



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 01:23 PM UTC

PDB ID : 3N2C / pdb_00003n2c
Title : Crystal structure of prolidase eah89906 complexed with n-methylphosphonat
e-l-proline
Authors : Patskovsky, Y.; Xu, C.; Sauder, J.M.; Burley, S.K.; Raushel, F.M.; Almo,
S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2010-05-17
Resolution : 2.81 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

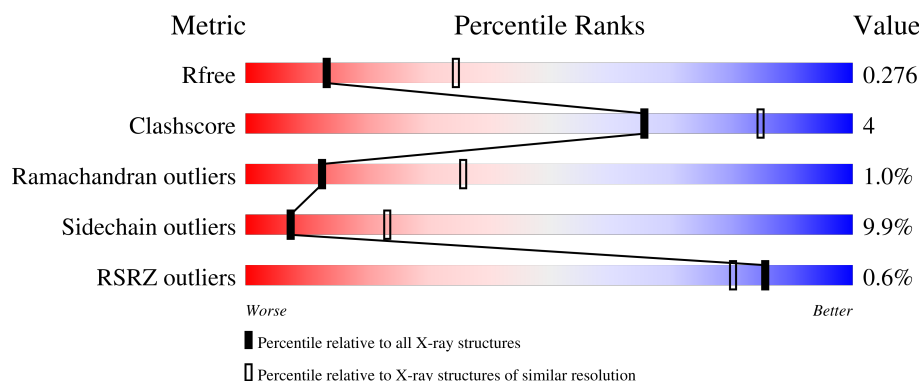
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.81 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	4591 (2.84-2.80)
Clashscore	190562	5010 (2.84-2.80)
Ramachandran outliers	187476	4916 (2.84-2.80)
Sidechain outliers	187428	4918 (2.84-2.80)
RSRZ outliers	180081	4594 (2.84-2.80)

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	423	 78% 16% . .
1	B	423	 81% 15% . .
1	C	423	 78% 17% . .
1	D	423	 80% 16% .
1	E	423	 80% 15% . .

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Mol	Chain	Length	Quality of chain
1	F	423	 81% 14% . .
1	G	423	 81% 15% .
1	H	423	%  81% 14% . .
1	I	423	%  79% 16% . .
1	J	423	%  81% 14% . .
1	K	423	%  79% 15% . .
1	L	423	2%  79% 16% . .
1	M	423	%  80% 15% . .
1	N	423	%  76% 19% . .
1	O	423	%  80% 15% . .
1	P	423	 81% 14% . .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 48752 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.

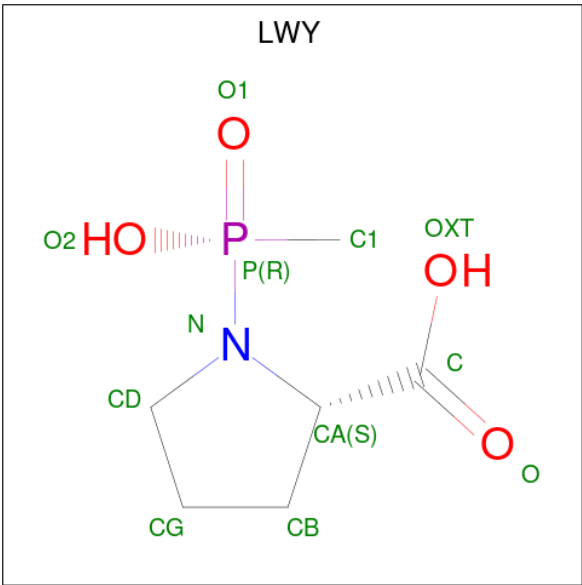
- Molecule 1 is a protein called PROLIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	408	Total	C	N	O	S	0	0	0
			3033	1887	549	582	15			
1	B	408	Total	C	N	O	S	0	0	0
			3033	1887	549	582	15			
1	C	408	Total	C	N	O	S	0	0	0
			3033	1887	549	582	15			
1	D	408	Total	C	N	O	S	0	0	0
			3033	1887	549	582	15			
1	E	408	Total	C	N	O	S	0	0	0
			3033	1887	549	582	15			
1	F	408	Total	C	N	O	S	0	0	0
			3033	1887	549	582	15			
1	G	408	Total	C	N	O	S	0	0	0
			3033	1887	549	582	15			
1	H	408	Total	C	N	O	S	0	0	0
			3033	1887	549	582	15			
1	I	408	Total	C	N	O	S	0	0	0
			3033	1887	549	582	15			
1	J	408	Total	C	N	O	S	0	0	0
			3033	1887	549	582	15			
1	K	408	Total	C	N	O	S	0	0	0
			3033	1887	549	582	15			
1	L	408	Total	C	N	O	S	0	0	0
			3033	1887	549	582	15			
1	M	408	Total	C	N	O	S	0	0	0
			3033	1887	549	582	15			
1	N	408	Total	C	N	O	S	0	0	0
			3033	1887	549	582	15			
1	O	408	Total	C	N	O	S	0	0	0
			3033	1887	549	582	15			
1	P	408	Total	C	N	O	S	0	0	0
			3033	1887	549	582	15			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total 2	Zn 2	0	0
2	B	2	Total 2	Zn 2	0	0
2	C	2	Total 2	Zn 2	0	0
2	D	2	Total 2	Zn 2	0	0
2	E	2	Total 2	Zn 2	0	0
2	F	2	Total 2	Zn 2	0	0
2	G	2	Total 2	Zn 2	0	0
2	H	2	Total 2	Zn 2	0	0
2	I	2	Total 2	Zn 2	0	0
2	J	2	Total 2	Zn 2	0	0
2	K	2	Total 2	Zn 2	0	0
2	L	2	Total 2	Zn 2	0	0
2	M	2	Total 2	Zn 2	0	0
2	N	2	Total 2	Zn 2	0	0
2	O	2	Total 2	Zn 2	0	0
2	P	2	Total 2	Zn 2	0	0

- Molecule 3 is 1-[(R)-hydroxy(methyl)phosphoryl]-L-proline (CCD ID: LWY) (formula: C₆H₁₂NO₄P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			12	6	1	4	1		
3	B	1	Total	C	N	O	P	0	0
			12	6	1	4	1		
3	C	1	Total	C	N	O	P	0	0
			12	6	1	4	1		
3	D	1	Total	C	N	O	P	0	0
			12	6	1	4	1		
3	E	1	Total	C	N	O	P	0	0
			12	6	1	4	1		
3	F	1	Total	C	N	O	P	0	0
			12	6	1	4	1		
3	G	1	Total	C	N	O	P	0	0
			12	6	1	4	1		
3	H	1	Total	C	N	O	P	0	0
			12	6	1	4	1		
3	I	1	Total	C	N	O	P	0	0
			12	6	1	4	1		
3	J	1	Total	C	N	O	P	0	0
			12	6	1	4	1		
3	K	1	Total	C	N	O	P	0	0
			12	6	1	4	1		
3	L	1	Total	C	N	O	P	0	0
			12	6	1	4	1		
3	M	1	Total	C	N	O	P	0	0
			12	6	1	4	1		
3	N	1	Total	C	N	O	P	0	0
			12	6	1	4	1		

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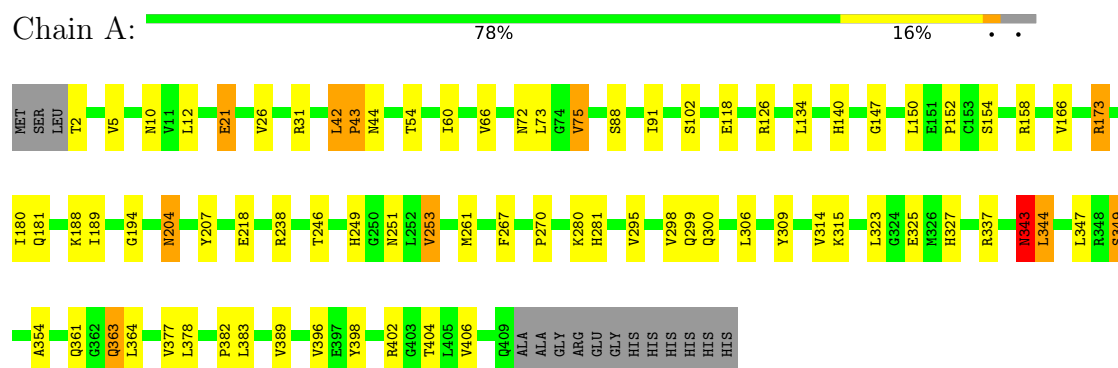
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	O	1	Total	C	N	O	P	0	0
			12	6	1	4	1		
3	P	1	Total	C	N	O	P	0	0
			12	6	1	4	1		

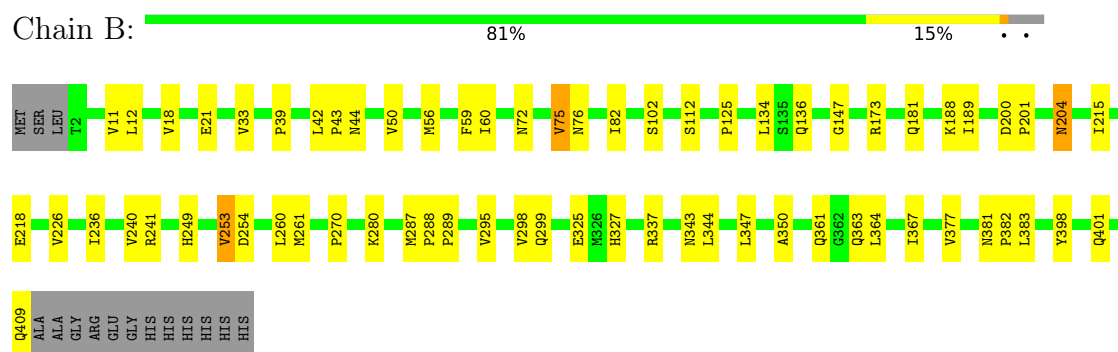
3 Residue-property plots

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.

