HG3	1:B:247:HIS:HD2	1.64	0.62
1:C:51:VAL:HA	1:C:54:MSE:CE	2.31	0.61
1:D:341:GLY:HA2	1:D:376:THR:HG21	1.82	0.61
1:D:341:GLY:HA2	1:D:376:THR:CG2	2.30	0.61
1:B:90:LEU:HD21	1:B:132:ILE:HD11	1.83	0.61
1:C:199:TRP:HZ2	1:C:376:THR:HG21	1.66	0.61
1:A:82:THR:HG22	1:A:104:LEU:HB2	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:VAL:HG11	1:A:343:PRO:HB2	1.81	0.61
1:A:176:MSE:HE3	1:A:178:LEU:HG	1.82	0.61
1:A:331:ASN:HD22	1:B:248:THR:HG22	1.65	0.61
1:A:183:GLU:HG3	1:A:190:VAL:CG2	2.33	0.59
1:C:23:ARG:HA	1:C:395:TYR:CE2	2.37	0.59
1:B:80:VAL:CG1	1:B:82:THR:HG23	2.33	0.59
1:C:279:GLN:O	1:C:283:ASN:ND2	2.36	0.59
1:D:224:VAL:HG11	1:D:265:LEU:HD13	1.85	0.59
1:B:149:ILE:HD11	1:B:186:THR:HG21	1.85	0.59
1:C:152:THR:HG23	1:C:195:ASP:HA	1.84	0.58
1:C:149:ILE:HD11	1:C:186:THR:HG21	1.85	0.58
1:D:90:LEU:HD21	1:D:132:ILE:HD11	1.86	0.58
1:B:287:SER:HB3	1:C:254:GLY:HA2	1.83	0.58
1:B:267:THR:HG22	1:B:268:ILE:HD12	1.86	0.58
1:B:217:GLN:O	1:B:226:ALA:HA	2.04	0.58
1:C:29:GLY:HA2	1:C:30:PRO:C	2.29	0.58
1:A:164:VAL:HG11	1:A:167:MSE:CE	2.33	0.57
1:C:149:ILE:HB	1:C:190:VAL:HG22	1.86	0.57
1:C:60:VAL:HG12	1:C:78:LEU:HD12	1.87	0.57
1:C:103:ASP:HB3	1:C:105:SER:H	1.70	0.57
1:A:33:ARG:HG2	1:A:47:ILE:HG23	1.86	0.57
1:D:196:ILE:HD13	1:D:225:GLY:HA3	1.87	0.56
1:B:183:GLU:HG3	1:B:190:VAL:HG23	1.87	0.56
1:B:236:HIS:O	1:B:237:ALA:C	2.49	0.56
1:A:332:LEU:HD21	1:B:329:MSE:HE3	1.88	0.56
1:A:394:MSE:SE	1:A:399:LEU:HD13	2.56	0.56
1:A:212:ALA:HA	1:A:336:GLN:HE22	1.71	0.56
1:B:25:ILE:HG22	1:B:80:VAL:HG23	1.88	0.56
1:B:25:ILE:HD12	1:B:54:MSE:CE	2.36	0.55
1:B:271:VAL:HA	1:B:274:ILE:HD12	1.88	0.55
1:C:120:ASP:CG	1:C:121:ASP:N	2.64	0.55
1:D:217:GLN:O	1:D:226:ALA:HA	2.06	0.55
1:C:51:VAL:HA	1:C:54:MSE:HE3	1.89	0.55
1:C:120:ASP:CG	1:C:121:ASP:H	2.15	0.55
1:B:103:ASP:HB3	1:B:105:SER:H	1.72	0.54
1:B:61:GLN:OE1	1:B:81:GLU:HG2	2.08	0.54
1:C:84:ALA:HA	1:C:144:GLU:HG2	1.90	0.54
1:D:25:ILE:HG22	1:D:80:VAL:HG23	1.90	0.54
1:B:270:SER:O	1:B:274:ILE:HG13	2.09	0.53
1:D:213:ARG:HH11	1:D:213:ARG:HB3	1.72	0.53
1:B:101:LEU:HB3	1:B:109:VAL:HB	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:394:MSE:SE	1:C:399:LEU:HD13	2.58	0.53
