



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:08 PM UTC

PDB ID : 3KLN / pdb_00003klh
Title : Vibrio cholerae VpsT
Authors : Krasteva, P.V.; Navarro, V.A.S.; Sondermann, H.
Deposited on : 2009-11-08
Resolution : 3.08 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

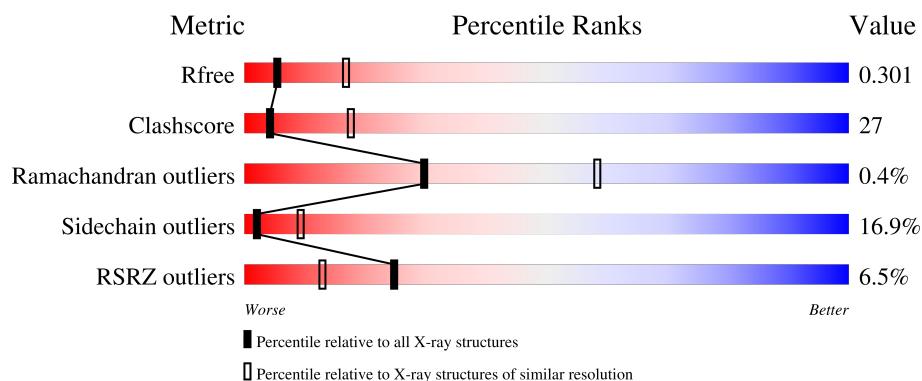
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.08 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	2010 (3.10-3.06)
Clashscore	190562	2102 (3.10-3.06)
Ramachandran outliers	187476	1982 (3.10-3.06)
Sidechain outliers	187428	1981 (3.10-3.06)
RSRZ outliers	180081	2010 (3.10-3.06)

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	225	3% 51% 34% 11% .
1	B	225	3% 46% 38% 11% .
1	C	225	6% 52% 33% 9% 5%
1	D	225	11% 40% 31% 6% 23%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6640 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 Transcriptional regulator, LuxR family.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	217	Total	C	N	O	S	0	0	0
			1756	1119	298	329	10			
1	B	215	Total	C	N	O	S	0	0	0
			1739	1110	296	323	10			
1	C	213	Total	C	N	O	S	0	0	0
			1728	1101	294	323	10			
1	D	173	Total	C	N	O	S	0	0	0
			1417	905	241	262	9			

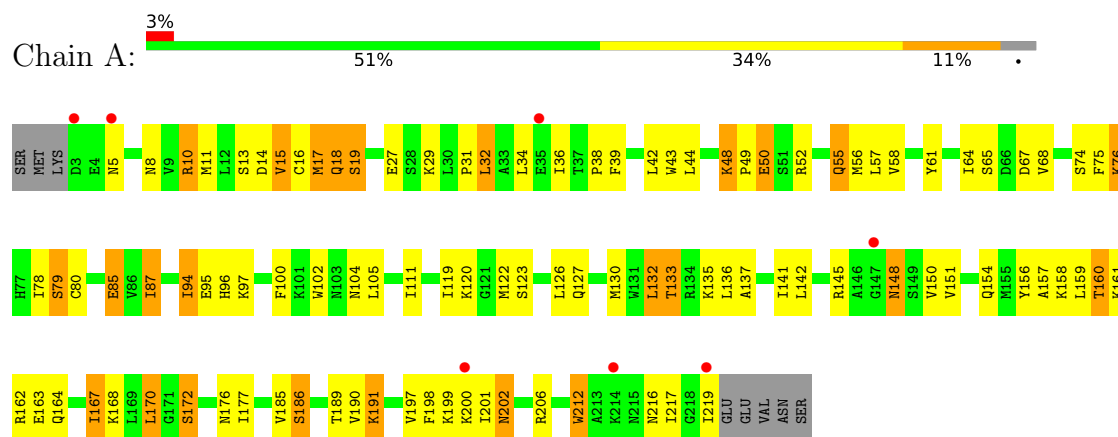
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP Q9KKZ8
B	0	SER	-	expression tag	UNP Q9KKZ8
C	0	SER	-	expression tag	UNP Q9KKZ8
D	0	SER	-	expression tag	UNP Q9KKZ8

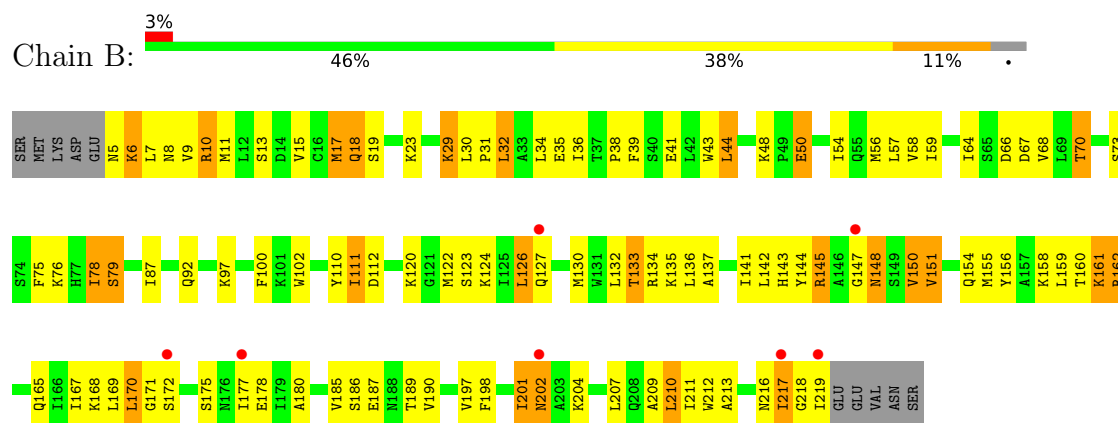
3 Residue-property plots

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.