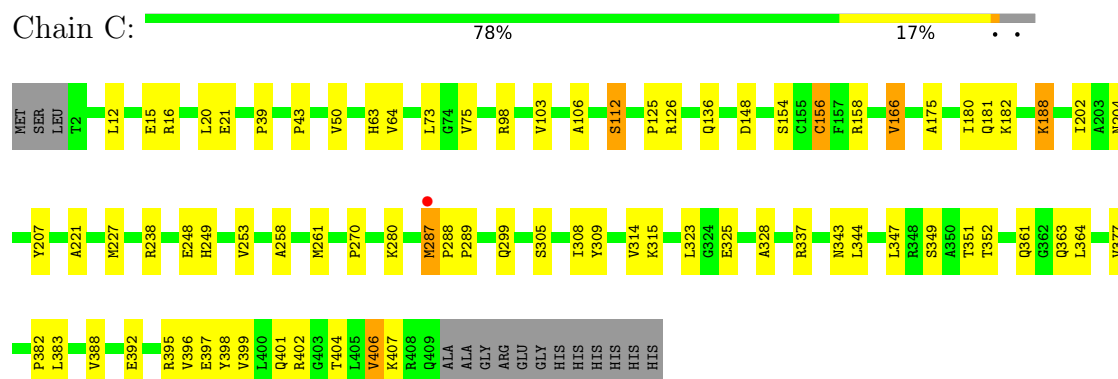
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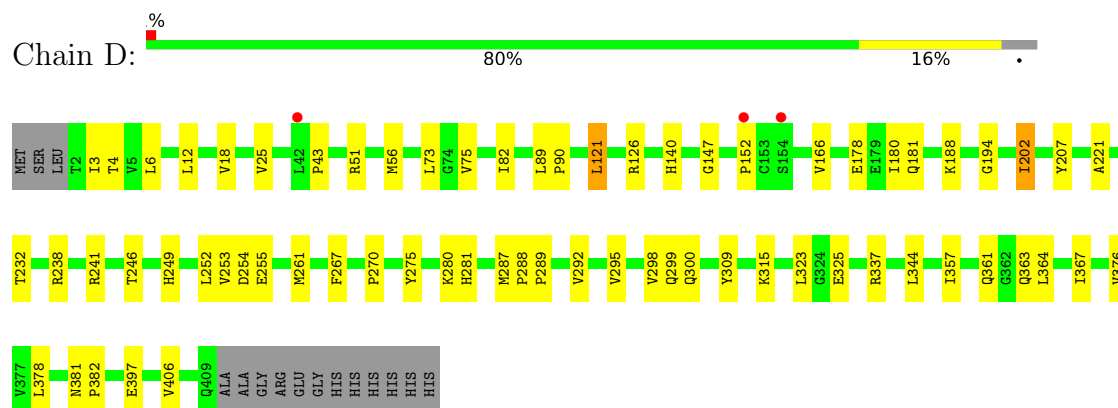
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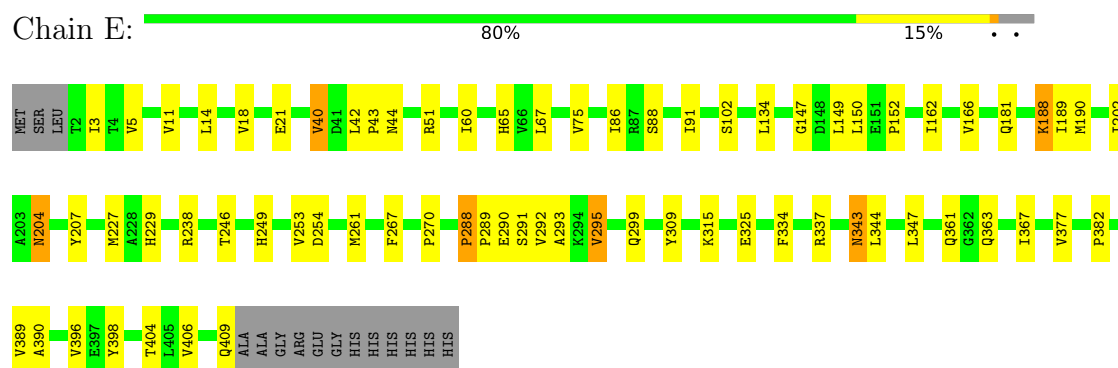
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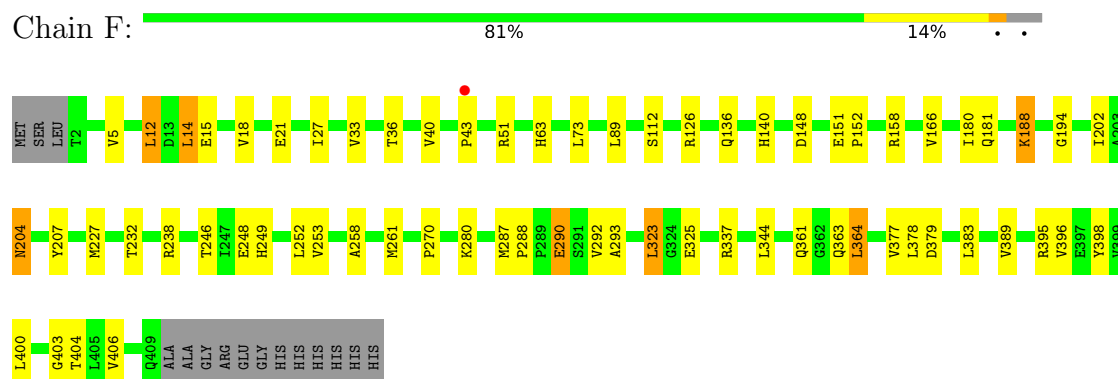
● Molecule 1: PROLIDASE



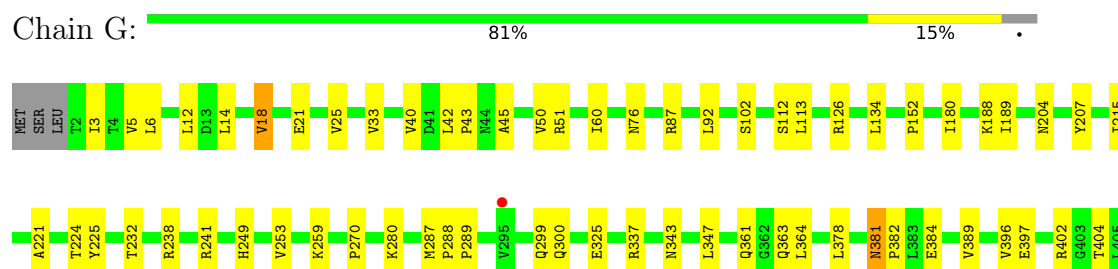
● Molecule 1: PROLIDASE

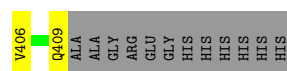


● Molecule 1: PROLIDASE

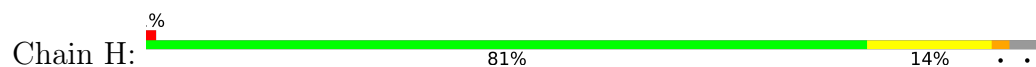


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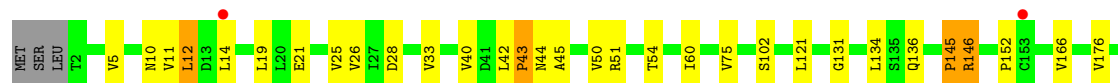
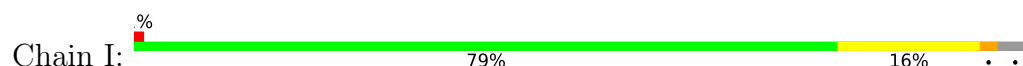




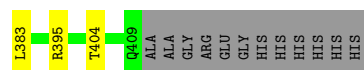
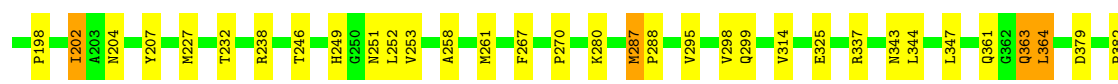
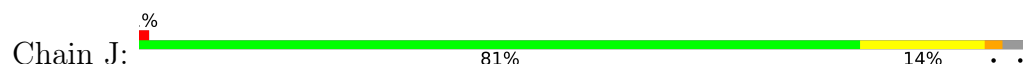
• Molecule 1: PROLIDASE



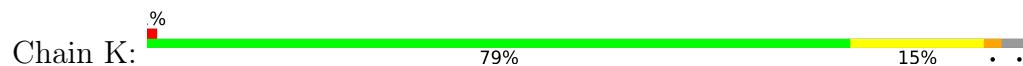
• Molecule 1: PROLIDASE

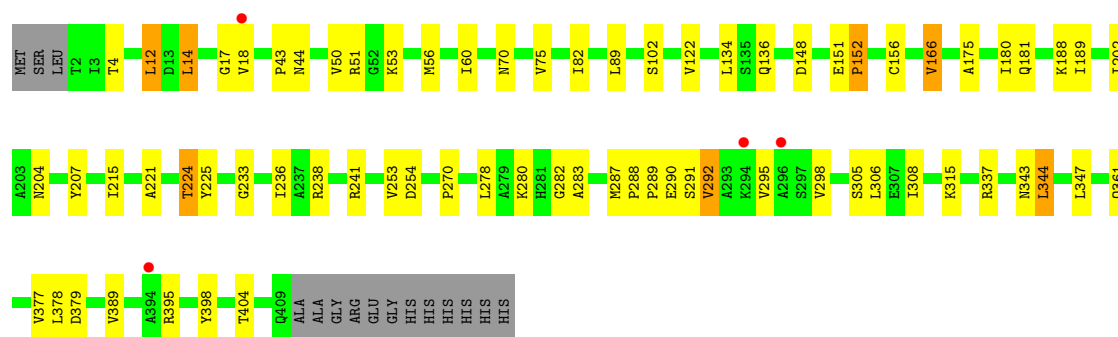


• Molecule 1: PROLIDASE

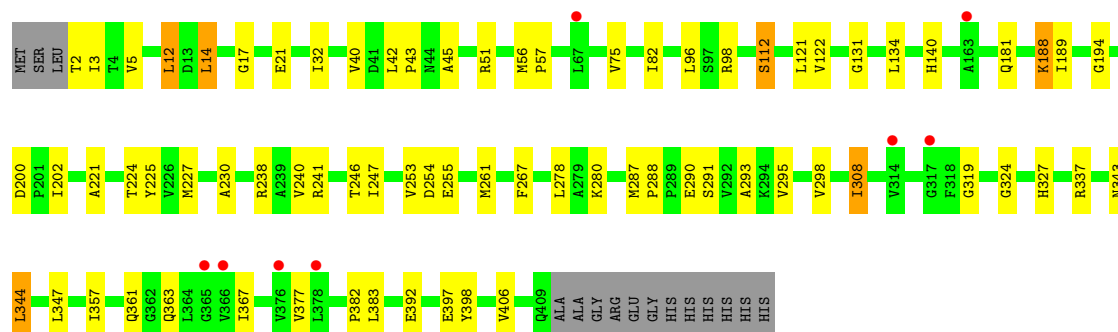


• Molecule 1: PROLIDASE

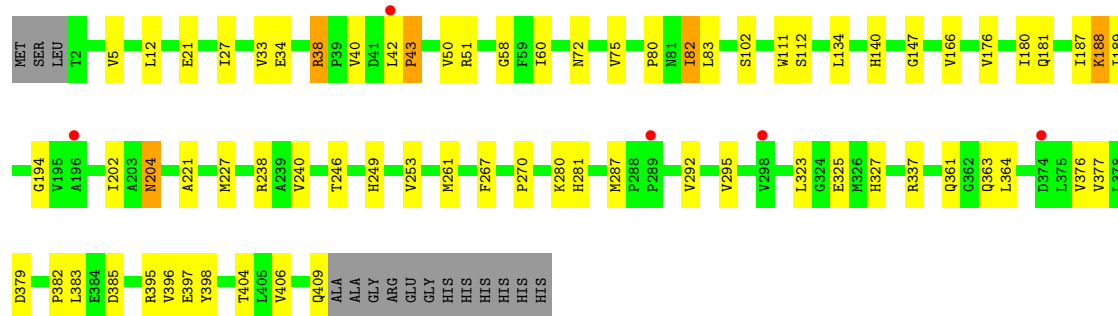
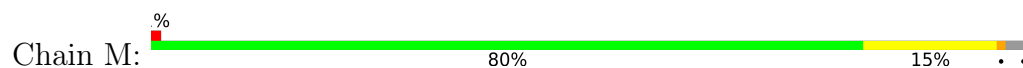




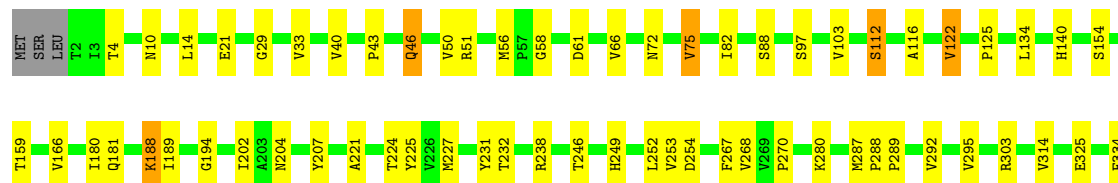
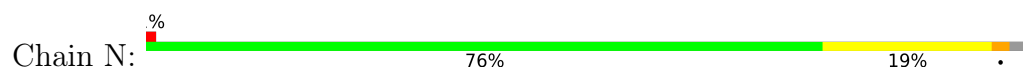
• Molecule 1: PROLIDASE

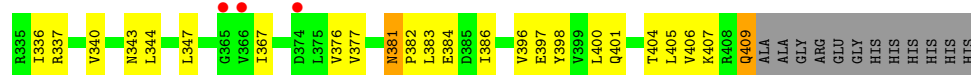


• Molecule 1: PROLIDASE

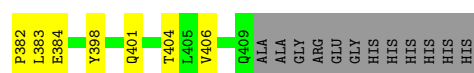
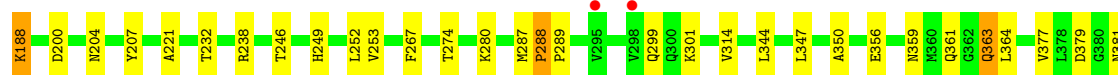
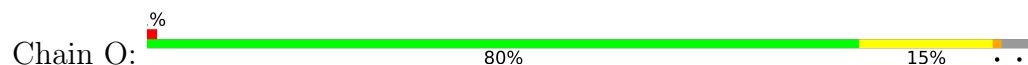


• Molecule 1: PROLIDASE

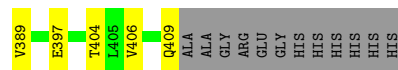
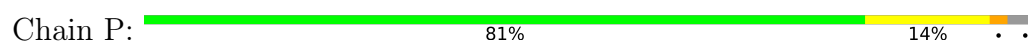




● Molecule 1: PROLIDASE



● Molecule 1: PROLIDASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	113.19Å 108.03Å 170.77Å 81.32° 80.47° 73.76°	Depositor
Resolution (Å)	40.00 – 2.81 40.00 – 2.81	Depositor EDS
% Data completeness (in resolution range)	89.9 (40.00-2.81) 90.2 (40.00-2.81)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.02 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.220 , 0.273 0.229 , 0.276	Depositor DCC
R_{free} test set	5054 reflections (2.71%)	wwPDB-VP
Wilson B-factor (Å ²)	72.7	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 47.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.014 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	48752	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% 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, LWY, KCX

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	0.51	0/3064	0.91	3/4156 (0.1%)
1	B	0.50	0/3064	0.92	3/4156 (0.1%)
1	C	0.49	0/3064	0.92	2/4156 (0.0%)
1	D	0.50	0/3064	0.91	2/4156 (0.0%)
1	E	0.52	0/3064	0.91	2/4156 (0.0%)
1	F	0.50	0/3064	0.91	4/4156 (0.1%)
1	G	0.49	0/3064	0.93	5/4156 (0.1%)
1	H	0.51	0/3064	0.90	1/4156 (0.0%)
1	I	0.53	0/3064	0.92	5/4156 (0.1%)
1	J	0.54	0/3064	0.94	3/4156 (0.1%)
1	K	0.53	0/3064	0.90	0/4156
1	L	0.52	0/3064	0.91	2/4156 (0.0%)
1	M	0.52	0/3064	0.93	2/4156 (0.0%)
1	N	0.53	0/3064	0.94	4/4156 (0.1%)
1	O	0.50	0/3064	0.92	4/4156 (0.1%)
1	P	0.51	0/3064	0.92	1/4156 (0.0%)
All	All	0.51	0/49024	0.92	43/66496 (0.1%)

There are no bond length outliers.