1:B:290:LEU:HD21	1:B:300:LEU:HA	1.91	0.53
1:D:109:VAL:HG12	1:D:110:VAL:HG22	1.91	0.53
1:A:206:PHE:CZ	1:A:391:LYS:HG3	2.39	0.52
1:B:199:TRP:CZ2	1:B:376:THR:HG21	2.42	0.52
1:A:216:ILE:CD1	1:A:335:PRO:HG3	2.37	0.52
1:D:189:PRO:HG2	1:D:399:LEU:HD23	1.91	0.52
1:C:331:ASN:HD21	1:C:363:ALA:HA	1.75	0.52
1:D:123:PRO:HD2	1:D:126:ASP:OD2	2.09	0.52
1:A:92:ILE:HD12	1:A:153:LEU:HD23	1.91	0.52
1:D:151:ILE:HB	1:D:192:ILE:HG12	1.91	0.52
1:D:340:ILE:HD13	1:D:373:VAL:HG13	1.92	0.52
1:B:376:THR:HG21	1:B:378:PHE:O	2.05	0.51
1:B:381:GLN:H	1:B:384:MSE:HE3	1.75	0.51
1:C:285:SER:OG	1:C:285:SER:CA	2.55	0.51
1:D:54:MSE:HG3	1:D:404:LEU:HD21	1.91	0.51
1:A:376:THR:HG23	1:A:378:PHE:O	2.09	0.51
1:B:136:PHE:O	1:B:140:GLN:HB2	2.11	0.51
1:C:394:MSE:HE3	1:C:400:LEU:HG	1.93	0.51
1:A:224:VAL:HG11	1:A:265:LEU:HD13	1.92	0.51
1:D:209:SER:HB2	1:D:215:VAL:HG21	1.93	0.51
1:D:148:SER:HA	1:D:188:VAL:CG1	2.39	0.51
1:A:147:THR:O	1:A:189:PRO:HD2	2.11	0.51
1:C:208:ALA:HB2	1:C:377:GLN:HB2	1.92	0.50
1:D:53:GLU:HB3	1:D:404:LEU:HD22	1.94	0.50
1:D:199:TRP:HD1	1:D:199:TRP:O	1.94	0.50
1:D:213:ARG:NH1	1:D:231:ASP:HA	2.26	0.50
1:B:384:MSE:CE	1:B:384:MSE:CG	2.89	0.50
1:D:57:ALA:O	1:D:85:TRP:HZ2	1.94	0.50
1:D:328:ILE:O	1:D:332:LEU:HG	2.10	0.50
1:B:91:ARG:HG3	1:B:152:THR:HG22	1.94	0.50
1:D:208:ALA:HB2	1:D:377:GLN:HB2	1.94	0.50
1:A:151:ILE:HB	1:A:192:ILE:HG12	1.93	0.50
1:A:278:ALA:O	1:A:282:LEU:HB2	2.12	0.50
1:A:251:ASP:O	1:A:263:GLY:HA3	2.12	0.50
1:B:25:ILE:HD12	1:B:54:MSE:HE1	1.93	0.50
1:D:247:HIS:HA	1:D:264:CYS:HB3	1.94	0.49
1:A:282:LEU:HD11	1:A:290:LEU:CB	2.43	0.49
1:B:126:ASP:O	1:B:127:ARG:C	2.55	0.49
1:B:286:MSE:HE1	1:C:318:VAL:HG22	1.93	0.49
1:C:55:LEU:HD21	1:C:78:LEU:HD11	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:199:TRP:CD1	1:D:217:GLN:HE22	2.31	0.49
1:B:339:LEU:HD23	1:B:374:GLU:HG3	1.94	0.49
1:D:22:TYR:CZ	1:D:394:MSE:HE2	2.48	0.49
1:D:201:MSE:HE3	1:D:234:LEU:HB2	1.95	0.49
1:B:159:THR:HG21	1:B:193:GLN:NE2	2.28	0.48
1:C:352:PHE:CD2	1:C:352:PHE:N	2.80	0.48
1:A:213:ARG:HB3	1:A:213:ARG:HH11	1.78	0.48
1:A:245:ILE:HD13	1:A:245:ILE:HG21	1.54	0.48