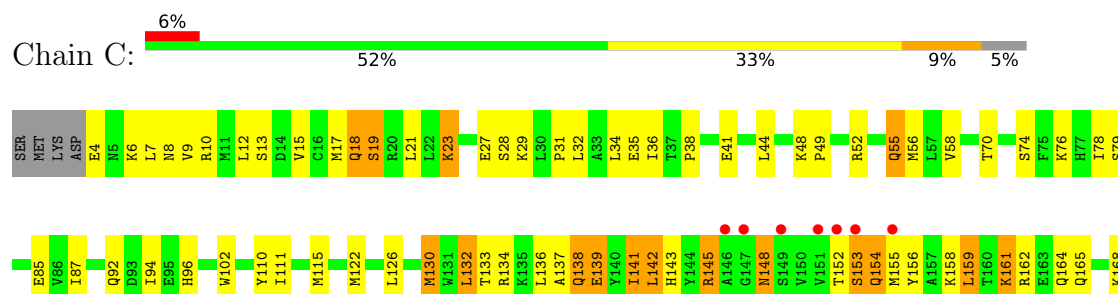
- Molecule 1: Transcriptional regulator, LuxR family

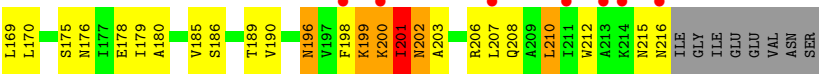


- Molecule 1: Transcriptional regulator, LuxR family

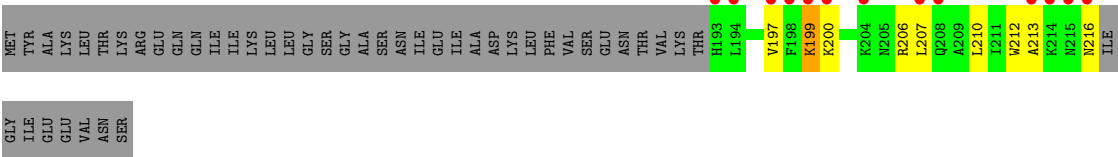
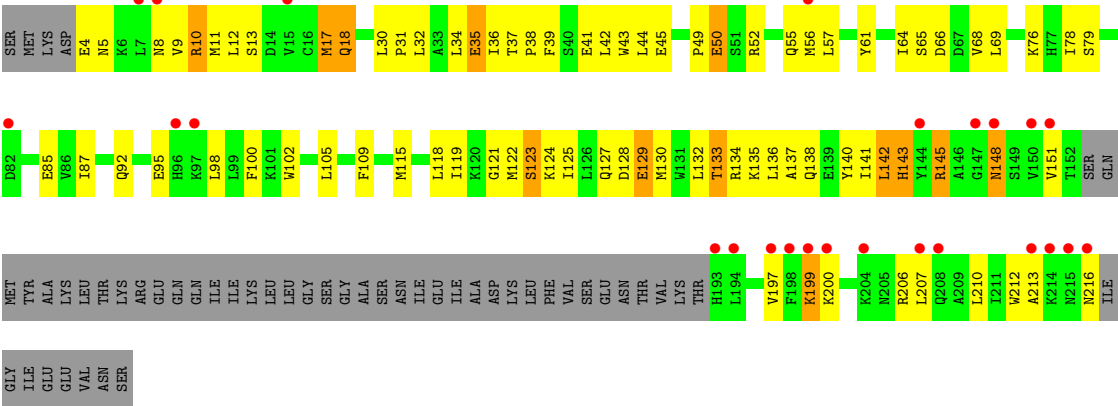


- Molecule 1: Transcriptional regulator, LuxR family





● Molecule 1: Transcriptional regulator, LuxR family



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	121.49Å 121.49Å 198.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.90 – 3.08 45.90 – 3.08	Depositor EDS
% Data completeness (in resolution range)	98.6 (45.90-3.08) 99.0 (45.90-3.08)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 3.07Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.247 , 0.308 0.251 , 0.301	Depositor DCC
R_{free} test set	1400 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	73.3	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 60.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6640	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 72.48 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.1867e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.79	0/1785	0.99	6/2407 (0.2%)
1	B	0.74	0/1768	0.94	6/2384 (0.3%)
1	C	0.54	0/1757	0.87	0/2369
1	D	0.57	0/1443	0.85	1/1947 (0.1%)
All	All	0.68	0/6753	0.92	13/9107 (0.1%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	48	LYS	CA-C-N	7.42	126.96	119.24
1	A	48	LYS	C-N-CA	7.42	126.96	119.24
1	B	78	ILE	N-CA-C	7.23	117.99	110.62
1	B	48	LYS	CA-C-N	6.23	125.72	119.24
1	B	48	LYS	C-N-CA	6.23	125.72	119.24
1	A	172	SER	N-CA-C	-6.07	104.38	112.94
1	B	172	SER	N-CA-C	-6.01	103.70	113.19
1	B	87	ILE	CB-CA-C	-5.59	103.97	110.91
1	A	14	ASP	CA-C-N	-5.56	113.60	122.50
1	A	14	ASP	C-N-CA	-5.56	113.60	122.50
1	A	212	TRP	N-CA-C	-5.56	104.44	111.11
1	D	78	ILE	N-CA-C	5.41	115.62	110.42
1	B	32	LEU	N-CA-C	5.14	117.22	109.41

There are no chirality outliers.

There are no planarity outliers.

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	1756	0	1796	86	0
1	B	1739	0	1786	114	0
1	C	1728	0	1767	88	0
1	D	1417	0	1435	84	0
All	All	6640	0	6784	365	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 27.