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	287	MET	CA-C-N	7.34	127.94	120.38
1	D	287	MET	C-N-CA	7.34	127.94	120.38
1	N	287	MET	CA-C-N	7.32	127.92	120.38
1	N	287	MET	C-N-CA	7.32	127.92	120.38
1	C	287	MET	CA-C-N	7.18	127.78	120.38
1	C	287	MET	C-N-CA	7.18	127.78	120.38
1	A	253	VAL	CB-CA-C	-6.30	104.39	111.45
1	B	287	MET	CA-C-N	6.23	126.80	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	287	MET	C-N-CA	6.23	126.80	120.38
1	M	287	MET	CA-C-N	6.20	126.76	120.38
1	M	287	MET	C-N-CA	6.20	126.76	120.38
1	I	287	MET	CA-C-N	6.02	126.58	120.38
1	I	287	MET	C-N-CA	6.02	126.58	120.38
1	F	288	PRO	O-C-N	5.85	123.90	121.15
1	I	131	GLY	N-CA-C	-5.81	106.33	111.67
1	J	363	GLN	N-CA-C	-5.76	108.05	114.62
1	G	287	MET	CA-C-N	5.75	126.30	120.38
1	G	287	MET	C-N-CA	5.75	126.30	120.38
1	O	287	MET	CA-C-N	5.73	126.28	120.38
1	O	287	MET	C-N-CA	5.73	126.28	120.38
1	O	288	PRO	CA-C-N	5.62	125.29	119.56
1	O	288	PRO	C-N-CA	5.62	125.29	119.56
1	H	33	VAL	CB-CA-C	-5.54	106.19	111.06
1	F	287	MET	CA-C-N	5.53	123.64	119.66
1	F	287	MET	C-N-CA	5.53	123.64	119.66
1	A	343	ASN	N-CA-C	5.49	117.26	111.28
1	P	3	ILE	N-CA-C	5.47	115.93	107.78
1	G	381	ASN	CA-C-N	5.44	124.96	119.19
1	G	381	ASN	C-N-CA	5.44	124.96	119.19
1	E	343	ASN	N-CA-C	5.36	119.44	113.01
1	B	253	VAL	CB-CA-C	-5.35	103.89	111.28
1	J	287	MET	CA-C-N	5.31	125.85	120.38
1	J	287	MET	C-N-CA	5.31	125.85	120.38
1	L	131	GLY	N-CA-C	-5.29	106.80	111.67
1	L	200	ASP	N-CA-C	5.22	116.25	109.72
1	F	36	THR	N-CA-C	5.20	116.97	109.07
1	G	18	VAL	N-CA-C	5.17	114.84	108.53
1	I	288	PRO	CA-C-N	5.16	124.83	119.56
1	I	288	PRO	C-N-CA	5.16	124.83	119.56
1	A	251	ASN	N-CA-C	5.06	116.80	111.28
1	N	381	ASN	CA-C-N	5.05	124.84	119.28
1	N	381	ASN	C-N-CA	5.05	124.84	119.28
1	E	288	PRO	N-CA-C	5.05	116.86	110.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3033	0	3038	35	0
1	B	3033	0	3037	21	0
1	C	3033	0	3037	28	0
1	D	3033	0	3037	20	0
1	E	3033	0	3037	22	0
1	F	3033	0	3037	21	0
1	G	3033	0	3037	21	0
1	H	3033	0	3037	18	0
1	I	3033	0	3037	23	0
1	J	3033	0	3037	20	0
1	K	3033	0	3037	29	0
1	L	3033	0	3037	33	0
1	M	3033	0	3037	23	0
1	N	3033	0	3037	30	0
1	O	3033	0	3037	23	0
1	P	3033	0	3037	20	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
2	I	2	0	0	0	0
2	J	2	0	0	0	0
2	K	2	0	0	0	0
2	L	2	0	0	0	0
2	M	2	0	0	0	0
2	N	2	0	0	0	0
2	O	2	0	0	0	0
2	P	2	0	0	0	0
3	A	12	0	10	2	0
3	B	12	0	10	0	0
3	C	12	0	10	0	0
3	D	12	0	10	0	0
3	E	12	0	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	12	0	10	0	0
3	G	12	0	10	0	0
3	H	12	0	10	0	0
3	I	12	0	10	0	0
3	J	12	0	10	1	0
3	K	12	0	10	0	0
3	L	12	0	10	1	0
3	M	12	0	10	1	0
3	N	12	0	10	0	0
3	O	12	0	10	0	0
3	P	12	0	10	0	0
All	All	48752	0	48753	368	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 4.