1:A:277:LEU:HD21	1:D:286:MSE:HE2	1.95	0.48
1:B:59:LEU:HD21	1:B:403:LEU:HD13	1.95	0.48
1:A:282:LEU:HD23	1:A:291:HIS:NE2	2.29	0.48
1:B:155:GLY:C	1:B:157:ILE:HD12	2.38	0.48
1:B:214:ASP:HA	1:B:229:ILE:O	2.13	0.48
1:D:251:ASP:HA	1:D:252:PRO:HD2	1.73	0.48
1:A:86:HIS:CD2	1:A:144:GLU:H	2.32	0.48
1:A:194:HIS:HD2	1:A:196:ILE:H	1.61	0.48
1:A:87:TYR:OH	1:A:387:ALA:HA	2.13	0.48
1:A:92:ILE:HB	1:A:153:LEU:HB3	1.96	0.48
1:C:309:LEU:O	1:C:313:ASP:HB3	2.14	0.48
1:B:343:PRO:O	1:B:346:LYS:HG2	2.14	0.47
1:B:251:ASP:O	1:B:263:GLY:HA3	2.13	0.47
1:A:282:LEU:HD11	1:A:290:LEU:HB3	1.96	0.47
1:D:167:MSE:HG2	1:D:173:VAL:CG2	2.40	0.47
1:C:51:VAL:HA	1:C:54:MSE:HE2	1.95	0.47
1:C:79:VAL:HG22	1:C:80:VAL:H	1.80	0.47
1:D:22:TYR:HB2	1:D:400:LEU:HD11	1.96	0.47
1:C:26:ASP:OD2	1:C:395:TYR:OH	2.33	0.47
1:A:80:VAL:CG1	1:A:82:THR:HG23	2.45	0.47
1:D:201:MSE:HE3	1:D:234:LEU:HD13	1.96	0.47
1:C:245:ILE:HG22	1:D:332:LEU:HD21	1.96	0.47
1:D:194:HIS:NE2	1:D:196:ILE:HD12	2.30	0.47
1:B:154:PRO:HB2	1:B:168:PRO:HG2	1.97	0.47
1:D:252:PRO:HB2	1:D:253:TYR:CD1	2.49	0.47
1:A:54:MSE:HB3	1:A:60:VAL:HB	1.96	0.47
1:B:166:ARG:HH11	1:B:166:ARG:CG	2.23	0.47
1:C:221:ASP:C	1:C:223:ASN:H	2.21	0.47
1:B:218:VAL:HG21	1:B:326:LEU:HD22	1.97	0.46
1:B:245:ILE:O	1:B:248:THR:CG2	2.59	0.46
1:B:255:LYS:CG	1:B:267:THR:HG23	2.45	0.46
1:A:255:LYS:HG3	1:A:267:THR:HG23	1.97	0.46
1:B:29:GLY:HA2	1:B:30:PRO:C	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:87:TYR:HE2	1:C:103:ASP:O	1.99	0.46
1:C:21:VAL:O	1:C:25:ILE:HG13	2.15	0.46
1:A:117:ALA:O	1:A:127:ARG:NH2	2.49	0.46
1:A:288:SER:OG	1:A:290:LEU:HD12	2.15	0.46
1:A:289:MSE:HE2	1:A:289:MSE:HB3	1.89	0.46
1:D:371:ILE:O	1:D:371:ILE:HG23	2.14	0.46
1:C:33:ARG:HG2	1:C:47:ILE:CG2	2.46	0.46
1:C:207:GLY:HA2	1:C:378:PHE:HE1	1.80	0.46
1:A:244:GLU:HG3	1:A:247:HIS:HD2	1.81	0.46
1:B:115:GLU:OE2	1:B:115:GLU:HA	2.16	0.46
1:A:87:TYR:CG	1:A:390:VAL:HG21	2.51	0.45
1:C:244:GLU:HG2	1:D:364:LEU:HD12	1.98	0.45
1:B:15:GLN:HA	1:B:401:ILE:HD13	1.98	0.45
1:C:178:LEU:HD22	1:C:182:LEU:CD1	2.36	0.45
1:C:399:LEU:HD22	1:C:403:LEU:HG	1.99	0.45
1:D:193:GLN:HB2	1:D:389:LEU:HD11	1.98	0.45
1:D:278:ALA:HB3	1:D:295:LEU:HD11	1.97	0.45