All (365) 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:B:145:ARG:HG2	1:B:145:ARG:HH11	1.04	1.16
1:B:130:MET:HE2	1:B:132:LEU:HD11	1.18	1.14
1:D:143:HIS:CE1	1:D:148:ASN:HB2	1.91	1.05
1:A:56:MET:HE1	1:A:122:MET:HE1	1.34	1.04
1:A:130:MET:HE2	1:A:132:LEU:HD11	1.08	1.02
1:A:130:MET:CE	1:A:132:LEU:HD11	1.91	0.99
1:D:18:GLN:H	1:D:18:GLN:NE2	1.61	0.99
1:D:18:GLN:HE21	1:D:18:GLN:N	1.61	0.98
1:B:56:MET:HE1	1:B:122:MET:HE1	1.44	0.97
1:B:18:GLN:HE21	1:B:18:GLN:N	1.63	0.96
1:B:18:GLN:H	1:B:18:GLN:NE2	1.63	0.96
1:C:18:GLN:H	1:C:18:GLN:HE21	0.95	0.94
1:B:201:ILE:O	1:B:202:ASN:HB3	1.71	0.91
1:B:130:MET:CE	1:B:132:LEU:HD11	2.01	0.90
1:A:18:GLN:H	1:A:18:GLN:HE21	1.10	0.90
1:B:186:SER:HB3	1:B:189:THR:OG1	1.72	0.88
1:A:18:GLN:H	1:A:18:GLN:NE2	1.70	0.88
1:B:145:ARG:HG2	1:B:145:ARG:NH1	1.86	0.86
1:C:130:MET:HE2	1:C:132:LEU:HD11	1.57	0.86
1:A:130:MET:HE2	1:A:132:LEU:CD1	2.01	0.86
1:C:201:ILE:HG22	1:C:203:ALA:H	1.41	0.86
1:D:143:HIS:ND1	1:D:148:ASN:HB2	1.91	0.85
1:C:145:ARG:HG2	1:C:145:ARG:HH11	1.38	0.85
1:B:143:HIS:HD2	1:B:144:TYR:CD2	1.94	0.84
1:C:18:GLN:HE21	1:C:18:GLN:N	1.76	0.84
1:C:153:SER:OG	1:C:216:ASN:HB3	1.76	0.84
1:C:18:GLN:H	1:C:18:GLN:NE2	1.76	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:148:ASN:N	1:D:148:ASN:HD22	1.76	0.83
1:B:145:ARG:HH11	1:B:145:ARG:CG	1.91	0.83
1:D:148:ASN:HD22	1:D:148:ASN:H	1.28	0.82
1:C:154:GLN:HA	1:C:154:GLN:NE2	1.96	0.80
1:C:145:ARG:HH11	1:C:145:ARG:CG	1.94	0.80
1:C:159:LEU:HD12	1:C:164:GLN:HG3	1.62	0.80
1:A:18:GLN:HE21	1:A:18:GLN:N	1.80	0.79
1:B:175:SER:HB3	1:B:178:GLU:HG3	1.64	0.79
1:C:199:LYS:H	1:C:199:LYS:HD3	1.47	0.79
1:D:130:MET:HE2	1:D:132:LEU:HD11	1.67	0.77
1:D:127:GLN:O	1:D:128:ASP:HB2	1.85	0.77
1:D:100:PHE:CE2	1:D:143:HIS:HD2	2.04	0.76
1:D:143:HIS:ND1	1:D:143:HIS:C	2.43	0.76
1:C:133:THR:HG23	1:C:136:LEU:H	1.51	0.75
1:B:150:VAL:HG11	1:B:218:GLY:H	1.52	0.73
1:B:162:ARG:HG3	1:B:162:ARG:HH11	1.52	0.73
1:D:37:THR:HG21	1:D:45:GLU:HG3	1.71	0.73
1:D:100:PHE:CD2	1:D:143:HIS:HD2	2.05	0.73
1:C:161:LYS:N	1:C:161:LYS:HD2	2.04	0.72
1:C:198:PHE:O	1:C:202:ASN:N	2.21	0.72
1:B:197:VAL:HG12	1:B:201:ILE:HD12	1.71	0.72
1:A:156:TYR:OH	1:A:168:LYS:HE3	1.90	0.72
1:B:56:MET:HE1	1:B:122:MET:CE	2.19	0.72
1:B:43:TRP:NE1	1:B:44:LEU:HD22	2.05	0.71
1:B:133:THR:CG2	1:B:136:LEU:H	2.02	0.71
1:D:207:LEU:HA	1:D:210:LEU:HD21	1.72	0.71
1:B:143:HIS:CD2	1:B:144:TYR:CD2	2.79	0.71
1:D:8:ASN:HB3	1:D:55:GLN:HG3	1.71	0.70
1:D:143:HIS:CE1	1:D:148:ASN:CB	2.73	0.70
1:C:148:ASN:N	1:C:148:ASN:HD22	1.88	0.70
1:A:56:MET:HE1	1:A:122:MET:CE	2.19	0.70
1:B:201:ILE:O	1:B:202:ASN:CB	2.39	0.70
1:D:124:LYS:O	1:D:129:GLU:HG3	1.91	0.70
1:A:133:THR:CG2	1:A:136:LEU:H	2.04	0.70
1:C:186:SER:HB3	1:C:189:THR:OG1	1.91	0.70
1:D:143:HIS:C	1:D:143:HIS:HD1	1.98	0.70
1:B:133:THR:HG22	1:B:136:LEU:H	1.57	0.69
1:B:132:LEU:HD23	1:B:136:LEU:HD23	1.75	0.69
1:A:96:HIS:HB3	1:A:136:LEU:CD1	2.22	0.69
1:B:130:MET:HE2	1:B:132:LEU:CD1	2.10	0.69
1:D:141:ILE:O	1:D:145:ARG:HB3	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:133:THR:HG22	1:D:135:LYS:N	2.08	0.68
1:D:56:MET:SD	1:D:122:MET:HE1	2.33	0.68
1:C:199:LYS:HD3	1:C:199:LYS:N	2.09	0.68
1:B:56:MET:CE	1:B:122:MET:HE1	2.22	0.67
1:B:43:TRP:CE2	1:B:44:LEU:HD22	2.30	0.67
1:B:177:ILE:HD12	1:B:177:ILE:H	1.59	0.66
1:A:127:GLN:HE22	1:C:6:LYS:HE3	1.60	0.65
1:A:133:THR:HG22	1:A:136:LEU:H	1.60	0.65
1:B:18:GLN:HE21	1:B:18:GLN:H	0.80	0.65
1:A:43:TRP:CE2	1:A:44:LEU:HG	2.32	0.65
1:A:13:SER:O	1:A:38:PRO:HA	1.97	0.65
1:B:132:LEU:CD2	1:B:136:LEU:HD23	2.27	0.65
1:B:75:PHE:O	1:B:79:SER:OG	2.14	0.64
1:A:56:MET:CE	1:A:122:MET:HE1	2.19	0.64
1:D:100:PHE:CE2	1:D:143:HIS:CD2	2.86	0.64
1:A:31:PRO:HD2	1:A:126:LEU:HD23	1.78	0.64
1:D:87:ILE:HG12	1:D:105:LEU:HD11	1.81	0.63
1:A:31:PRO:HD2	1:A:126:LEU:CD2	2.30	0.62
1:A:76:LYS:HE2	1:A:80:CYS:O	1.98	0.62
1:C:156:TYR:OH	1:C:168:LYS:HE2	1.98	0.62
1:A:198:PHE:O	1:A:199:LYS:HD2	1.99	0.62
1:B:148:ASN:N	1:B:148:ASN:OD1	2.30	0.62
1:C:74:SER:O	1:C:78:ILE:HG12	1.99	0.62