All (368) 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:K:278:LEU:HD22	1:K:287:MET:HE1	1.32	1.12
1:K:278:LEU:CD2	1:K:287:MET:HE1	1.81	1.08
1:L:287:MET:HG3	1:L:288:PRO:HD2	1.34	1.07
1:A:343:ASN:ND2	1:A:343:ASN:H	1.50	0.97
1:A:343:ASN:H	1:A:343:ASN:HD22	1.07	0.89
1:K:278:LEU:HD22	1:K:287:MET:CE	2.01	0.89
1:L:278:LEU:HD13	1:L:287:MET:HE1	1.59	0.84
1:L:287:MET:HG3	1:L:288:PRO:CD	2.10	0.81
1:A:343:ASN:ND2	1:A:343:ASN:N	2.30	0.74
1:K:287:MET:HG3	1:K:288:PRO:HD2	1.73	0.71
1:A:343:ASN:HD22	1:A:343:ASN:N	1.85	0.69
1:K:278:LEU:HD21	1:K:287:MET:HE1	1.75	0.68
1:J:347:LEU:HD11	1:J:382:PRO:HB2	1.75	0.68
1:I:299:GLN:HG3	1:I:300:GLN:HE21	1.60	0.66
1:F:290:GLU:OE1	1:F:290:GLU:N	2.30	0.64
1:G:347:LEU:HD11	1:G:382:PRO:HB2	1.79	0.64
1:E:347:LEU:HD11	1:E:382:PRO:HB2	1.79	0.64
1:O:377:VAL:HB	1:O:398:TYR:HB2	1.81	0.63
1:F:377:VAL:HB	1:F:398:TYR:HB2	1.81	0.63
1:D:56:MET:HA	1:D:367:ILE:HD11	1.80	0.63
1:E:246:THR:HG22	1:E:267:PHE:HB2	1.84	0.60
1:H:377:VAL:HB	1:H:398:TYR:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:MET:HA	1:B:367:ILE:HD11	1.83	0.59
1:J:204:ASN:HB2	1:P:221:ALA:O	2.03	0.59
1:E:290:GLU:HG2	1:E:291:SER:N	2.16	0.59
1:I:42:LEU:HB2	1:I:45:ALA:HB3	1.84	0.58
1:K:60:ILE:HG12	1:K:102:SER:HB2	1.85	0.58
1:E:261:MET:HE1	1:E:309:TYR:HE1	1.69	0.57
1:C:347:LEU:HD11	1:C:382:PRO:HB2	1.86	0.57
1:K:224:THR:OG1	1:K:225:TYR:N	2.38	0.57
1:H:188:KCX:HD2	1:H:227:MET:HE2	1.87	0.57
1:D:270:PRO:O	1:D:337:ARG:NH2	2.38	0.56
1:A:173:ARG:HG2	1:A:218:GLU:HG3	1.88	0.56
1:I:347:LEU:HD11	1:I:382:PRO:HB2	1.89	0.55
1:L:278:LEU:HD22	1:L:287:MET:HE2	1.88	0.55
1:E:377:VAL:HB	1:E:398:TYR:HB2	1.88	0.55
1:G:381:ASN:HD22	1:G:384:GLU:HG2	1.72	0.55
1:F:290:GLU:CD	1:F:290:GLU:H	2.09	0.55
1:G:134:LEU:HB2	1:G:189:ILE:HG22	1.89	0.55
1:I:5:VAL:HG11	1:I:40:VAL:HG21	1.87	0.55
1:J:154:SER:HB2	1:J:158:ARG:HG2	1.89	0.55
1:J:251:ASN:HD22	1:J:298:VAL:HB	1.72	0.55
1:B:204:ASN:HB2	1:H:221:ALA:O	2.08	0.54
1:G:378:LEU:HD21	1:G:389:VAL:HG22	1.90	0.54
1:G:42:LEU:HB2	1:G:45:ALA:HB3	1.90	0.54
1:A:246:THR:HG22	1:A:267:PHE:HB2	1.89	0.54
1:G:5:VAL:HG11	1:G:40:VAL:HG21	1.89	0.54
1:O:381:ASN:HD22	1:O:384:GLU:HG2	1.73	0.54
1:F:258:ALA:HA	1:F:261:MET:HE3	1.89	0.54
1:A:126:ARG:HH22	1:A:402:ARG:HD3	1.73	0.53
1:B:173:ARG:HG2	1:B:218:GLU:HG3	1.89	0.53
1:O:4:THR:HG23	1:O:46:GLN:HB3	1.91	0.53
1:A:73:LEU:HD11	3:A:427:LWY:H1B	1.91	0.53
1:I:204:ASN:HB2	1:O:221:ALA:O	2.09	0.53
1:A:204:ASN:HB2	1:G:221:ALA:O	2.08	0.53
1:A:377:VAL:HB	1:A:398:TYR:HB2	1.90	0.53
1:G:270:PRO:O	1:G:337:ARG:NH2	2.42	0.53
1:A:31:ARG:HH22	1:A:363:GLN:HG3	1.74	0.52
1:J:258:ALA:HA	1:J:261:MET:HE3	1.91	0.52
1:P:57:PRO:HG3	1:P:367:ILE:HG13	1.92	0.52
1:M:246:THR:HG22	1:M:267:PHE:HB2	1.90	0.52
1:H:73:LEU:HD21	1:H:323:LEU:HD22	1.92	0.52
1:J:80:PRO:HB2	1:J:83:LEU:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:5:VAL:HG11	1:P:40:VAL:HG21	1.92	0.51
1:G:299:GLN:HG3	1:G:300:GLN:HE21	1.74	0.51
1:F:140:HIS:CE1	1:F:194:GLY:HA3	2.46	0.51
1:A:347:LEU:HD11	1:A:382:PRO:HB2	1.92	0.51
1:A:270:PRO:O	1:A:337:ARG:NH2	2.43	0.51
1:N:154:SER:HB3	1:P:150:LEU:HD21	1.93	0.51
1:O:106:ALA:HB1	1:O:188:KCX:HZ	1.76	0.51
1:I:10:ASN:HA	1:I:21:GLU:HA	1.92	0.51
1:I:261:MET:HE1	1:I:309:TYR:HE1	1.76	0.51
1:L:17:GLY:HA2	1:L:344:LEU:HD21	1.93	0.51
1:N:377:VAL:HB	1:N:398:TYR:HB2	1.92	0.51
1:O:347:LEU:HD11	1:O:382:PRO:HB2	1.92	0.51
1:C:270:PRO:O	1:C:337:ARG:NH2	2.44	0.50
1:K:17:GLY:HA2	1:K:344:LEU:HD21	1.92	0.50
1:N:116:ALA:HB1	1:N:122:VAL:HB	1.91	0.50
1:K:56:MET:HE1	1:K:347:LEU:HD22	1.94	0.50
1:L:140:HIS:NE2	3:L:427:LWY:O1	2.43	0.50
1:J:134:LEU:HB2	1:J:189:ILE:HG22	1.93	0.50
1:C:305:SER:HA	1:C:308:ILE:HD12	1.94	0.49
1:B:134:LEU:HB2	1:B:189:ILE:HG22	1.94	0.49
1:C:98:ARG:HD3	1:C:392:GLU:HG2	1.93	0.49
1:D:246:THR:HG22	1:D:267:PHE:HB2	1.94	0.49
1:J:10:ASN:HD22	1:J:21:GLU:HA	1.77	0.49
1:K:134:LEU:HB2	1:K:189:ILE:HG22	1.92	0.49
1:A:134:LEU:HB2	1:A:189:ILE:HG22	1.94	0.49
1:B:11:VAL:HG13	1:B:367:ILE:HD12	1.93	0.49
1:B:241:ARG:HG3	1:B:260:LEU:HD21	1.95	0.49
1:K:288:PRO:O	1:K:291:SER:HB2	2.11	0.49
1:K:377:VAL:HB	1:K:398:TYR:HB2	1.94	0.49
1:F:73:LEU:HD21	1:F:323:LEU:HD22	1.95	0.49
1:I:134:LEU:HB2	1:I:189:ILE:HG22	1.94	0.49
1:K:12:LEU:HD22	1:K:14:LEU:HG	1.95	0.49
1:M:60:ILE:HG12	1:M:102:SER:HB2	1.94	0.48
1:N:56:MET:HA	1:N:367:ILE:HD11	1.95	0.48
1:N:347:LEU:HD11	1:N:382:PRO:HB2	1.95	0.48
1:P:378:LEU:HD21	1:P:389:VAL:HG22	1.95	0.48
1:B:347:LEU:HD11	1:B:382:PRO:HB2	1.95	0.48
1:E:134:LEU:HB2	1:E:189:ILE:HG22	1.94	0.48
1:O:53:LYS:HG2	1:O:379:ASP:HA	1.96	0.48
1:B:60:ILE:HA	1:B:102:SER:O	2.13	0.48
1:B:189:ILE:HG21	1:B:215:ILE:HD13	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:126:ARG:HH22	1:C:402:ARG:HD3	1.79	0.48
1:J:379:ASP:HB3	1:J:395:ARG:HB3	1.96	0.48
1:N:188:KCX:HD2	1:N:227:MET:HE2	1.95	0.48
1:O:59:PHE:HB3	1:O:350:ALA:HB1	1.94	0.48
1:O:356:GLU:HA	1:O:361:GLN:HG2	1.95	0.48
1:C:258:ALA:HA	1:C:261:MET:HE3	1.95	0.48
1:A:261:MET:HE1	1:A:309:TYR:HE1	1.79	0.48
1:H:134:LEU:HB2	1:H:189:ILE:HG22	1.96	0.48
1:I:188:KCX:HD2	1:I:227:MET:HE2	1.95	0.48
1:L:134:LEU:HB2	1:L:189:ILE:HG22	1.96	0.48
1:J:246:THR:HG22	1:J:267:PHE:HB2	1.95	0.48
1:I:378:LEU:HD21	1:I:389:VAL:HG22	1.96	0.48
1:M:82:ILE:HG23	1:N:112:SER:HB2	1.96	0.48
1:P:60:ILE:HG12	1:P:102:SER:HB2	1.96	0.48
1:A:60:ILE:HG12	1:A:102:SER:HB2	1.95	0.47
1:D:6:LEU:HD12	1:D:25:VAL:HB	1.96	0.47
1:G:126:ARG:HH22	1:G:402:ARG:HD3	1.79	0.47
1:I:377:VAL:HB	1:I:398:TYR:HB2	1.96	0.47
1:N:125:PRO:HA	1:N:401:GLN:HE22	1.79	0.47
1:A:140:HIS:NE2	3:A:427:LWY:O1	2.47	0.47
1:B:236:ILE:HG21	1:B:261:MET:HE2	1.95	0.47
1:F:379:ASP:HB3	1:F:395:ARG:HB3	1.96	0.47
1:J:126:ARG:HH11	1:J:364:LEU:HD11	1.80	0.47
1:K:233:GLY:HA2	1:K:236:ILE:HD12	1.96	0.47
1:L:347:LEU:HD11	1:L:382:PRO:HB2	1.96	0.47
1:A:344:LEU:C	1:A:344:LEU:CD2	2.87	0.47
1:D:73:LEU:HD21	1:D:323:LEU:HD22	1.97	0.47
1:G:189:ILE:HG21	1:G:215:ILE:HD13	1.95	0.47
1:L:42:LEU:HB2	1:L:45:ALA:HB3	1.96	0.47
1:M:40:VAL:HG13	1:M:42:LEU:HD22	1.96	0.47
1:N:400:LEU:HA	1:N:405:LEU:HA	1.96	0.47
1:A:54:THR:HB	1:A:378:LEU:HB3	1.95	0.47
1:C:106:ALA:HB1	1:C:188:KCX:HZ	1.79	0.47
1:D:178:GLU:HG2	1:E:149:LEU:HD13	1.96	0.47
1:G:60:ILE:HG12	1:G:102:SER:HB2	1.96	0.47
1:K:166:VAL:HG11	1:K:175:ALA:HB2	1.97	0.47
1:L:224:THR:OG1	1:L:225:TYR:N	2.43	0.47
1:O:31:ARG:HH22	1:O:363:GLN:HG3	1.80	0.47
1:C:399:VAL:HB	1:C:407:LYS:HB2	1.96	0.47
1:H:343:ASN:HB3	1:H:386:ILE:HD13	1.96	0.47
1:I:19:LEU:HD21	1:I:54:THR:HG23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:240:VAL:HG21	1:B:261:MET:HG2	1.98	0.47
1:D:221:ALA:O	1:E:204:ASN:HB2	2.15	0.47
1:O:288:PRO:HA	1:O:289:PRO:HD3	1.78	0.47
1:C:377:VAL:HB	1:C:398:TYR:HB2	1.97	0.46
1:C:16:ARG:HH12	1:C:20:LEU:HD21	1.81	0.46
1:D:288:PRO:HA	1:D:289:PRO:HD3	1.83	0.46
1:L:5:VAL:HG11	1:L:40:VAL:HG21	1.97	0.46
1:B:377:VAL:HB	1:B:398:TYR:HB2	1.97	0.46
1:H:401:GLN:HB2	1:H:406:VAL:HG21	1.97	0.46
1:A:88:SER:HA	1:A:91:ILE:HD12	1.97	0.46
1:E:288:PRO:HA	1:E:289:PRO:HD3	1.75	0.46
1:B:59:PHE:HB3	1:B:350:ALA:HB1	1.97	0.46
1:E:88:SER:HA	1:E:91:ILE:HD12	1.97	0.46
1:N:397:GLU:HA	1:N:409:GLN:HB2	1.97	0.46
1:F:12:LEU:HD22	1:F:14:LEU:HG	1.98	0.46
1:M:221:ALA:O	1:P:204:ASN:HB2	2.15	0.46
1:E:334:PHE:HB2	1:E:390:ALA:HB2	1.97	0.46
1:C:156:CYS:SG	1:C:182:LYS:NZ	2.89	0.46
1:D:261:MET:HE1	1:D:309:TYR:HE1	1.81	0.46
1:D:89:LEU:HB2	1:D:90:PRO:HD3	1.98	0.46
1:L:278:LEU:HD22	1:L:287:MET:CE	2.45	0.46
1:L:377:VAL:HB	1:L:398:TYR:HB2	1.97	0.46
1:M:377:VAL:HB	1:M:398:TYR:HB2	1.97	0.46
1:J:66:VAL:HG12	1:J:88:SER:HB2	1.98	0.45
1:C:112:SER:HB2	1:H:82:ILE:HB	1.97	0.45
1:L:240:VAL:HG21	1:L:261:MET:HG2	1.98	0.45
1:E:5:VAL:HG11	1:E:40:VAL:HG21	1.98	0.45
1:G:270:PRO:HD2	1:G:337:ARG:HH12	1.81	0.45
1:I:189:ILE:HG21	1:I:215:ILE:HD13	1.98	0.45
1:J:188:KCX:HD2	1:J:227:MET:HE2	1.98	0.45
1:J:202:ILE:HD11	1:J:252:LEU:HD11	1.97	0.45
1:P:347:LEU:HD11	1:P:382:PRO:HB2	1.99	0.45
1:F:5:VAL:HG11	1:F:40:VAL:HG21	1.99	0.45
1:B:72:ASN:HB3	1:B:75:VAL:HG12	1.98	0.45
1:E:86:ILE:HD12	1:F:89:LEU:HD11	1.98	0.45
1:H:288:PRO:HA	1:H:289:PRO:HD3	1.82	0.45
1:N:381:ASN:HB3	1:N:384:GLU:HB2	1.99	0.45
1:P:80:PRO:HB2	1:P:83:LEU:HB2	1.98	0.45
1:M:176:VAL:HG13	1:M:187:ILE:HG13	1.98	0.45
1:L:56:MET:HE1	1:L:347:LEU:HD22	1.98	0.45
1:O:126:ARG:HH11	1:O:364:LEU:HD11	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:379:ASP:HB3	1:K:395:ARG:HB3	1.99	0.45
1:N:10:ASN:HA	1:N:21:GLU:HA	1.98	0.44
1:P:270:PRO:O	1:P:337:ARG:NH2	2.50	0.44
1:P:105:ASP:HB3	1:P:129:PRO:HA	1.99	0.44
1:H:55:VAL:HG22	1:H:377:VAL:HG22	1.99	0.44
1:N:4:THR:HG23	1:N:46:GLN:HB3	1.99	0.44
1:E:11:VAL:HG13	1:E:367:ILE:HD12	2.00	0.44
1:F:63:HIS:ND1	1:F:248:GLU:OE1	2.43	0.44