1:C:13:ILE:HD13	1:D:39:LEU:O	2.16	0.45
1:A:322:VAL:HG12	1:A:326:LEU:HD22	1.97	0.45
1:A:235:LEU:O	1:A:236:HIS:HB2	2.16	0.45
1:A:212:ALA:HA	1:A:336:GLN:NE2	2.30	0.45
1:C:105:SER:O	1:C:106:SER:CB	2.63	0.45
1:B:92:ILE:O	1:B:154:PRO:HD3	2.17	0.45
1:B:147:THR:O	1:B:148:SER:HB3	2.16	0.45
1:C:251:ASP:O	1:C:263:GLY:HA3	2.16	0.45
1:A:289:MSE:C	1:A:291:HIS:H	2.25	0.45
1:A:91:ARG:HD2	1:A:382:GLY:O	2.17	0.44
1:B:396:ASN:OD1	1:B:396:ASN:C	2.59	0.44
1:D:199:TRP:CD1	1:D:199:TRP:C	2.95	0.44
1:C:352:PHE:N	1:C:352:PHE:HD2	2.14	0.44
1:C:365:PRO:HG2	1:D:259:CYS:O	2.18	0.44
1:B:365:PRO:O	1:B:369:GLN:HB2	2.17	0.44
1:C:157:ILE:O	1:C:240:SER:HB2	2.17	0.44
1:A:42:LEU:HD23	1:A:46:SER:HB3	1.99	0.44
1:B:33:ARG:HG2	1:B:47:ILE:HG22	2.00	0.44
1:D:245:ILE:HG13	1:D:246:GLY:N	2.33	0.44
1:B:182:LEU:HB3	1:B:190:VAL:HG21	1.99	0.44
1:B:304:ALA:CB	1:B:315:ILE:HD12	2.48	0.44
1:C:181:ALA:O	1:C:185:HIS:HB2	2.18	0.44
1:A:200:THR:HA	1:A:217:GLN:OE1	2.18	0.44
1:C:305:LEU:HD23	1:C:350:ILE:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:363:ALA:O	1:C:364:LEU:C	2.61	0.44
1:B:384:MSE:HG3	1:B:385:ALA:N	2.32	0.43
1:C:305:LEU:HD21	1:C:347:ALA:HA	1.99	0.43
1:A:259:CYS:O	1:B:365:PRO:HG2	2.17	0.43
1:A:383:THR:C	1:A:385:ALA:H	2.25	0.43
1:C:322:VAL:HG12	1:C:326:LEU:HD22	2.01	0.43
1:A:147:THR:HG22	1:A:403:LEU:HD21	1.99	0.43
1:A:234:LEU:HA	1:A:234:LEU:HD12	1.69	0.43
1:A:63:LEU:HD12	1:A:79:VAL:HG21	1.99	0.43
1:A:90:LEU:HA	1:A:90:LEU:HD12	1.70	0.43
1:A:214:ASP:OD1	1:A:230:THR:HG22	2.19	0.43
1:B:148:SER:HA	1:B:188:VAL:CG1	2.40	0.43
1:C:383:THR:C	1:C:385:ALA:H	2.27	0.43
1:D:217:GLN:HG3	1:D:339:LEU:HB2	2.00	0.43
1:C:14:LYS:HB2	1:D:41:GLN:HE22	1.82	0.43
1:C:87:TYR:CE2	1:C:103:ASP:O	2.72	0.43
1:C:218:VAL:HG13	1:C:245:ILE:HD11	2.00	0.43
1:C:22:TYR:HB2	1:C:400:LEU:HD11	2.01	0.43
1:D:80:VAL:HG12	1:D:82:THR:HG23	2.01	0.43
1:A:22:TYR:HB2	1:A:400:LEU:HD11	2.01	0.43
1:A:151:ILE:HD11	1:A:182:LEU:CD1	2.49	0.43
1:D:86:HIS:HA	1:D:102:ARG:O	2.19	0.43
1:C:87:TYR:CG	1:C:390:VAL:HG21	2.54	0.42
1:A:82:THR:HG22	1:A:104:LEU:CB	2.48	0.42
1:A:284:GLN:HE21	1:D:293:GLN:C	2.26	0.42