1:A:199:LYS:HE3	1:A:200:LYS:HA	1.80	0.62
1:C:185:VAL:CG1	1:C:189:THR:HB	2.29	0.61
1:D:148:ASN:N	1:D:148:ASN:ND2	2.46	0.61
1:D:143:HIS:HE1	1:D:148:ASN:C	2.09	0.61
1:C:130:MET:CE	1:C:132:LEU:HD11	2.29	0.61
1:C:27:GLU:HG2	1:C:32:LEU:O	2.00	0.60
1:D:9:VAL:HG21	1:D:32:LEU:HD22	1.83	0.60
1:B:59:ILE:HD13	1:B:102:TRP:CZ3	2.36	0.60
1:A:156:TYR:CE2	1:A:164:GLN:HG2	2.37	0.60
1:C:148:ASN:N	1:C:148:ASN:ND2	2.44	0.60
1:D:76:LYS:HE2	1:D:85:GLU:OE2	2.01	0.60
1:B:213:ALA:O	1:B:217:ILE:HG22	2.00	0.60
1:D:143:HIS:HD1	1:D:148:ASN:HB2	1.67	0.60
1:B:185:VAL:HG12	1:B:189:THR:HB	1.82	0.60
1:A:156:TYR:C	1:A:156:TYR:CD2	2.80	0.60
1:B:120:LYS:O	1:B:123:SER:OG	2.18	0.59
1:A:160:THR:HG23	1:A:163:GLU:CD	2.28	0.59
1:B:175:SER:HB3	1:B:178:GLU:CG	2.31	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:LYS:HB2	1:A:191:LYS:HZ2	1.67	0.59
1:D:133:THR:CG2	1:D:135:LYS:H	2.16	0.59
1:B:10:ARG:HB3	1:B:57:LEU:HD23	1.85	0.59
1:B:137:ALA:O	1:B:141:ILE:HG13	2.03	0.58
1:D:123:SER:O	1:D:127:GLN:HG2	2.03	0.58
1:C:145:ARG:HG2	1:C:145:ARG:NH1	2.14	0.58
1:A:75:PHE:O	1:A:79:SER:OG	2.22	0.58
1:A:176:ASN:OD1	1:A:206:ARG:NH1	2.36	0.58
1:A:27:GLU:HG2	1:A:32:LEU:O	2.04	0.58
1:C:137:ALA:O	1:C:141:ILE:HG13	2.04	0.57
1:D:49:PRO:HA	1:D:52:ARG:NH1	2.19	0.57
1:B:13:SER:O	1:B:38:PRO:HA	2.05	0.57
1:C:137:ALA:HB1	1:D:137:ALA:HB1	1.86	0.57
1:A:141:ILE:O	1:A:145:ARG:HB2	2.04	0.57
1:D:130:MET:CE	1:D:132:LEU:HD11	2.34	0.57
1:B:143:HIS:CE1	1:B:148:ASN:HB2	2.40	0.57
1:D:210:LEU:H	1:D:210:LEU:HD23	1.69	0.57
1:B:11:MET:HE2	1:B:36:ILE:HG12	1.86	0.57
1:A:185:VAL:HG12	1:A:189:THR:HB	1.86	0.57
1:B:171:GLY:HA3	1:B:213:ALA:HB1	1.85	0.57
1:B:39:PHE:HB3	1:B:68:VAL:HG11	1.86	0.56
1:B:197:VAL:CG1	1:B:201:ILE:HD12	2.35	0.56
1:A:97:LYS:HA	1:A:100:PHE:CE2	2.40	0.56
1:A:186:SER:HB3	1:A:189:THR:OG1	2.05	0.56
1:D:137:ALA:O	1:D:141:ILE:HG13	2.05	0.56
1:C:96:HIS:HB2	1:C:139:GLU:HG2	1.87	0.56
1:A:39:PHE:HB3	1:A:68:VAL:HG11	1.88	0.56
1:D:39:PHE:O	1:D:42:LEU:HB2	2.05	0.56
1:B:143:HIS:CD2	1:B:144:TYR:CE2	2.94	0.56
1:C:8:ASN:HB3	1:C:55:GLN:HG3	1.87	0.56
1:C:156:TYR:C	1:C:156:TYR:CD2	2.84	0.56
1:B:31:PRO:HD2	1:B:126:LEU:HD23	1.87	0.55
1:C:56:MET:HE1	1:C:122:MET:HE1	1.88	0.55
1:D:10:ARG:HB3	1:D:57:LEU:HD23	1.89	0.55
1:C:56:MET:HE3	1:C:58:VAL:CG2	2.37	0.55
1:D:12:LEU:HA	1:D:37:THR:O	2.06	0.55
1:D:41:GLU:O	1:D:41:GLU:HG2	2.07	0.55
1:A:96:HIS:HB3	1:A:136:LEU:HD12	1.89	0.55
1:B:156:TYR:CE1	1:B:217:ILE:HD11	2.41	0.54
1:B:97:LYS:HA	1:B:100:PHE:CE2	2.42	0.54
1:A:49:PRO:HA	1:A:52:ARG:NH2	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:133:THR:HG22	1:D:135:LYS:H	1.70	0.54
1:C:200:LYS:O	1:C:201:ILE:C	2.50	0.54
1:D:52:ARG:HA	1:D:79:SER:O	2.07	0.54
1:C:31:PRO:HD2	1:C:126:LEU:CD2	2.36	0.54
1:C:85:GLU:OE2	1:C:102:TRP:HB3	2.07	0.54
1:A:148:ASN:OD1	1:A:148:ASN:N	2.41	0.54
1:A:154:GLN:O	1:A:158:LYS:HG3	2.06	0.54
1:D:4:GLU:HG3	1:D:5:ASN:H	1.72	0.54
1:D:207:LEU:HA	1:D:210:LEU:CD2	2.36	0.54
1:C:207:LEU:HA	1:C:210:LEU:HD23	1.89	0.54
1:D:9:VAL:HG12	1:D:10:ARG:N	2.23	0.54
1:B:43:TRP:CE2	1:B:44:LEU:CD2	2.91	0.53
1:B:154:GLN:O	1:B:158:LYS:HG3	2.08	0.53
1:D:95:GLU:HB3	1:D:98:LEU:HG	1.89	0.53
1:D:43:TRP:CE2	1:D:44:LEU:HG	2.43	0.53
1:B:19:SER:HB3	1:B:36:ILE:HD13	1.91	0.53
1:D:100:PHE:CD2	1:D:143:HIS:CD2	2.93	0.53
1:A:8:ASN:HB3	1:A:55:GLN:HG3	1.91	0.52
1:A:19:SER:HB3	1:A:36:ILE:HD13	1.91	0.52
1:B:144:TYR:O	1:B:147:GLY:N	2.40	0.52
1:C:31:PRO:HD2	1:C:126:LEU:HD23	1.91	0.52
1:C:19:SER:HB3	1:C:36:ILE:HD13	1.92	0.52
1:D:109:PHE:CE1	1:D:118:LEU:HA	2.44	0.52
1:B:168:LYS:HG2	1:B:217:ILE:HG13	1.91	0.52
1:C:154:GLN:NE2	1:C:154:GLN:CA	2.70	0.52
1:B:29:LYS:O	1:B:30:LEU:HD23	2.11	0.51
1:D:17:MET:HE3	1:D:17:MET:HA	1.91	0.51
1:A:10:ARG:HB3	1:A:57:LEU:HD23	1.91	0.51
1:B:177:ILE:HD12	1:B:177:ILE:N	2.24	0.51
1:C:141:ILE:HD13	1:D:140:TYR:CD2	2.46	0.51
1:A:94:ILE:HD13	1:A:95:GLU:N	2.26	0.51
1:D:212:TRP:CZ2	1:D:216:ASN:ND2	2.68	0.51
1:C:52:ARG:HA	1:C:79:SER:O	2.10	0.51
1:D:132:LEU:HD22	1:D:136:LEU:HD23	1.92	0.51
1:A:132:LEU:HD22	1:A:136:LEU:HD23	1.93	0.51