1:N:246:THR:HG22	1:N:267:PHE:HB2	2.00	0.44
1:A:344:LEU:CD2	1:A:344:LEU:O	2.66	0.44
1:G:381:ASN:HA	1:G:382:PRO:HD2	1.82	0.44
1:C:188:KCX:HD2	1:C:227:MET:HE2	1.99	0.44
1:E:292:VAL:O	1:E:295:VAL:HG12	2.17	0.44
1:G:126:ARG:HH11	1:G:364:LEU:HD21	1.82	0.44
1:H:50:VAL:HG12	1:H:50:VAL:O	2.17	0.44
1:N:72:ASN:HB3	1:N:75:VAL:HG12	2.00	0.44
1:O:56:MET:HE1	1:O:347:LEU:HD22	1.99	0.44
1:A:140:HIS:CE1	1:A:194:GLY:HA3	2.52	0.44
1:J:287:MET:HA	1:J:288:PRO:HD2	1.81	0.44
1:P:154:SER:HA	1:P:157:PHE:HB2	1.99	0.44
1:F:151:GLU:HA	1:F:152:PRO:HD3	1.86	0.44
1:H:268:VAL:HG21	1:H:309:TYR:CE1	2.53	0.44
1:K:287:MET:HB2	1:K:287:MET:HE2	1.51	0.44
1:M:379:ASP:HB3	1:M:395:ARG:HB3	1.99	0.44
1:N:61:ASP:HB3	1:N:103:VAL:HG12	2.00	0.44
1:A:126:ARG:HH11	1:A:364:LEU:HD21	1.83	0.43
1:C:63:HIS:ND1	1:C:248:GLU:OE1	2.50	0.43
1:D:82:ILE:HG21	1:G:113:LEU:HG	2.00	0.43
1:I:5:VAL:HG22	1:I:26:VAL:HA	1.99	0.43
1:O:246:THR:HG22	1:O:267:PHE:HB2	2.00	0.43
1:A:349:SER:O	1:A:354:ALA:HB2	2.18	0.43
1:B:60:ILE:HG12	1:B:102:SER:HB2	2.00	0.43
1:I:42:LEU:HA	1:I:43:PRO:HD3	1.78	0.43
1:M:80:PRO:HB2	1:M:83:LEU:HB2	2.01	0.43
1:H:280:LYS:HE3	1:H:280:LYS:HB2	1.93	0.43
1:O:59:PHE:HB2	1:O:100:PHE:CD1	2.53	0.43
1:F:27:ILE:HG21	1:F:403:GLY:HA2	1.99	0.43
1:G:288:PRO:HA	1:G:289:PRO:HD3	1.77	0.43
1:J:140:HIS:NE2	3:J:427:LWY:O1	2.48	0.43
1:K:53:LYS:HE3	1:K:53:LYS:HB2	1.78	0.43
1:M:134:LEU:HB2	1:M:189:ILE:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:240:VAL:HG21	1:M:261:MET:HG2	2.01	0.43
1:O:176:VAL:HG13	1:O:187:ILE:HG13	2.01	0.43
1:H:258:ALA:HA	1:H:261:MET:HE3	2.00	0.43
1:K:270:PRO:HD2	1:K:337:ARG:HH22	1.83	0.43
1:P:6:LEU:HB3	1:P:50:VAL:HG21	2.01	0.43
1:A:73:LEU:HD21	1:A:323:LEU:HD22	2.01	0.43
1:C:288:PRO:HA	1:C:289:PRO:HD3	1.83	0.43
1:J:154:SER:HA	1:J:157:PHE:HB2	2.00	0.43
1:L:57:PRO:HG3	1:L:367:ILE:HG13	2.01	0.43
1:A:118:GLU:HG2	1:A:402:ARG:HH22	1.83	0.43
1:C:388:VAL:HA	1:C:395:ARG:HH11	1.84	0.43
1:D:299:GLN:HG3	1:D:300:GLN:HE21	1.84	0.43
1:L:140:HIS:CE1	1:L:194:GLY:HA3	2.54	0.43
1:L:288:PRO:HG2	1:L:291:SER:OG	2.19	0.43
1:L:308:ILE:H	1:L:308:ILE:HG13	1.70	0.43
1:M:270:PRO:HD2	1:M:337:ARG:HH22	1.83	0.43
1:P:188:KCX:HD2	1:P:227:MET:HE2	2.01	0.43
1:A:154:SER:HB2	1:A:158:ARG:HD3	2.01	0.43
1:E:60:ILE:HG12	1:E:102:SER:HB2	2.01	0.43
1:E:188:KCX:HD2	1:E:227:MET:HE2	2.00	0.43
1:F:290:GLU:O	1:F:293:ALA:HB3	2.19	0.43
1:K:282:GLY:O	1:K:287:MET:HB3	2.19	0.43
1:P:268:VAL:HG21	1:P:309:TYR:CE1	2.54	0.43
1:C:328:ALA:O	1:C:392:GLU:HG3	2.19	0.42
1:D:275:TYR:HB3	1:D:299:GLN:HB3	2.00	0.42
1:F:270:PRO:O	1:F:337:ARG:NH2	2.52	0.42
1:L:98:ARG:HD3	1:L:392:GLU:HG3	2.01	0.42
1:C:73:LEU:HD21	1:C:323:LEU:HD22	2.01	0.42
1:N:97:SER:HA	1:N:407:LYS:HG3	2.00	0.42
1:F:126:ARG:HH11	1:F:364:LEU:HD11	1.84	0.42
1:N:232:THR:HA	1:N:252:LEU:HB2	2.01	0.42
1:N:270:PRO:O	1:N:337:ARG:NH2	2.53	0.42
1:A:299:GLN:HG3	1:A:300:GLN:HE21	1.84	0.42
1:E:65:HIS:HD1	1:E:162:ILE:HD12	1.85	0.42
1:I:12:LEU:HD22	1:I:14:LEU:HG	2.01	0.42
1:M:382:PRO:HA	1:M:385:ASP:O	2.20	0.42
1:P:166:VAL:HG11	1:P:175:ALA:HB2	2.01	0.42
1:A:378:LEU:HD21	1:A:389:VAL:HG22	2.01	0.42
1:J:232:THR:HA	1:J:252:LEU:HB2	2.01	0.42
1:K:221:ALA:O	1:N:204:ASN:HB2	2.18	0.42
1:D:232:THR:HA	1:D:252:LEU:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:188:KCX:HD2	1:F:227:MET:HE2	2.02	0.42
1:H:299:GLN:HG3	1:H:300:GLN:HE21	1.83	0.42
1:M:111:TRP:CD2	1:P:146:ARG:HG2	2.55	0.42
1:N:194:GLY:HA2	1:N:231:TYR:HE2	1.85	0.42
1:A:10:ASN:HA	1:A:21:GLU:HA	2.01	0.42
1:B:125:PRO:HA	1:B:401:GLN:HE22	1.84	0.42
1:N:224:THR:OG1	1:N:225:TYR:N	2.50	0.42
1:N:303:ARG:HH21	1:N:336:ILE:HG12	1.85	0.42
1:I:11:VAL:HG13	1:I:367:ILE:HD12	2.01	0.42
1:K:189:ILE:HG21	1:K:215:ILE:HD13	2.01	0.42
1:M:140:HIS:NE2	3:M:427:LWY:O1	2.52	0.42
1:D:140:HIS:CE1	1:D:194:GLY:HA3	2.55	0.42
1:M:5:VAL:HG21	1:M:40:VAL:HG21	2.01	0.42
1:M:58:GLY:HA2	1:M:376:VAL:HG23	2.01	0.42
1:N:288:PRO:HA	1:N:289:PRO:HD3	1.87	0.42
1:H:113:LEU:HD23	1:H:113:LEU:HA	1.94	0.41
1:N:140:HIS:CE1	1:N:194:GLY:HA3	2.55	0.41
1:O:232:THR:HA	1:O:252:LEU:HB2	2.02	0.41
1:B:200:ASP:HA	1:B:201:PRO:HD3	1.89	0.41
1:B:270:PRO:O	1:B:337:ARG:NH2	2.52	0.41
1:G:397:GLU:HA	1:G:409:GLN:HB2	2.02	0.41
1:L:290:GLU:O	1:L:293:ALA:HB3	2.20	0.41
1:N:334:PHE:HB3	1:N:386:ILE:HD11	2.02	0.41
1:O:125:PRO:HA	1:O:401:GLN:HE22	1.84	0.41
1:C:221:ALA:O	1:F:204:ASN:HB2	2.20	0.41
1:H:43:PRO:HB2	1:H:44:ASN:H	1.62	0.41
1:L:246:THR:HG22	1:L:267:PHE:HB2	2.01	0.41
1:P:72:ASN:HB3	1:P:75:VAL:HG12	2.02	0.41
1:C:287:MET:HA	1:C:288:PRO:HD2	1.89	0.41
1:D:121:LEU:HD21	1:G:87:ARG:HG2	2.03	0.41
1:D:202:ILE:HD12	1:D:298:VAL:HG13	2.02	0.41
1:D:246:THR:HG21	1:D:357:ILE:HG23	2.03	0.41
1:E:190:MET:HA	1:E:229:HIS:HB3	2.01	0.41
1:E:270:PRO:O	1:E:337:ARG:NH2	2.53	0.41
1:H:409:GLN:HE21	1:H:409:GLN:HB2	1.75	0.41
1:L:32:ILE:HD13	1:L:367:ILE:HG23	2.03	0.41
1:L:221:ALA:O	1:M:204:ASN:HB2	2.20	0.41
1:I:145:PRO:HB2	1:I:146:ARG:H	1.67	0.41
1:L:96:LEU:HD21	1:L:406:VAL:HG11	2.02	0.41
1:L:324:GLY:O	1:L:327:HIS:ND1	2.48	0.41
1:M:38:ARG:H	1:M:38:ARG:HG2	1.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:66:VAL:HG12	1:N:88:SER:HB2	2.03	0.41
1:B:288:PRO:HA	1:B:289:PRO:HD3	1.88	0.41
1:C:401:GLN:HB2	1:C:406:VAL:HG21	2.03	0.41
1:F:158:ARG:HA	1:F:158:ARG:HD2	1.95	0.41
1:J:270:PRO:O	1:J:337:ARG:NH2	2.53	0.41
1:K:151:GLU:HA	1:K:152:PRO:HD3	1.94	0.41
1:L:230:ALA:HB3	1:L:247:ILE:HG23	2.03	0.41
1:O:16:ARG:HH12	1:O:20:LEU:HD21	1.85	0.41
1:C:154:SER:O	1:C:158:ARG:HG2	2.21	0.41
1:F:378:LEU:HD21	1:F:389:VAL:HG22	2.03	0.41
1:I:318:PHE:CZ	1:I:333:GLU:HB3	2.56	0.41
1:K:89:LEU:HD22	1:K:122:VAL:HG11	2.03	0.41
1:K:378:LEU:HD21	1:K:389:VAL:HG22	2.02	0.41
1:A:5:VAL:HG22	1:A:26:VAL:HG13	2.01	0.41
1:G:6:LEU:HB2	1:G:25:VAL:HB	2.03	0.41
1:I:60:ILE:HG12	1:I:102:SER:HB2	2.03	0.41
1:I:288:PRO:HA	1:I:289:PRO:HD3	1.77	0.41
1:J:53:LYS:HE3	1:J:53:LYS:HB2	1.83	0.41
1:L:12:LEU:HD22	1:L:14:LEU:HG	2.03	0.41
1:L:288:PRO:HG2	1:L:291:SER:CB	2.50	0.41
1:M:42:LEU:HA	1:M:43:PRO:HD3	1.89	0.41
1:A:72:ASN:HB3	1:A:75:VAL:HG12	2.02	0.41
1:A:154:SER:O	1:A:158:ARG:HG2	2.21	0.41
1:B:215:ILE:HG22	1:B:226:VAL:HG21	2.02	0.41
1:D:126:ARG:HH11	1:D:364:LEU:HD21	1.86	0.41
1:I:40:VAL:HG13	1:I:42:LEU:HD22	2.02	0.41
1:K:288:PRO:HA	1:K:289:PRO:HD3	1.89	0.41
1:L:246:THR:HG21	1:L:357:ILE:HG23	2.02	0.41
1:N:58:GLY:HA2	1:N:376:VAL:HG23	2.03	0.41
1:P:140:HIS:CE1	1:P:194:GLY:HA3	2.56	0.41
1:C:125:PRO:HA	1:C:401:GLN:HE22	1.86	0.41
1:C:126:ARG:HH11	1:C:364:LEU:HD21	1.86	0.41
1:C:166:VAL:HG11	1:C:175:ALA:HB2	2.03	0.41
1:F:232:THR:HA	1:F:252:LEU:HB2	2.03	0.41
1:G:224:THR:OG1	1:G:225:TYR:N	2.54	0.41
1:L:188:KCX:HD2	1:L:227:MET:HE2	2.02	0.41
1:L:319:GLY:H	1:L:337:ARG:HH21	1.69	0.41
1:O:359:ASN:HD22	1:O:361:GLN:HE21	1.67	0.41
1:B:381:ASN:HA	1:B:382:PRO:HD2	1.97	0.40
1:K:305:SER:HA	1:K:308:ILE:HD12	2.04	0.40
1:O:42:LEU:HB2	1:O:45:ALA:HB3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:42:LEU:HA	1:P:43:PRO:HD3	1.93	0.40
1:C:347:LEU:O	1:C:351:THR:OG1	2.32	0.40
1:D:381:ASN:HA	1:D:382:PRO:HD2	1.90	0.40
1:M:72:ASN:HB3	1:M:75:VAL:HG12	2.03	0.40
1:C:64:VAL:HG21	1:C:103:VAL:HB	2.03	0.40
1:K:361:GLN:H	1:K:361:GLN:CD	2.30	0.40
1:L:112:SER:HB2	1:O:82:ILE:HG23	2.02	0.40
1:N:134:LEU:HB2	1:N:189:ILE:HG22	2.02	0.40
1:A:270:PRO:HD2	1:A:337:ARG:HH22	1.86	0.40
1:E:290:GLU:O	1:E:293:ALA:HB3	2.20	0.40
1:I:176:VAL:HG11	1:I:218:GLU:HB3	2.04	0.40
1:M:188:KCX:HD2	1:M:227:MET:HE2	2.03	0.40
1:A:42:LEU:HA	1:A:43:PRO:HD3	1.86	0.40
1:C:261:MET:HE1	1:C:309:TYR:HE1	1.86	0.40
1:E:21:GLU:H	1:E:21:GLU:CD	2.29	0.40
1:K:283:ALA:HB2	1:K:292:VAL:HG21	2.03	0.40
1:M:140:HIS:CE1	1:M:194:GLY:HA3	2.56	0.40
1:N:221:ALA:O	1:O:204:ASN:HB2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	405/423 (96%)	385 (95%)	15 (4%)	5 (1%)	10	31
1	B	405/423 (96%)	381 (94%)	20 (5%)	4 (1%)	12	36
1	C	405/423 (96%)	380 (94%)	21 (5%)	4 (1%)	12	36
1	D	405/423 (96%)	379 (94%)	21 (5%)	5 (1%)	10	31
1	E	405/423 (96%)	380 (94%)	20 (5%)	5 (1%)	10	31
1	F	405/423 (96%)	379 (94%)	23 (6%)	3 (1%)	18	45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	405/423 (96%)	375 (93%)	26 (6%)	4 (1%)	12	36
1	H	405/423 (96%)	383 (95%)	18 (4%)	4 (1%)	12	36
1	I	405/423 (96%)	377 (93%)	23 (6%)	5 (1%)	10	31
1	J	405/423 (96%)	374 (92%)	26 (6%)	5 (1%)	10	31
1	K	405/423 (96%)	378 (93%)	24 (6%)	3 (1%)	18	45
1	L	405/423 (96%)	377 (93%)	27 (7%)	1 (0%)	43	71
1	M	405/423 (96%)	383 (95%)	19 (5%)	3 (1%)	18	45
1	N	405/423 (96%)	371 (92%)	30 (7%)	4 (1%)	12	36
1	O	405/423 (96%)	375 (93%)	27 (7%)	3 (1%)	18	45
1	P	405/423 (96%)	375 (93%)	25 (6%)	5 (1%)	10	31
All	All	6480/6768 (96%)	6052 (93%)	365 (6%)	63 (1%)	12	36