1:C:91:ARG:HA	1:C:152:THR:O	2.18	0.42
1:B:160:GLU:OE1	1:B:238:GLY:O	2.38	0.42
1:C:148:SER:HA	1:C:188:VAL:CG1	2.38	0.42
1:C:224:VAL:HG11	1:C:265:LEU:HD13	2.00	0.42
1:C:17:ASN:OD1	1:C:42:LEU:HD11	2.20	0.42
1:C:15:GLN:HA	1:C:401:ILE:HD13	2.02	0.42
1:D:293:GLN:CD	1:D:299:SER:HB2	2.44	0.42
1:B:369:GLN:HG3	1:B:370:HIS:ND1	2.34	0.42
1:C:218:VAL:HG21	1:C:326:LEU:HD21	2.01	0.42
1:C:221:ASP:C	1:C:223:ASN:N	2.78	0.42
1:B:90:LEU:HD21	1:B:132:ILE:CD1	2.49	0.42
1:B:152:THR:HG23	1:B:195:ASP:HA	2.02	0.42
1:C:290:LEU:HD11	1:C:311:ALA:HB2	2.01	0.42
1:D:37:SER:HA	1:D:47:ILE:HD13	2.02	0.42
1:A:90:LEU:HD12	1:A:99:LEU:HA	2.01	0.41
1:B:178:LEU:CD2	1:B:182:LEU:CD1	2.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:173:VAL:O	1:D:173:VAL:HG23	2.19	0.41
1:B:193:GLN:HG3	1:B:197:SER:OG	2.19	0.41
1:D:83:GLU:C	1:D:85:TRP:H	2.27	0.41
1:A:385:ALA:O	1:A:386:GLY:C	2.62	0.41
1:B:153:LEU:CD1	1:B:157:ILE:HG12	2.50	0.41
1:C:17:ASN:O	1:C:21:VAL:HG23	2.21	0.41
1:B:25:ILE:HD12	1:B:54:MSE:HE3	2.02	0.41
1:B:116:LEU:O	1:B:117:ALA:C	2.63	0.41
1:B:266:GLU:O	1:B:270:SER:HB3	2.21	0.41
1:C:194:HIS:O	1:C:195:ASP:C	2.63	0.41
1:D:219:VAL:O	1:D:224:VAL:HA	2.20	0.41
1:A:255:LYS:HE2	1:A:267:THR:HG23	2.03	0.41
1:A:270:SER:O	1:A:271:VAL:C	2.63	0.41
1:C:194:HIS:CD2	1:C:196:ILE:H	2.24	0.41
1:D:191:TYR:OH	1:D:399:LEU:HG	2.20	0.41
1:D:218:VAL:HG21	1:D:326:LEU:CD1	2.42	0.41
1:B:153:LEU:HD13	1:B:157:ILE:HD11	2.02	0.41
1:B:255:LYS:HG3	1:B:267:THR:HG23	2.03	0.41
1:C:116:LEU:HD13	1:C:124:LEU:HD11	2.03	0.41
1:C:196:ILE:HD12	1:C:225:GLY:HA3	2.03	0.41
1:C:383:THR:O	1:C:385:ALA:N	2.54	0.41
1:D:199:TRP:O	1:D:199:TRP:CD1	2.72	0.41
1:A:343:PRO:O	1:A:346:LYS:HG2	2.21	0.41
1:C:15:GLN:O	1:C:16:THR:C	2.64	0.41
1:C:326:LEU:HD12	1:C:326:LEU:HA	1.83	0.41
1:D:48:THR:O	1:D:52:HIS:HB2	2.20	0.41
1:D:117:ALA:O	1:D:127:ARG:NH2	2.54	0.41
1:A:217:GLN:O	1:A:226:ALA:HA	2.21	0.41
1:C:120:ASP:OD2	1:C:127:ARG:HD2	2.20	0.41
1:D:331:ASN:HD21	1:D:363:ALA:HA	1.86	0.41
1:D:368:SER:O	1:D:369:GLN:C	2.64	0.41
1:A:285:SER:C	1:A:287:SER:H	2.25	0.40
1:B:247:HIS:HA	1:B:264:CYS:HB3	2.02	0.40
1:D:311:ALA:O	1:D:312:LYS:C	2.61	0.40