1:A:170:LEU:HD21	1:A:206:ARG:NH2	2.27	0.50
1:B:150:VAL:CG1	1:B:218:GLY:H	2.20	0.50
1:C:154:GLN:CA	1:C:154:GLN:HE21	2.24	0.50
1:C:180:ALA:HB1	1:C:185:VAL:O	2.11	0.50
1:A:16:CYS:O	1:A:17:MET:C	2.54	0.50
1:C:56:MET:SD	1:C:122:MET:HE1	2.51	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:169:LEU:HD12	1:C:179:ILE:HG23	1.92	0.50
1:C:196:ASN:N	1:C:196:ASN:ND2	2.57	0.50
1:B:17:MET:HE3	1:B:17:MET:CA	2.42	0.50
1:C:92:GLN:OE1	1:C:110:TYR:HB3	2.11	0.50
1:B:207:LEU:HD12	1:B:210:LEU:HD23	1.92	0.50
1:C:212:TRP:O	1:C:216:ASN:HB2	2.12	0.50
1:C:196:ASN:N	1:C:196:ASN:HD22	2.07	0.50
1:B:202:ASN:CG	1:B:202:ASN:O	2.55	0.50
1:D:17:MET:HE3	1:D:17:MET:CA	2.42	0.49
1:A:11:MET:HE2	1:A:36:ILE:HG12	1.94	0.49
1:D:13:SER:O	1:D:38:PRO:HA	2.11	0.49
1:A:15:VAL:O	1:A:16:CYS:HB3	2.12	0.49
1:D:30:LEU:HD13	1:D:122:MET:HB3	1.95	0.49
1:A:11:MET:HB2	1:A:34:LEU:HD21	1.93	0.49
1:B:162:ARG:HG3	1:B:162:ARG:NH1	2.25	0.49
1:C:165:GLN:O	1:C:169:LEU:HG	2.13	0.49
1:D:85:GLU:OE1	1:D:102:TRP:HE3	1.96	0.49
1:B:212:TRP:CD1	1:B:216:ASN:HD22	2.31	0.49
1:C:164:GLN:O	1:C:168:LYS:HG3	2.13	0.49
1:A:177:ILE:H	1:A:177:ILE:HD12	1.77	0.48
1:A:199:LYS:HE3	1:A:199:LYS:HA	1.95	0.48
1:B:202:ASN:O	1:B:202:ASN:OD1	2.30	0.48
1:C:145:ARG:HH11	1:C:145:ARG:CB	2.26	0.48
1:C:9:VAL:HG13	1:C:56:MET:HE2	1.96	0.48
1:D:148:ASN:H	1:D:148:ASN:ND2	2.04	0.48
1:A:50:GLU:CD	1:A:50:GLU:H	2.22	0.48
1:C:56:MET:HE3	1:C:58:VAL:HG23	1.96	0.48
1:A:74:SER:O	1:A:78:ILE:HG12	2.14	0.48
1:A:185:VAL:CG1	1:A:189:THR:HB	2.43	0.48
1:B:9:VAL:HG12	1:B:10:ARG:N	2.27	0.48
1:C:154:GLN:HA	1:C:154:GLN:HE21	1.71	0.48
1:D:50:GLU:H	1:D:50:GLU:CD	2.22	0.48
1:D:206:ARG:O	1:D:210:LEU:HD23	2.14	0.48
1:B:17:MET:HE3	1:B:17:MET:HA	1.96	0.47
1:C:41:GLU:HG3	1:C:44:LEU:HD12	1.96	0.47
1:C:49:PRO:HA	1:C:52:ARG:NH2	2.29	0.47
1:D:17:MET:HE2	1:D:17:MET:HB3	1.71	0.47
1:B:31:PRO:HD2	1:B:126:LEU:CD2	2.44	0.47
1:A:185:VAL:HG12	1:A:186:SER:N	2.28	0.47
1:C:175:SER:HB3	1:C:178:GLU:HG3	1.97	0.47
1:D:132:LEU:HD22	1:D:136:LEU:CD2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:LEU:O	1:A:48:LYS:HE3	2.15	0.47
1:C:134:ARG:NH2	1:D:124:LYS:HD3	2.29	0.47
1:C:185:VAL:HG12	1:C:189:THR:HB	1.97	0.47
1:D:133:THR:CG2	1:D:134:ARG:N	2.77	0.47
1:D:49:PRO:HA	1:D:52:ARG:HH12	1.79	0.47
1:D:66:ASP:HA	1:D:69:LEU:HD12	1.97	0.47
1:B:185:VAL:HG12	1:B:186:SER:N	2.30	0.47
1:A:104:ASN:O	1:A:105:LEU:C	2.58	0.46
1:D:143:HIS:HE1	1:D:148:ASN:CB	2.26	0.46
1:A:132:LEU:CD2	1:A:136:LEU:HD23	2.46	0.46
1:C:74:SER:HB3	1:C:208:GLN:HG2	1.98	0.46
1:A:137:ALA:HB1	1:B:137:ALA:HB1	1.96	0.46
1:A:212:TRP:CD1	1:A:216:ASN:HD22	2.33	0.46
1:B:23:LYS:HE3	1:B:34:LEU:O	2.16	0.46
1:B:133:THR:HG23	1:B:135:LYS:N	2.31	0.46
1:B:165:GLN:O	1:B:169:LEU:HG	2.16	0.46
1:A:97:LYS:HA	1:A:100:PHE:CD2	2.51	0.46
1:A:120:LYS:O	1:A:123:SER:OG	2.31	0.46
1:B:207:LEU:O	1:B:211:ILE:HG13	2.15	0.46
1:B:70:THR:HG21	1:B:201:ILE:O	2.16	0.46
1:B:17:MET:HE2	1:B:17:MET:HB3	1.79	0.45
1:C:138:GLN:OE1	1:D:129:GLU:HA	2.16	0.45
1:C:155:MET:HA	1:C:158:LYS:HG3	1.97	0.45
1:A:167:ILE:HD12	1:A:167:ILE:HA	1.85	0.45
1:A:198:PHE:O	1:A:202:ASN:N	2.48	0.45
1:C:199:LYS:N	1:C:199:LYS:CD	2.72	0.45
1:D:65:SER:OG	1:D:68:VAL:HG22	2.16	0.45
1:D:121:GLY:O	1:D:125:ILE:HG13	2.16	0.45
1:A:156:TYR:HH	1:A:168:LYS:HE3	1.80	0.45
1:B:150:VAL:HG13	1:B:151:VAL:N	2.31	0.45
1:C:9:VAL:CG1	1:C:56:MET:HE2	2.46	0.45
1:D:87:ILE:HG12	1:D:105:LEU:CD1	2.46	0.45
1:B:124:LYS:O	1:B:127:GLN:HB2	2.16	0.45
1:B:180:ALA:HB1	1:B:185:VAL:O	2.17	0.45
1:A:18:GLN:NE2	1:A:18:GLN:N	2.50	0.45
1:B:177:ILE:HG13	1:B:187:GLU:HG3	1.98	0.45
1:C:153:SER:HG	1:C:216:ASN:HB3	1.81	0.45
1:A:49:PRO:HA	1:A:52:ARG:HH22	1.82	0.45
1:D:61:TYR:O	1:D:64:ILE:HG22	2.16	0.45
1:D:133:THR:HG22	1:D:136:LEU:H	1.81	0.45
1:D:143:HIS:HE1	1:D:148:ASN:HB2	1.67	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:212:TRP:O	1:D:216:ASN:HB2	2.17	0.45
1:B:50:GLU:H	1:B:50:GLU:CD	2.25	0.44
1:C:133:THR:HG22	1:C:136:LEU:HB3	1.98	0.44
1:A:122:MET:HB3	1:A:122:MET:HE3	1.63	0.44
1:B:156:TYR:CE1	1:B:217:ILE:CD1	3.00	0.44