All (63) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	43	PRO
1	C	43	PRO
1	D	43	PRO
1	E	43	PRO
1	F	43	PRO
1	H	43	PRO
1	I	43	PRO
1	L	43	PRO
1	M	43	PRO
1	P	43	PRO
1	B	43	PRO
1	B	147	GLY
1	G	43	PRO
1	I	145	PRO
1	N	43	PRO
1	O	207	TYR
1	P	147	GLY
1	A	207	TYR
1	A	249	HIS
1	B	39	PRO
1	D	249	HIS
1	E	207	TYR
1	F	249	HIS

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Mol	Chain	Res	Type
1	K	43	PRO
1	M	147	GLY
1	O	43	PRO
1	P	249	HIS
1	A	152	PRO
1	B	249	HIS
1	C	249	HIS
1	D	207	TYR
1	F	207	TYR
1	G	152	PRO
1	G	207	TYR
1	G	249	HIS
1	H	207	TYR
1	H	249	HIS
1	I	249	HIS
1	J	43	PRO
1	J	198	PRO
1	J	207	TYR
1	K	207	TYR
1	M	249	HIS
1	N	249	HIS
1	O	249	HIS
1	P	152	PRO
1	A	147	GLY
1	C	207	TYR
1	D	147	GLY
1	E	249	HIS
1	I	207	TYR
1	J	249	HIS
1	N	207	TYR
1	P	207	TYR
1	H	198	PRO
1	D	152	PRO
1	E	152	PRO
1	N	29	GLY
1	C	39	PRO
1	I	152	PRO
1	J	147	GLY
1	E	147	GLY
1	K	152	PRO

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	314/325 (97%)	281 (90%)	33 (10%)	6	21
1	B	314/325 (97%)	285 (91%)	29 (9%)	8	26
1	C	314/325 (97%)	282 (90%)	32 (10%)	7	22
1	D	314/325 (97%)	285 (91%)	29 (9%)	8	26
1	E	314/325 (97%)	284 (90%)	30 (10%)	8	24
1	F	314/325 (97%)	282 (90%)	32 (10%)	7	22
1	G	314/325 (97%)	288 (92%)	26 (8%)	10	31
1	H	314/325 (97%)	276 (88%)	38 (12%)	5	16
1	I	314/325 (97%)	281 (90%)	33 (10%)	6	21
1	J	314/325 (97%)	285 (91%)	29 (9%)	8	26
1	K	314/325 (97%)	281 (90%)	33 (10%)	6	21
1	L	314/325 (97%)	286 (91%)	28 (9%)	9	27
1	M	314/325 (97%)	281 (90%)	33 (10%)	6	21
1	N	314/325 (97%)	282 (90%)	32 (10%)	7	22
1	O	314/325 (97%)	286 (91%)	28 (9%)	9	27
1	P	314/325 (97%)	282 (90%)	32 (10%)	7	22
All	All	5024/5200 (97%)	4527 (90%)	497 (10%)	7	23

All (497) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	12	LEU
1	A	21	GLU
1	A	42	LEU
1	A	44	ASN
1	A	66	VAL
1	A	75	VAL
1	A	150	LEU

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Mol	Chain	Res	Type
1	A	166	VAL
1	A	173	ARG
1	A	180	ILE
1	A	181	GLN
1	A	204	ASN
1	A	238	ARG
1	A	253	VAL
1	A	280	LYS
1	A	281	HIS
1	A	295	VAL
1	A	298	VAL
1	A	306	LEU
1	A	314	VAL
1	A	315	LYS
1	A	325	GLU
1	A	327	HIS
1	A	343	ASN
1	A	344	LEU
1	A	349	SER
1	A	361	GLN
1	A	363	GLN
1	A	383	LEU
1	A	396	VAL
1	A	404	THR
1	A	406	VAL
1	B	12	LEU
1	B	18	VAL
1	B	21	GLU
1	B	33	VAL
1	B	42	LEU
1	B	44	ASN
1	B	50	VAL
1	B	75	VAL
1	B	76	ASN
1	B	82	ILE
1	B	112	SER
1	B	136	GLN
1	B	181	GLN
1	B	204	ASN
1	B	253	VAL
1	B	254	ASP
1	B	280	LYS

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Mol	Chain	Res	Type
1	B	295	VAL
1	B	298	VAL
1	B	299	GLN
1	B	325	GLU
1	B	327	HIS
1	B	343	ASN
1	B	344	LEU
1	B	361	GLN
1	B	363	GLN
1	B	364	LEU
1	B	383	LEU
1	B	409	GLN
1	C	12	LEU
1	C	15	GLU
1	C	21	GLU
1	C	50	VAL
1	C	75	VAL
1	C	112	SER
1	C	136	GLN
1	C	148	ASP
1	C	156	CYS
1	C	166	VAL
1	C	180	ILE
1	C	181	GLN
1	C	202	ILE
1	C	204	ASN
1	C	238	ARG
1	C	253	VAL
1	C	280	LYS
1	C	299	GLN
1	C	314	VAL
1	C	315	LYS
1	C	325	GLU
1	C	343	ASN
1	C	344	LEU
1	C	349	SER
1	C	352	THR
1	C	361	GLN
1	C	363	GLN
1	C	383	LEU
1	C	396	VAL
1	C	397	GLU

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Mol	Chain	Res	Type
1	C	404	THR
1	C	406	VAL
1	D	3	ILE
1	D	4	THR
1	D	12	LEU
1	D	18	VAL
1	D	51	ARG
1	D	75	VAL
1	D	121	LEU
1	D	166	VAL
1	D	180	ILE
1	D	181	GLN
1	D	202	ILE
1	D	238	ARG
1	D	241	ARG
1	D	253	VAL
1	D	254	ASP
1	D	255	GLU
1	D	280	LYS
1	D	281	HIS
1	D	292	VAL
1	D	295	VAL
1	D	315	LYS
1	D	325	GLU
1	D	344	LEU
1	D	361	GLN
1	D	363	GLN
1	D	376	VAL
1	D	378	LEU
1	D	397	GLU
1	D	406	VAL
1	E	3	ILE
1	E	14	LEU
1	E	18	VAL
1	E	40	VAL
1	E	42	LEU
1	E	44	ASN
1	E	51	ARG
1	E	67	LEU
1	E	75	VAL
1	E	150	LEU
1	E	166	VAL

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Mol	Chain	Res	Type
1	E	181	GLN
1	E	202	ILE
1	E	204	ASN
1	E	238	ARG
1	E	253	VAL
1	E	254	ASP
1	E	295	VAL
1	E	299	GLN
1	E	315	LYS
1	E	325	GLU
1	E	343	ASN
1	E	344	LEU
1	E	361	GLN
1	E	363	GLN
1	E	389	VAL
1	E	396	VAL
1	E	404	THR
1	E	406	VAL
1	E	409	GLN
1	F	12	LEU
1	F	14	LEU
1	F	15	GLU
1	F	18	VAL
1	F	21	GLU
1	F	33	VAL
1	F	51	ARG
1	F	112	SER
1	F	136	GLN
1	F	148	ASP
1	F	166	VAL
1	F	180	ILE
1	F	181	GLN
1	F	202	ILE
1	F	204	ASN
1	F	238	ARG
1	F	246	THR
1	F	253	VAL
1	F	280	LYS
1	F	290	GLU
1	F	292	VAL
1	F	323	LEU
1	F	325	GLU

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Mol	Chain	Res	Type
1	F	344	LEU
1	F	361	GLN
1	F	363	GLN
1	F	364	LEU
1	F	383	LEU
1	F	396	VAL
1	F	400	LEU
1	F	404	THR
1	F	406	VAL
1	G	3	ILE
1	G	12	LEU
1	G	14	LEU
1	G	18	VAL
1	G	21	GLU
1	G	33	VAL
1	G	50	VAL
1	G	51	ARG
1	G	76	ASN
1	G	92	LEU
1	G	112	SER
1	G	180	ILE
1	G	204	ASN
1	G	232	THR
1	G	238	ARG
1	G	241	ARG
1	G	253	VAL
1	G	259	LYS
1	G	280	LYS
1	G	325	GLU
1	G	343	ASN
1	G	361	GLN
1	G	363	GLN
1	G	396	VAL
1	G	404	THR
1	G	406	VAL
1	H	2	THR
1	H	3	ILE
1	H	12	LEU
1	H	15	GLU
1	H	18	VAL
1	H	21	GLU
1	H	33	VAL

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Mol	Chain	Res	Type
1	H	36	THR
1	H	51	ARG
1	H	70	ASN
1	H	118	GLU
1	H	123	SER
1	H	136	GLN
1	H	166	VAL
1	H	180	ILE
1	H	181	GLN
1	H	202	ILE
1	H	238	ARG
1	H	253	VAL
1	H	254	ASP
1	H	280	LYS
1	H	281	HIS
1	H	292	VAL
1	H	295	VAL
1	H	298	VAL
1	H	306	LEU
1	H	325	GLU
1	H	327	HIS
1	H	343	ASN
1	H	344	LEU
1	H	361	GLN
1	H	363	GLN
1	H	376	VAL
1	H	383	LEU
1	H	388	VAL
1	H	404	THR
1	H	406	VAL
1	H	409	GLN
1	I	12	LEU
1	I	25	VAL
1	I	28	ASP
1	I	33	VAL
1	I	44	ASN
1	I	50	VAL
1	I	51	ARG
1	I	75	VAL
1	I	121	LEU
1	I	136	GLN
1	I	146	ARG

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Mol	Chain	Res	Type
1	I	166	VAL
1	I	204	ASN
1	I	238	ARG
1	I	241	ARG
1	I	253	VAL
1	I	274	THR
1	I	280	LYS
1	I	295	VAL
1	I	298	VAL
1	I	315	LYS
1	I	325	GLU
1	I	343	ASN
1	I	344	LEU
1	I	349	SER
1	I	361	GLN
1	I	363	GLN
1	I	383	LEU
1	I	396	VAL
1	I	397	GLU
1	I	404	THR
1	I	406	VAL
1	I	409	GLN
1	J	12	LEU
1	J	14	LEU
1	J	21	GLU
1	J	27	ILE
1	J	33	VAL
1	J	44	ASN
1	J	50	VAL
1	J	51	ARG
1	J	75	VAL
1	J	82	ILE
1	J	158	ARG
1	J	166	VAL
1	J	180	ILE
1	J	181	GLN
1	J	202	ILE
1	J	238	ARG
1	J	253	VAL
1	J	280	LYS
1	J	295	VAL
1	J	299	GLN