1:A:133:ASP:O	1:A:137:ILE:HG13	2.21	0.40
1:A:244:GLU:CG	1:A:247:HIS:HD2	2.35	0.40
1:B:203:GLU:HA	1:B:207:GLY:HA3	2.04	0.40
1:D:139:HIS:O	1:D:140:GLN:C	2.64	0.40
1:C:167:MSE:O	1:C:168:PRO:C	2.64	0.40
1:D:91:ARG:NE	1:D:380:ASN:HD21	2.10	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	378/406 (93%)	346 (92%)	25 (7%)	7 (2%)	6	17
1	B	378/406 (93%)	353 (93%)	25 (7%)	0	100	100
1	C	378/406 (93%)	344 (91%)	31 (8%)	3 (1%)	16	37
1	D	378/406 (93%)	351 (93%)	24 (6%)	3 (1%)	16	37
All	All	1512/1624 (93%)	1394 (92%)	105 (7%)	13 (1%)	14	35

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	290	LEU
1	C	106	SER
1	D	369	GLN
1	A	286	MSE
1	C	294	PRO
1	A	94	ARG
1	D	288	SER
1	A	106	SER
1	A	232	GLY
1	A	271	VAL
1	C	168	PRO
1	D	380	ASN
1	A	382	GLY

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	321/329 (98%)	271 (84%)	50 (16%)	2	7
1	B	321/329 (98%)	268 (84%)	53 (16%)	2	6
1	C	321/329 (98%)	262 (82%)	59 (18%)	1	4
1	D	321/329 (98%)	272 (85%)	49 (15%)	3	7
All	All	1284/1316 (98%)	1073 (84%)	211 (16%)	2	6

All (211) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	ARG
1	A	47	ILE
1	A	54	MSE
1	A	78	LEU
1	A	80	VAL
1	A	82	THR
1	A	88	LEU
1	A	90	LEU
1	A	96	GLU
1	A	99	LEU
1	A	101	LEU
1	A	110	VAL
1	A	115	GLU
1	A	116	LEU
1	A	125	LEU
1	A	127	ARG
1	A	138	ARG
1	A	143	LEU
1	A	152	THR
1	A	153	LEU
1	A	157	ILE
1	A	159	THR
1	A	178	LEU
1	A	188	VAL
1	A	213	ARG
1	A	230	THR
1	A	231	ASP
1	A	241	SER
1	A	255	LYS
1	A	265	LEU
1	A	267	THR
1	A	273	SER
1	A	282	LEU

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Mol	Chain	Res	Type
1	A	285	SER
1	A	287	SER
1	A	288	SER
1	A	289	MSE
1	A	293	GLN
1	A	295	LEU
1	A	297	VAL
1	A	300	LEU
1	A	310	LEU
1	A	326	LEU
1	A	340	ILE
1	A	351	LEU
1	A	364	LEU
1	A	384	MSE
1	A	399	LEU
1	A	401	ILE
1	A	405	GLN
1	B	13	ILE
1	B	33	ARG
1	B	42	LEU
1	B	54	MSE
1	B	78	LEU
1	B	79	VAL
1	B	80	VAL
1	B	83	GLU
1	B	88	LEU
1	B	90	LEU
1	B	101	LEU
1	B	107	LYS
1	B	110	VAL
1	B	115	GLU
1	B	125	LEU
1	B	143	LEU
1	B	144	GLU
1	B	145	ARG
1	B	152	THR
1	B	153	LEU
1	B	157	ILE
1	B	178	LEU
1	B	182	LEU
1	B	188	VAL
1	B	213	ARG

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Mol	Chain	Res	Type