1:D:43:TRP:CH2	1:D:44:LEU:HD21	2.52	0.44
1:B:162:ARG:NH1	1:B:162:ARG:CG	2.78	0.44
1:C:13:SER:O	1:C:38:PRO:HA	2.18	0.44
1:B:161:LYS:H	1:B:161:LYS:HD2	1.82	0.44
1:B:11:MET:HB2	1:B:34:LEU:HD21	1.98	0.44
1:B:161:LYS:HD2	1:B:161:LYS:N	2.32	0.44
1:A:197:VAL:C	1:A:199:LYS:N	2.74	0.44
1:B:156:TYR:CZ	1:B:217:ILE:HD11	2.52	0.44
1:B:212:TRP:CD1	1:B:216:ASN:ND2	2.86	0.44
1:A:156:TYR:CZ	1:A:164:GLN:HG2	2.52	0.43
1:C:52:ARG:HG3	1:C:52:ARG:HH21	1.84	0.43
1:C:115:MET:HE3	1:C:115:MET:HB3	1.81	0.43
1:D:30:LEU:HA	1:D:31:PRO:HD3	1.82	0.43
1:A:133:THR:HG23	1:A:135:LYS:N	2.33	0.43
1:C:41:GLU:O	1:C:41:GLU:HG2	2.19	0.43
1:D:199:LYS:HA	1:D:200:LYS:HA	1.73	0.43
1:B:209:ALA:O	1:B:212:TRP:HB3	2.19	0.43
1:C:23:LYS:CE	1:C:34:LEU:O	2.66	0.43
1:B:70:THR:HG21	1:B:202:ASN:HB3	2.00	0.43
1:C:145:ARG:HH11	1:C:145:ARG:HB3	1.83	0.43
1:B:97:LYS:HA	1:B:100:PHE:CD2	2.52	0.43
1:B:156:TYR:CD1	1:B:217:ILE:CD1	3.01	0.43
1:B:122:MET:HB3	1:B:122:MET:HE3	1.64	0.43
1:B:167:ILE:HD12	1:B:167:ILE:HA	1.92	0.43
1:B:8:ASN:OD1	1:B:54:ILE:HA	2.18	0.43
1:C:215:ASN:O	1:C:216:ASN:OD1	2.36	0.43
1:D:34:LEU:HD23	1:D:35:GLU:N	2.34	0.43
1:A:200:LYS:O	1:A:201:ILE:C	2.62	0.43
1:C:48:LYS:HA	1:C:49:PRO:HD3	1.86	0.43
1:D:11:MET:HB2	1:D:34:LEU:HD21	2.00	0.43
1:C:142:LEU:HA	1:C:142:LEU:HD12	1.72	0.42
1:B:162:ARG:HA	1:B:162:ARG:HD3	1.83	0.42
1:D:115:MET:HE3	1:D:115:MET:HB3	1.92	0.42
1:B:43:TRP:CH2	1:B:44:LEU:HD11	2.55	0.42
1:C:9:VAL:HG21	1:C:32:LEU:HD22	2.01	0.42
1:A:119:ILE:HD13	1:A:119:ILE:HA	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:LYS:HA	1:A:199:LYS:CE	2.49	0.42
1:B:198:PHE:N	1:B:198:PHE:CD1	2.86	0.42
1:C:159:LEU:CD1	1:C:164:GLN:HG3	2.42	0.42
1:A:156:TYR:HD2	1:A:157:ALA:N	2.16	0.42
1:B:92:GLN:NE2	1:B:112:ASP:OD1	2.47	0.42
1:B:180:ALA:HB2	1:B:187:GLU:HA	2.00	0.42
1:C:176:ASN:OD1	1:C:206:ARG:NH1	2.52	0.42
1:B:30:LEU:HA	1:B:31:PRO:HD3	1.86	0.42
1:D:115:MET:O	1:D:119:ILE:HG12	2.20	0.42
1:A:87:ILE:HD13	1:A:105:LEU:HD13	2.02	0.42
1:A:160:THR:HG23	1:A:163:GLU:OE1	2.20	0.42
1:A:170:LEU:C	1:A:172:SER:H	2.28	0.42
1:B:120:LYS:O	1:B:124:LYS:HG3	2.20	0.42
1:D:210:LEU:O	1:D:213:ALA:HB3	2.20	0.42
1:B:177:ILE:H	1:B:177:ILE:CD1	2.31	0.41
1:A:48:LYS:HA	1:A:49:PRO:HD3	1.83	0.41
1:A:156:TYR:CE1	1:A:217:ILE:HD13	2.55	0.41
1:A:61:TYR:O	1:A:64:ILE:HG22	2.20	0.41
1:B:212:TRP:NE1	1:B:216:ASN:ND2	2.69	0.41
1:C:215:ASN:O	1:C:216:ASN:CG	2.62	0.41
1:B:56:MET:HE3	1:B:58:VAL:CG2	2.50	0.41
1:C:44:LEU:O	1:C:48:LYS:HE3	2.20	0.41
1:D:52:ARG:HG2	1:D:79:SER:O	2.20	0.41
1:A:56:MET:HE3	1:A:58:VAL:CG2	2.50	0.41
1:A:170:LEU:HD23	1:A:170:LEU:HA	1.82	0.41
1:B:110:TYR:O	1:B:111:ILE:C	2.63	0.41
1:B:170:LEU:HD23	1:B:170:LEU:HA	1.85	0.41
1:A:127:GLN:NE2	1:C:6:LYS:HE3	2.32	0.41
1:B:218:GLY:HA2	1:B:219:ILE:HA	1.84	0.41
1:C:161:LYS:HD2	1:C:161:LYS:H	1.81	0.41
1:A:43:TRP:CH2	1:A:44:LEU:HD21	2.56	0.41
1:A:85:GLU:OE2	1:A:102:TRP:HB3	2.20	0.41
1:D:37:THR:HA	1:D:38:PRO:HD3	1.91	0.41
1:B:9:VAL:HG13	1:B:56:MET:HB3	2.03	0.41
1:B:39:PHE:C	1:B:41:GLU:H	2.29	0.41
1:B:66:ASP:HB3	1:B:155:MET:CE	2.50	0.41
1:B:111:ILE:HG22	1:B:112:ASP:N	2.36	0.41
1:B:144:TYR:CD2	1:B:144:TYR:N	2.89	0.41
1:B:145:ARG:NH1	1:B:145:ARG:CG	2.62	0.41
1:A:65:SER:O	1:A:68:VAL:HG22	2.21	0.41
1:A:159:LEU:HB3	1:A:163:GLU:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:LEU:HD12	1:B:7:LEU:HA	1.76	0.40
1:C:7:LEU:HD12	1:C:7:LEU:HA	1.94	0.40
1:B:43:TRP:CZ2	1:B:44:LEU:HD21	2.57	0.40
1:B:56:MET:SD	1:B:122:MET:HE1	2.61	0.40
1:C:21:LEU:HD12	1:C:21:LEU:HA	1.71	0.40
1:C:34:LEU:C	1:C:34:LEU:HD23	2.47	0.40
1:B:6:LYS:HE3	1:B:6:LYS:HB3	1.87	0.40
1:C:153:SER:OG	1:C:216:ASN:CB	2.60	0.40
1:C:185:VAL:HG12	1:C:186:SER:O	2.21	0.40
1:D:138:GLN:O	1:D:142:LEU:HB2	2.22	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	215/225 (96%)	203 (94%)	12 (6%)	0	100	100
1	B	213/225 (95%)	198 (93%)	14 (7%)	1 (0%)	24	54
1	C	211/225 (94%)	200 (95%)	9 (4%)	2 (1%)	14	41
1	D	169/225 (75%)	152 (90%)	17 (10%)	0	100	100
All	All	808/900 (90%)	753 (93%)	52 (6%)	3 (0%)	30	58