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Mol	Chain	Res	Type
1	J	314	VAL
1	J	325	GLU
1	J	343	ASN
1	J	344	LEU
1	J	361	GLN
1	J	363	GLN
1	J	364	LEU
1	J	383	LEU
1	J	404	THR
1	K	4	THR
1	K	12	LEU
1	K	14	LEU
1	K	18	VAL
1	K	44	ASN
1	K	50	VAL
1	K	51	ARG
1	K	70	ASN
1	K	75	VAL
1	K	82	ILE
1	K	136	GLN
1	K	148	ASP
1	K	156	CYS
1	K	166	VAL
1	K	180	ILE
1	K	181	GLN
1	K	202	ILE
1	K	204	ASN
1	K	224	THR
1	K	238	ARG
1	K	241	ARG
1	K	253	VAL
1	K	254	ASP
1	K	280	LYS
1	K	290	GLU
1	K	292	VAL
1	K	295	VAL
1	K	298	VAL
1	K	306	LEU
1	K	315	LYS
1	K	343	ASN
1	K	344	LEU
1	K	404	THR

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Mol	Chain	Res	Type
1	L	2	THR
1	L	3	ILE
1	L	12	LEU
1	L	14	LEU
1	L	21	GLU
1	L	51	ARG
1	L	75	VAL
1	L	82	ILE
1	L	112	SER
1	L	121	LEU
1	L	122	VAL
1	L	181	GLN
1	L	202	ILE
1	L	238	ARG
1	L	241	ARG
1	L	253	VAL
1	L	254	ASP
1	L	255	GLU
1	L	280	LYS
1	L	295	VAL
1	L	298	VAL
1	L	308	ILE
1	L	343	ASN
1	L	344	LEU
1	L	361	GLN
1	L	363	GLN
1	L	383	LEU
1	L	397	GLU
1	M	12	LEU
1	M	21	GLU
1	M	27	ILE
1	M	33	VAL
1	M	34	GLU
1	M	38	ARG
1	M	50	VAL
1	M	51	ARG
1	M	82	ILE
1	M	112	SER
1	M	166	VAL
1	M	180	ILE
1	M	181	GLN
1	M	202	ILE

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Mol	Chain	Res	Type
1	M	204	ASN
1	M	238	ARG
1	M	253	VAL
1	M	280	LYS
1	M	281	HIS
1	M	292	VAL
1	M	295	VAL
1	M	323	LEU
1	M	325	GLU
1	M	327	HIS
1	M	361	GLN
1	M	363	GLN
1	M	364	LEU
1	M	383	LEU
1	M	396	VAL
1	M	397	GLU
1	M	404	THR
1	M	406	VAL
1	M	409	GLN
1	N	14	LEU
1	N	33	VAL
1	N	40	VAL
1	N	46	GLN
1	N	50	VAL
1	N	51	ARG
1	N	75	VAL
1	N	82	ILE
1	N	112	SER
1	N	122	VAL
1	N	159	THR
1	N	166	VAL
1	N	180	ILE
1	N	181	GLN
1	N	202	ILE
1	N	238	ARG
1	N	253	VAL
1	N	254	ASP
1	N	268	VAL
1	N	280	LYS
1	N	292	VAL
1	N	295	VAL
1	N	314	VAL

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Mol	Chain	Res	Type
1	N	325	GLU
1	N	340	VAL
1	N	343	ASN
1	N	344	LEU
1	N	383	LEU
1	N	396	VAL
1	N	404	THR
1	N	406	VAL
1	N	409	GLN
1	O	2	THR
1	O	18	VAL
1	O	21	GLU
1	O	33	VAL
1	O	42	LEU
1	O	50	VAL
1	O	51	ARG
1	O	66	VAL
1	O	75	VAL
1	O	82	ILE
1	O	112	SER
1	O	136	GLN
1	O	166	VAL
1	O	180	ILE
1	O	181	GLN
1	O	200	ASP
1	O	238	ARG
1	O	253	VAL
1	O	274	THR
1	O	280	LYS
1	O	299	GLN
1	O	301	LYS
1	O	314	VAL
1	O	344	LEU
1	O	363	GLN
1	O	383	LEU
1	O	404	THR
1	O	406	VAL
1	P	12	LEU
1	P	16	ARG
1	P	21	GLU
1	P	33	VAL
1	P	42	LEU

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Mol	Chain	Res	Type
1	P	46	GLN
1	P	50	VAL
1	P	51	ARG
1	P	75	VAL
1	P	76	ASN
1	P	82	ILE
1	P	83	LEU
1	P	112	SER
1	P	136	GLN
1	P	156	CYS
1	P	166	VAL
1	P	202	ILE
1	P	204	ASN
1	P	238	ARG
1	P	253	VAL
1	P	260	LEU
1	P	280	LYS
1	P	298	VAL
1	P	314	VAL
1	P	325	GLU
1	P	343	ASN
1	P	344	LEU
1	P	361	GLN
1	P	397	GLU
1	P	404	THR
1	P	406	VAL
1	P	409	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (95) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	223	ASN
1	A	251	ASN
1	A	281	HIS
1	A	299	GLN
1	A	300	GLN
1	A	343	ASN
1	A	359	ASN
1	A	363	GLN
1	A	409	GLN
1	B	46	GLN
1	B	299	GLN

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Mol	Chain	Res	Type
1	B	401	GLN
1	B	409	GLN
1	C	46	GLN
1	C	79	GLN
1	C	299	GLN
1	C	300	GLN
1	C	401	GLN
1	C	409	GLN
1	D	10	ASN
1	D	44	ASN
1	D	262	HIS
1	D	299	GLN
1	D	300	GLN
1	E	10	ASN
1	E	359	ASN
1	E	361	GLN
1	F	10	ASN
1	F	23	HIS
1	F	44	ASN
1	F	262	HIS
1	F	299	GLN
1	F	359	ASN
1	F	409	GLN
1	G	7	GLN
1	G	23	HIS
1	G	44	ASN
1	G	262	HIS
1	G	299	GLN
1	G	300	GLN
1	G	401	GLN
1	H	10	ASN
1	H	44	ASN
1	H	46	GLN
1	H	299	GLN
1	H	300	GLN
1	H	343	ASN
1	H	361	GLN
1	H	409	GLN
1	I	300	GLN
1	I	359	ASN
1	I	361	GLN
1	J	10	ASN

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Mol	Chain	Res	Type
1	J	251	ASN
1	J	299	GLN
1	J	343	ASN
1	J	363	GLN
1	K	10	ASN
1	K	23	HIS
1	K	281	HIS
1	K	299	GLN
1	K	300	GLN
1	K	311	ASN
1	K	409	GLN
1	L	10	ASN
1	L	44	ASN
1	L	65	HIS
1	L	299	GLN
1	L	361	GLN
1	M	70	ASN
1	M	281	HIS
1	M	299	GLN
1	M	300	GLN
1	M	311	ASN
1	M	401	GLN
1	N	46	GLN
1	N	262	HIS
1	N	299	GLN
1	N	300	GLN
1	N	359	ASN
1	N	401	GLN
1	O	10	ASN
1	O	206	GLN
1	O	299	GLN
1	O	300	GLN
1	O	361	GLN
1	O	363	GLN
1	O	401	GLN
1	P	10	ASN
1	P	44	ASN
1	P	46	GLN
1	P	223	ASN
1	P	299	GLN
1	P	300	GLN
1	P	343	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

16 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z > 2$
1	KCX	C	188	1,2	10,11,12	0.88	0	6,12,14	1.22	1 (16%)
1	KCX	P	188	1,2	10,11,12	0.89	0	6,12,14	0.99	1 (16%)
1	KCX	H	188	1,2	10,11,12	0.92	0	6,12,14	1.12	1 (16%)
1	KCX	J	188	1,2	10,11,12	0.91	0	6,12,14	1.10	1 (16%)
1	KCX	O	188	1,2	10,11,12	0.92	0	6,12,14	1.19	1 (16%)
1	KCX	L	188	1,2	10,11,12	0.96	0	6,12,14	1.07	1 (16%)
1	KCX	E	188	1,2	10,11,12	0.89	0	6,12,14	1.13	1 (16%)
1	KCX	B	188	1,2	10,11,12	0.93	0	6,12,14	1.11	1 (16%)
1	KCX	K	188	1,2	10,11,12	0.86	0	6,12,14	1.06	1 (16%)
1	KCX	A	188	1,2	10,11,12	0.90	0	6,12,14	1.45	1 (16%)
1	KCX	G	188	1,2	10,11,12	0.95	0	6,12,14	1.14	1 (16%)
1	KCX	N	188	1,2	10,11,12	0.94	0	6,12,14	1.08	1 (16%)
1	KCX	I	188	1,2	10,11,12	0.92	0	6,12,14	1.18	1 (16%)
1	KCX	F	188	1,2	10,11,12	0.90	0	6,12,14	1.04	1 (16%)
1	KCX	M	188	1,2	10,11,12	0.88	0	6,12,14	1.13	1 (16%)
1	KCX	D	188	1,2	10,11,12	0.92	0	6,12,14	1.04	1 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	KCX	C	188	1,2	-	0/9/10/12	-
1	KCX	P	188	1,2	-	0/9/10/12	-
1	KCX	H	188	1,2	-	1/9/10/12	-
1	KCX	J	188	1,2	-	1/9/10/12	-
1	KCX	O	188	1,2	-	0/9/10/12	-
1	KCX	L	188	1,2	-	0/9/10/12	-
1	KCX	E	188	1,2	-	0/9/10/12	-
1	KCX	B	188	1,2	-	0/9/10/12	-
1	KCX	K	188	1,2	-	0/9/10/12	-
1	KCX	A	188	1,2	-	0/9/10/12	-
1	KCX	G	188	1,2	-	1/9/10/12	-
1	KCX	N	188	1,2	-	2/9/10/12	-
1	KCX	I	188	1,2	-	1/9/10/12	-
1	KCX	F	188	1,2	-	0/9/10/12	-
1	KCX	M	188	1,2	-	0/9/10/12	-
1	KCX	D	188	1,2	-	1/9/10/12	-

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	188	KCX	OQ1-CX-NZ	-3.25	119.99	124.92
1	I	188	KCX	OQ1-CX-NZ	-2.75	120.74	124.92
1	C	188	KCX	OQ1-CX-NZ	-2.73	120.77	124.92
1	O	188	KCX	OQ1-CX-NZ	-2.71	120.80	124.92
1	G	188	KCX	OQ1-CX-NZ	-2.67	120.87	124.92
1	E	188	KCX	OQ1-CX-NZ	-2.66	120.89	124.92
1	J	188	KCX	OQ1-CX-NZ	-2.62	120.94	124.92
1	M	188	KCX	OQ1-CX-NZ	-2.60	120.96	124.92
1	H	188	KCX	OQ1-CX-NZ	-2.57	121.01	124.92
1	B	188	KCX	OQ1-CX-NZ	-2.55	121.05	124.92
1	N	188	KCX	OQ1-CX-NZ	-2.54	121.06	124.92
1	L	188	KCX	OQ1-CX-NZ	-2.48	121.16	124.92
1	K	188	KCX	OQ1-CX-NZ	-2.46	121.19	124.92
1	F	188	KCX	OQ1-CX-NZ	-2.40	121.28	124.92
1	D	188	KCX	OQ1-CX-NZ	-2.34	121.37	124.92
1	P	188	KCX	OQ1-CX-NZ	-2.29	121.45	124.92

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	J	188	KCX	CG-CD-CE-NZ
1	N	188	KCX	CG-CD-CE-NZ
1	N	188	KCX	C-CA-CB-CG
1	I	188	KCX	CG-CD-CE-NZ
1	G	188	KCX	CG-CD-CE-NZ
1	D	188	KCX	C-CA-CB-CG
1	H	188	KCX	CG-CD-CE-NZ

There are no ring outliers.