1	B	230	THR
1	B	248	THR
1	B	250	VAL
1	B	255	LYS
1	B	265	LEU
1	B	267	THR
1	B	268	ILE
1	B	273	SER
1	B	282	LEU
1	B	287	SER
1	B	293	GLN
1	B	295	LEU
1	B	297	VAL
1	B	300	LEU
1	B	302	GLN
1	B	310	LEU
1	B	325	ILE
1	B	336	GLN
1	B	351	LEU
1	B	364	LEU
1	B	365	PRO
1	B	371	ILE
1	B	375	SER
1	B	376	THR
1	B	399	LEU
1	B	400	LEU
1	B	401	ILE
1	B	405	GLN
1	C	12	GLN
1	C	16	THR
1	C	33	ARG
1	C	37	SER
1	C	42	LEU
1	C	47	ILE
1	C	78	LEU
1	C	80	VAL
1	C	81	GLU
1	C	88	LEU
1	C	89	SER
1	C	90	LEU
1	C	101	LEU
1	C	104	LEU

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Mol	Chain	Res	Type
1	C	105	SER
1	C	106	SER
1	C	108	LEU
1	C	110	VAL
1	C	111	GLU
1	C	125	LEU
1	C	143	LEU
1	C	144	GLU
1	C	145	ARG
1	C	152	THR
1	C	153	LEU
1	C	178	LEU
1	C	184	GLN
1	C	188	VAL
1	C	195	ASP
1	C	213	ARG
1	C	230	THR
1	C	265	LEU
1	C	268	ILE
1	C	277	LEU
1	C	284	GLN
1	C	287	SER
1	C	293	GLN
1	C	295	LEU
1	C	297	VAL
1	C	298	ASP
1	C	300	LEU
1	C	301	CYS
1	C	309	LEU
1	C	310	LEU
1	C	316	THR
1	C	326	LEU
1	C	328	ILE
1	C	340	ILE
1	C	351	LEU
1	C	357	ASP
1	C	361	GLN
1	C	364	LEU
1	C	371	ILE
1	C	376	THR
1	C	384	MSE
1	C	399	LEU

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Mol	Chain	Res	Type
1	C	400	LEU
1	C	401	ILE
1	C	402	ARG
1	D	13	ILE
1	D	33	ARG
1	D	35	ASP
1	D	42	LEU
1	D	47	ILE
1	D	50	ILE
1	D	54	MSE
1	D	62	GLU
1	D	78	LEU
1	D	79	VAL
1	D	81	GLU
1	D	88	LEU
1	D	108	LEU
1	D	110	VAL
1	D	122	LEU
1	D	125	LEU
1	D	138	ARG
1	D	143	LEU
1	D	152	THR
1	D	153	LEU
1	D	178	LEU
1	D	184	GLN
1	D	197	SER
1	D	213	ARG
1	D	230	THR
1	D	239	SER
1	D	242	LEU
1	D	265	LEU
1	D	280	LEU
1	D	282	LEU
1	D	293	GLN
1	D	295	LEU
1	D	300	LEU
1	D	302	GLN
1	D	306	ARG
1	D	310	LEU
1	D	316	THR
1	D	325	ILE
1	D	326	LEU

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Mol	Chain	Res	Type
1	D	351	LEU
1	D	360	ARG
1	D	364	LEU
1	D	374	GLU
1	D	375	SER
1	D	381	GLN
1	D	399	LEU
1	D	400	LEU
1	D	402	ARG
1	D	405	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	HIS
1	A	184	GLN
1	A	262	HIS
1	A	279	GLN
1	A	284	GLN
1	A	334	ASN
1	A	362	GLN
1	B	15	GLN
1	B	86	HIS
1	B	184	GLN
1	B	193	GLN
1	B	194	HIS
1	B	262	HIS
1	B	279	GLN
1	B	293	GLN
1	B	334	ASN
1	B	361	GLN