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	202	ASN
1	C	143	HIS
1	C	201	ILE

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	199/207 (96%)	165 (83%)	34 (17%)	2	9
1	B	197/207 (95%)	160 (81%)	37 (19%)	1	7
1	C	196/207 (95%)	157 (80%)	39 (20%)	1	5
1	D	161/207 (78%)	144 (89%)	17 (11%)	6	24
All	All	753/828 (91%)	626 (83%)	127 (17%)	2	9

All (127) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	10	ARG
1	A	15	VAL
1	A	17	MET
1	A	18	GLN
1	A	19	SER
1	A	29	LYS
1	A	32	LEU
1	A	42	LEU
1	A	50	GLU
1	A	55	GLN
1	A	67	ASP
1	A	76	LYS
1	A	79	SER
1	A	85	GLU
1	A	87	ILE
1	A	94	ILE
1	A	111	ILE
1	A	132	LEU
1	A	133	THR
1	A	142	LEU
1	A	148	ASN
1	A	150	VAL
1	A	151	VAL

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Mol	Chain	Res	Type
1	A	160	THR
1	A	161	LYS
1	A	162	ARG
1	A	167	ILE
1	A	170	LEU
1	A	186	SER
1	A	190	VAL
1	A	191	LYS
1	A	202	ASN
1	A	219	ILE
1	B	5	ASN
1	B	6	LYS
1	B	10	ARG
1	B	15	VAL
1	B	17	MET
1	B	18	GLN
1	B	29	LYS
1	B	32	LEU
1	B	35	GLU
1	B	44	LEU
1	B	50	GLU
1	B	64	ILE
1	B	67	ASP
1	B	70	THR
1	B	73	SER
1	B	76	LYS
1	B	78	ILE
1	B	79	SER
1	B	111	ILE
1	B	126	LEU
1	B	133	THR
1	B	134	ARG
1	B	142	LEU
1	B	145	ARG
1	B	148	ASN
1	B	150	VAL
1	B	151	VAL
1	B	159	LEU
1	B	160	THR
1	B	161	LYS
1	B	162	ARG
1	B	170	LEU