11 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	188	KCX	2	0
1	P	188	KCX	1	0
1	H	188	KCX	1	0
1	J	188	KCX	1	0
1	O	188	KCX	1	0
1	L	188	KCX	1	0
1	E	188	KCX	1	0
1	N	188	KCX	1	0
1	I	188	KCX	1	0
1	F	188	KCX	1	0
1	M	188	KCX	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 48 ligands modelled in this entry, 32 are monoatomic - leaving 16 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	$\# Z > 2$
3	LWY	E	427	2	10,12,12	1.82	2 (20%)	10,18,18	0.98	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	LWY	I	427	2	10,12,12	1.74	2 (20%)	10,18,18	1.10	0
3	LWY	A	427	2	10,12,12	1.77	2 (20%)	10,18,18	1.09	0
3	LWY	C	427	2	10,12,12	1.79	2 (20%)	10,18,18	1.05	0
3	LWY	P	427	2	10,12,12	1.82	2 (20%)	10,18,18	0.91	0
3	LWY	B	427	2	10,12,12	1.78	2 (20%)	10,18,18	1.13	0
3	LWY	M	427	2	10,12,12	1.80	2 (20%)	10,18,18	1.05	0
3	LWY	D	427	2	10,12,12	1.80	2 (20%)	10,18,18	1.00	0
3	LWY	L	427	2	10,12,12	1.77	2 (20%)	10,18,18	1.05	0
3	LWY	F	427	2	10,12,12	1.78	2 (20%)	10,18,18	0.99	0
3	LWY	J	427	2	10,12,12	1.77	2 (20%)	10,18,18	1.02	0
3	LWY	K	427	2	10,12,12	1.80	2 (20%)	10,18,18	0.93	0
3	LWY	G	427	2	10,12,12	1.83	2 (20%)	10,18,18	1.01	0
3	LWY	N	427	2	10,12,12	1.76	2 (20%)	10,18,18	0.99	0
3	LWY	H	427	2	10,12,12	1.80	2 (20%)	10,18,18	1.03	0
3	LWY	O	427	2	10,12,12	1.81	2 (20%)	10,18,18	1.01	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LWY	E	427	2	-	0/4/20/20	0/1/1/1
3	LWY	I	427	2	-	0/4/20/20	0/1/1/1
3	LWY	A	427	2	-	0/4/20/20	0/1/1/1
3	LWY	C	427	2	-	0/4/20/20	0/1/1/1
3	LWY	P	427	2	-	0/4/20/20	0/1/1/1
3	LWY	B	427	2	-	0/4/20/20	0/1/1/1
3	LWY	M	427	2	-	0/4/20/20	0/1/1/1
3	LWY	D	427	2	-	0/4/20/20	0/1/1/1
3	LWY	L	427	2	-	0/4/20/20	0/1/1/1
3	LWY	F	427	2	-	0/4/20/20	0/1/1/1
3	LWY	J	427	2	-	0/4/20/20	0/1/1/1
3	LWY	K	427	2	-	0/4/20/20	0/1/1/1
3	LWY	G	427	2	-	0/4/20/20	0/1/1/1
3	LWY	N	427	2	-	0/4/20/20	0/1/1/1
3	LWY	H	427	2	-	0/4/20/20	0/1/1/1
3	LWY	O	427	2	-	0/4/20/20	0/1/1/1

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	427	LWY	P-O1	4.71	1.61	1.46
3	E	427	LWY	P-O1	4.71	1.61	1.46
3	O	427	LWY	P-O1	4.69	1.61	1.46
3	P	427	LWY	P-O1	4.68	1.61	1.46
3	B	427	LWY	P-O1	4.68	1.61	1.46
3	K	427	LWY	P-O1	4.66	1.61	1.46
3	M	427	LWY	P-O1	4.63	1.61	1.46
3	C	427	LWY	P-O1	4.62	1.61	1.46
3	D	427	LWY	P-O1	4.61	1.61	1.46
3	H	427	LWY	P-O1	4.59	1.61	1.46
3	F	427	LWY	P-O1	4.58	1.61	1.46
3	N	427	LWY	P-O1	4.56	1.61	1.46
3	L	427	LWY	P-O1	4.56	1.61	1.46
3	A	427	LWY	P-O1	4.55	1.60	1.46
3	J	427	LWY	P-O1	4.54	1.60	1.46
3	I	427	LWY	P-O1	4.52	1.60	1.46
3	P	427	LWY	P-O2	-2.22	1.50	1.56
3	E	427	LWY	P-O2	-2.17	1.51	1.56
3	F	427	LWY	P-O2	-2.16	1.51	1.56
3	G	427	LWY	P-O2	-2.16	1.51	1.56
3	A	427	LWY	P-O2	-2.14	1.51	1.56
3	H	427	LWY	P-O2	-2.14	1.51	1.56
3	B	427	LWY	P-O2	-2.13	1.51	1.56
3	J	427	LWY	P-O2	-2.13	1.51	1.56
3	O	427	LWY	P-O2	-2.12	1.51	1.56
3	M	427	LWY	P-O2	-2.11	1.51	1.56
3	L	427	LWY	P-O2	-2.10	1.51	1.56
3	K	427	LWY	P-O2	-2.08	1.51	1.56
3	D	427	LWY	P-O2	-2.08	1.51	1.56
3	C	427	LWY	P-O2	-2.06	1.51	1.56
3	N	427	LWY	P-O2	-2.06	1.51	1.56
3	I	427	LWY	P-O2	-2.00	1.51	1.56

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	427	LWY	2	0
3	M	427	LWY	1	0
3	L	427	LWY	1	0
3	J	427	LWY	1	0

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	407/423 (96%)	-0.12	0 100 100	50, 78, 119, 133	0
1	B	407/423 (96%)	-0.27	0 100 100	32, 67, 107, 137	0
1	C	407/423 (96%)	-0.09	1 (0%) 91 89	48, 73, 114, 142	0
1	D	407/423 (96%)	-0.27	3 (0%) 84 78	42, 63, 97, 154	0
1	E	407/423 (96%)	-0.24	0 100 100	42, 70, 112, 142	0
1	F	407/423 (96%)	-0.21	1 (0%) 91 89	49, 73, 113, 134	0
1	G	407/423 (96%)	-0.13	1 (0%) 91 89	48, 81, 118, 145	0
1	H	407/423 (96%)	-0.28	4 (0%) 79 72	39, 64, 107, 140	0
1	I	407/423 (96%)	0.18	4 (0%) 79 72	58, 94, 134, 150	0
1	J	407/423 (96%)	0.15	3 (0%) 84 78	64, 96, 140, 154	0
1	K	407/423 (96%)	0.21	4 (0%) 79 72	59, 99, 137, 153	0
1	L	407/423 (96%)	0.31	8 (1%) 65 55	67, 106, 136, 150	0
1	M	407/423 (96%)	0.16	5 (1%) 76 68	52, 96, 132, 155	0
1	N	407/423 (96%)	0.24	3 (0%) 84 78	51, 97, 134, 160	0
1	O	407/423 (96%)	-0.03	3 (0%) 84 78	40, 86, 126, 154	0
1	P	407/423 (96%)	-0.18	1 (0%) 91 89	45, 76, 121, 142	0
All	All	6512/6768 (96%)	-0.04	41 (0%) 85 80	32, 82, 128, 160	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	N	365	GLY	3.4
1	N	366	VAL	3.3
1	I	365	GLY	3.1
1	M	298	VAL	3.1
1	D	42	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	M	196	ALA	2.7
1	C	287	MET	2.7
1	D	154	SER	2.7
1	O	298	VAL	2.7
1	K	296	ALA	2.6
1	D	152	PRO	2.6
1	H	152	PRO	2.6
1	H	42	LEU	2.6
1	N	374	ASP	2.6
1	F	43	PRO	2.6
1	L	378	LEU	2.6
1	G	295	VAL	2.6
1	L	365	GLY	2.5
1	M	42	LEU	2.5
1	K	394	ALA	2.4
1	J	148	ASP	2.4
1	O	295	VAL	2.3
1	M	374	ASP	2.3
1	K	294	LYS	2.3
1	K	18	VAL	2.3
1	L	317	GLY	2.3
1	L	67	LEU	2.3
1	J	42	LEU	2.2
1	O	6	LEU	2.2
1	H	147	GLY	2.2
1	L	366	VAL	2.2
1	L	376	VAL	2.1
1	I	183	GLY	2.1
1	L	163	ALA	2.1
1	H	283	ALA	2.1
1	I	153	CYS	2.0
1	M	289	PRO	2.0
1	I	14	LEU	2.0
1	J	25	VAL	2.0
1	P	42	LEU	2.0
1	L	314	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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
1	KCX	L	188	12/13	0.90	0.12	76,91,120,127	0
1	KCX	K	188	12/13	0.92	0.11	75,89,99,100	0
1	KCX	C	188	12/13	0.93	0.10	48,63,78,85	0
1	KCX	D	188	12/13	0.93	0.12	48,54,72,82	0
1	KCX	H	188	12/13	0.93	0.11	51,59,94,107	0
1	KCX	A	188	12/13	0.93	0.12	64,77,107,111	0
1	KCX	B	188	12/13	0.93	0.10	41,46,88,89	0
1	KCX	J	188	12/13	0.94	0.09	62,79,108,108	0
1	KCX	I	188	12/13	0.95	0.13	61,74,110,111	0
1	KCX	M	188	12/13	0.95	0.09	67,75,92,103	0
1	KCX	O	188	12/13	0.95	0.10	41,61,79,94	0
1	KCX	F	188	12/13	0.96	0.11	52,61,115,124	0
1	KCX	G	188	12/13	0.96	0.07	55,64,92,97	0
1	KCX	E	188	12/13	0.96	0.08	48,52,78,86	0
1	KCX	P	188	12/13	0.96	0.06	52,64,90,93	0
1	KCX	N	188	12/13	0.97	0.08	68,78,133,140	0

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	LWY	K	427	12/12	0.93	0.11	127,133,135,135	0
3	LWY	I	427	12/12	0.94	0.10	102,106,112,113	0
3	LWY	M	427	12/12	0.94	0.11	103,113,116,116	0
3	LWY	L	427	12/12	0.95	0.11	101,111,114,115	0
3	LWY	B	427	12/12	0.95	0.10	73,77,81,83	0
3	LWY	O	427	12/12	0.95	0.09	81,90,93,95	0
3	LWY	C	427	12/12	0.96	0.09	89,94,98,100	0
3	LWY	E	427	12/12	0.96	0.09	81,88,90,90	0
3	LWY	F	427	12/12	0.96	0.08	97,98,101,106	0
3	LWY	A	427	12/12	0.96	0.08	95,103,107,108	0
3	LWY	N	427	12/12	0.97	0.07	109,111,112,115	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	LWY	J	427	12/12	0.97	0.07	90,105,106,107	0
3	LWY	P	427	12/12	0.97	0.08	74,87,89,92	0
2	ZN	I	426	1/1	0.98	0.08	115,115,115,115	0
2	ZN	L	426	1/1	0.98	0.06	108,108,108,108	0
3	LWY	G	427	12/12	0.98	0.07	85,91,95,97	0
3	LWY	H	427	12/12	0.98	0.07	77,81,88,88	0
2	ZN	M	426	1/1	0.98	0.05	103,103,103,103	0
3	LWY	D	427	12/12	0.98	0.05	63,71,80,81	0
2	ZN	P	426	1/1	0.99	0.03	94,94,94,94	0
2	ZN	C	425	1/1	0.99	0.02	90,90,90,90	0
2	ZN	C	426	1/1	0.99	0.03	91,91,91,91	0
2	ZN	E	426	1/1	0.99	0.03	84,84,84,84	0
2	ZN	F	426	1/1	0.99	0.03	89,89,89,89	0
2	ZN	I	425	1/1	0.99	0.08	100,100,100,100	0
2	ZN	A	426	1/1	0.99	0.04	99,99,99,99	0
2	ZN	J	425	1/1	0.99	0.04	102,102,102,102	0
2	ZN	J	426	1/1	0.99	0.02	101,101,101,101	0
2	ZN	K	425	1/1	0.99	0.04	125,125,125,125	0
2	ZN	K	426	1/1	0.99	0.05	110,110,110,110	0
2	ZN	L	425	1/1	0.99	0.04	102,102,102,102	0
2	ZN	B	425	1/1	0.99	0.03	78,78,78,78	0
2	ZN	M	425	1/1	0.99	0.05	114,114,114,114	0
2	ZN	B	426	1/1	0.99	0.04	84,84,84,84	0
2	ZN	N	426	1/1	0.99	0.03	95,95,95,95	0
2	ZN	O	426	1/1	0.99	0.03	93,93,93,93	0
2	ZN	H	426	1/1	1.00	0.04	92,92,92,92	0
2	ZN	D	426	1/1	1.00	0.02	72,72,72,72	0
2	ZN	N	425	1/1	1.00	0.02	90,90,90,90	0
2	ZN	E	425	1/1	1.00	0.02	79,79,79,79	0
2	ZN	O	425	1/1	1.00	0.04	92,92,92,92	0
2	ZN	A	425	1/1	1.00	0.05	86,86,86,86	0
2	ZN	P	425	1/1	1.00	0.03	87,87,87,87	0
2	ZN	F	425	1/1	1.00	0.04	96,96,96,96	0
2	ZN	D	425	1/1	1.00	0.01	73,73,73,73	0
2	ZN	G	425	1/1	1.00	0.03	84,84,84,84	0
2	ZN	G	426	1/1	1.00	0.03	95,95,95,95	0
2	ZN	H	425	1/1	1.00	0.03	89,89,89,89	0

6.5 Other polymers ⓘ

There are no such residues in this entry.