1	B	405	GLN
1	C	139	HIS
1	C	184	GLN
1	C	185	HIS
1	C	194	HIS
1	C	262	HIS
1	C	279	GLN
1	C	283	ASN
1	C	284	GLN
1	C	334	ASN
1	C	405	GLN

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Mol	Chain	Res	Type
1	D	15	GLN
1	D	41	GLN
1	D	86	HIS
1	D	161	ASN
1	D	185	HIS
1	D	193	GLN
1	D	223	ASN
1	D	361	GLN
1	D	369	GLN
1	D	380	ASN
1	D	381	GLN

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	373/406 (91%)	0.50	17 (4%) 37 34	57, 71, 78, 87	0
1	B	373/406 (91%)	0.10	5 (1%) 75 73	61, 71, 78, 87	0
1	C	373/406 (91%)	0.45	11 (2%) 53 50	61, 71, 77, 84	0
1	D	373/406 (91%)	0.61	26 (6%) 22 19	60, 71, 77, 86	0
All	All	1492/1624 (91%)	0.41	59 (3%) 42 38	57, 71, 78, 87	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	77	GLY	6.0
1	D	381	GLN	5.9
1	D	382	GLY	5.5
1	D	194	HIS	4.9
1	A	77	GLY	4.2
1	C	385	ALA	4.1
1	B	77	GLY	4.0
1	D	34	ILE	3.9
1	D	193	GLN	3.7
1	D	174	LYS	3.5
1	A	13	ILE	3.3
1	A	59	LEU	3.0
1	D	156	ILE	3.0
1	A	288	SER	3.0
1	A	63	LEU	3.0
1	D	123	PRO	2.9
1	A	382	GLY	2.9
1	A	293	GLN	2.8
1	A	78	LEU	2.8
1	A	168	PRO	2.7
1	A	378	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	406	GLY	2.6
1	D	13	ILE	2.6
1	C	261	ASN	2.5
1	C	383	THR	2.5
1	C	120	ASP	2.5
1	D	146	LEU	2.5
1	A	363	ALA	2.5
1	C	229	ILE	2.5
1	D	163	ILE	2.4
1	D	122	LEU	2.4
1	D	84	ALA	2.4
1	D	157	ILE	2.3
1	B	406	GLY	2.3
1	D	119	LYS	2.3
1	D	195	ASP	2.3
1	D	108	LEU	2.3
1	A	57	ALA	2.2
1	D	173	VAL	2.2
1	D	404	LEU	2.2
1	A	364	LEU	2.2
1	C	15	GLN	2.2
1	B	172	ASP	2.2
1	D	385	ALA	2.2
1	D	166	ARG	2.2
1	C	382	GLY	2.2
1	D	386	GLY	2.2
1	D	91	ARG	2.1
1	D	168	PRO	2.1
1	D	143	LEU	2.1
1	A	302	GLN	2.1
1	C	61	GLN	2.1
1	C	22	TYR	2.1
1	C	309	LEU	2.1
1	A	172	ASP	2.0
1	B	357	ASP	2.0
1	D	363	ALA	2.0
1	B	298	ASP	2.0
1	A	164	VAL	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 [i](#)

There are no oligosaccharides 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($\text{\AA}^2$)	Q<0.9
2	ZN	A	501	1/1	0.99	0.16	55,55,55,55	0
2	ZN	B	502	1/1	0.99	0.16	46,46,46,46	0
2	ZN	C	503	1/1	0.99	0.12	71,71,71,71	0
2	ZN	D	504	1/1	0.99	0.17	86,86,86,86	0

6.5 Other polymers [i](#)

There are no such residues in this entry.