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Mol	Chain	Res	Type
1	B	190	VAL
1	B	201	ILE
1	B	204	LYS
1	B	210	LEU
1	B	217	ILE
1	C	4	GLU
1	C	10	ARG
1	C	12	LEU
1	C	15	VAL
1	C	17	MET
1	C	18	GLN
1	C	19	SER
1	C	23	LYS
1	C	28	SER
1	C	29	LYS
1	C	35	GLU
1	C	55	GLN
1	C	70	THR
1	C	76	LYS
1	C	87	ILE
1	C	94	ILE
1	C	111	ILE
1	C	130	MET
1	C	132	LEU
1	C	138	GLN
1	C	139	GLU
1	C	141	ILE
1	C	142	LEU
1	C	145	ARG
1	C	148	ASN
1	C	152	THR
1	C	153	SER
1	C	154	GLN
1	C	159	LEU
1	C	161	LYS
1	C	162	ARG
1	C	170	LEU
1	C	190	VAL
1	C	196	ASN
1	C	199	LYS
1	C	200	LYS
1	C	201	ILE

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Mol	Chain	Res	Type
1	C	202	ASN
1	C	210	LEU
1	D	10	ARG
1	D	17	MET
1	D	18	GLN
1	D	35	GLU
1	D	36	ILE
1	D	50	GLU
1	D	92	GLN
1	D	123	SER
1	D	129	GLU
1	D	133	THR
1	D	142	LEU
1	D	143	HIS
1	D	145	ARG
1	D	148	ASN
1	D	151	VAL
1	D	197	VAL
1	D	199	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	18	GLN
1	A	55	GLN
1	A	77	HIS
1	A	92	GLN
1	A	103	ASN
1	A	127	GLN
1	A	154	GLN
1	B	5	ASN
1	B	18	GLN
1	B	96	HIS
1	B	104	ASN
1	B	143	HIS
1	B	176	ASN
1	B	188	ASN
1	B	195	HIS
1	B	216	ASN
1	C	18	GLN
1	C	55	GLN

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Mol	Chain	Res	Type
1	C	89	ASN
1	C	103	ASN
1	C	148	ASN
1	C	154	GLN
1	C	196	ASN
1	D	5	ASN
1	D	8	ASN
1	D	18	GLN
1	D	55	GLN
1	D	89	ASN
1	D	103	ASN
1	D	143	HIS
1	D	148	ASN

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	217/225 (96%)	0.13	7 (3%)	50	28	33, 58, 93, 126	0
1	B	215/225 (95%)	0.16	7 (3%)	49	28	39, 62, 109, 121	0
1	C	213/225 (94%)	0.35	14 (6%)	24	12	47, 80, 121, 135	0
1	D	173/225 (76%)	0.85	25 (14%)	6	3	60, 84, 125, 137	0
All	All	818/900 (90%)	0.35	53 (6%)	25	13	33, 74, 118, 137	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	219	ILE	5.6
1	A	3	ASP	4.4
1	C	147	GLY	4.3
1	B	219	ILE	4.2
1	D	215	ASN	4.0
1	D	213	ALA	3.5
1	A	147	GLY	3.3
1	D	151	VAL	3.2
1	D	216	ASN	3.1
1	D	214	LYS	3.1
1	C	216	ASN	3.0
1	C	207	LEU	3.0
1	C	152	THR	3.0
1	D	204	LYS	2.9
1	A	35	GLU	2.9
1	B	217	ILE	2.8
1	D	8	ASN	2.8
1	D	193	HIS	2.7
1	C	155	MET	2.7
1	B	202	ASN	2.6
1	C	213	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	148	ASN	2.5
1	D	82	ASP	2.4
1	D	199	LYS	2.4
1	D	147	GLY	2.4
1	B	172	SER	2.4
1	A	200	LYS	2.4
1	D	150	VAL	2.4
1	D	97	LYS	2.3
1	C	149	SER	2.3
1	C	151	VAL	2.3
1	D	198	PHE	2.3
1	C	198	PHE	2.2
1	D	96	HIS	2.2
1	C	153	SER	2.2
1	A	5	ASN	2.2
1	C	200	LYS	2.2
1	C	211	ILE	2.2
1	D	56	MET	2.2
1	D	7	LEU	2.2
1	C	146	ALA	2.2
1	B	147	GLY	2.1
1	D	144	TYR	2.1
1	D	208	GLN	2.1
1	D	194	LEU	2.1
1	B	127	GLN	2.1
1	D	197	VAL	2.1
1	D	207	LEU	2.1
1	A	214	LYS	2.0
1	C	214	LYS	2.0
1	D	15	VAL	2.0
1	B	177	ILE	2.0
1	D	200	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.