Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2023 – 04:45 AM EDT

PDB ID	:	3N2C
Title	:	Crystal structure of prolidase eah89906 complexed with n-methylphosphonate-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)

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

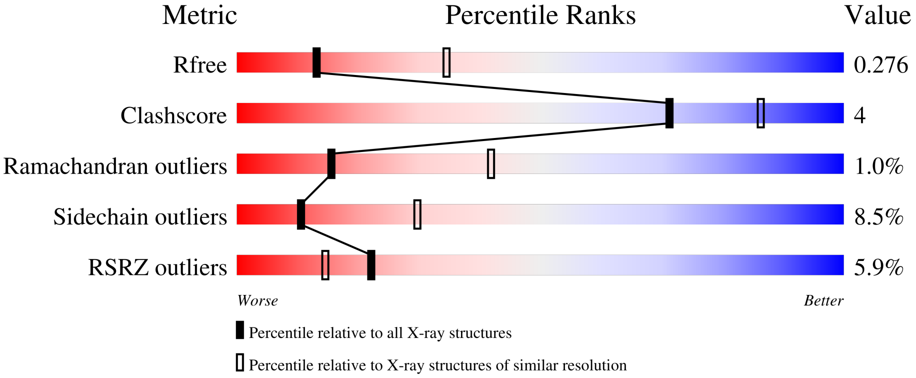
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

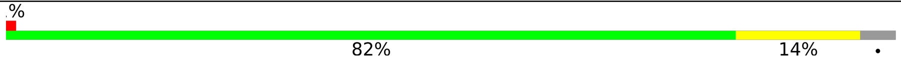
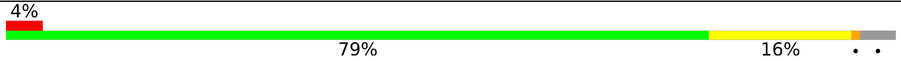
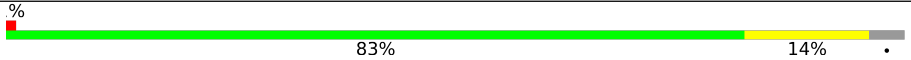
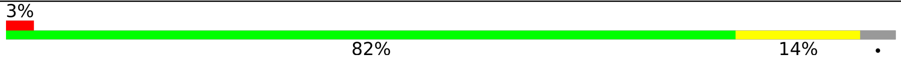
The reported resolution of this entry is 2.81 Å.

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}	130704	3617 (2.84-2.80)
Clashscore	141614	4060 (2.84-2.80)
Ramachandran outliers	138981	3978 (2.84-2.80)
Sidechain outliers	138945	3980 (2.84-2.80)
RSRZ outliers	127900	3552 (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 <=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	
1	B	423	
1	C	423	
1	D	423	
1	E	423	

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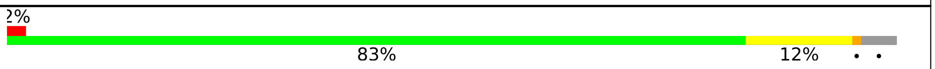
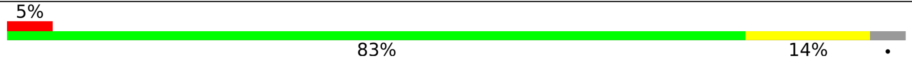
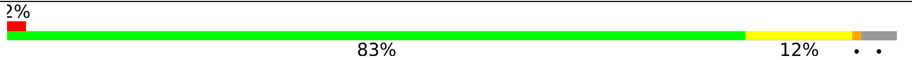
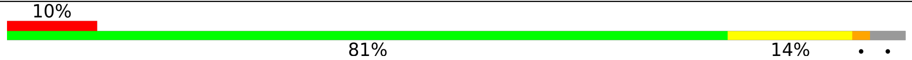
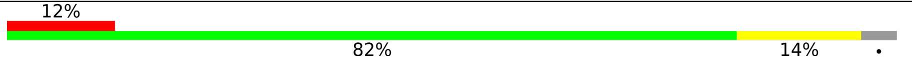
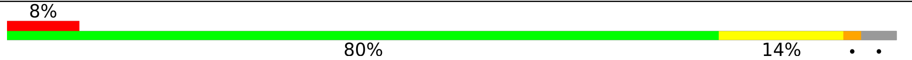
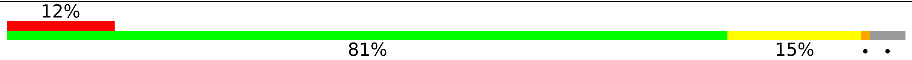
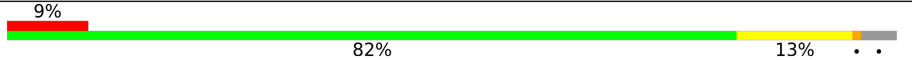
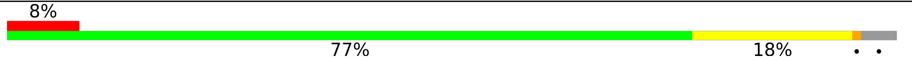
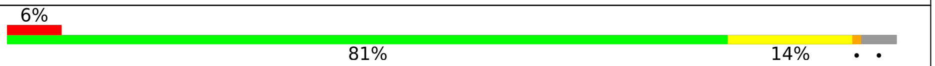
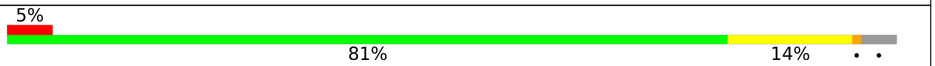
Mol	Chain	Length	Quality of chain
1	F	423	
1	G	423	
1	H	423	
1	I	423	
1	J	423	
1	K	423	
1	L	423	
1	M	423	
1	N	423	
1	O	423	
1	P	423	

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.

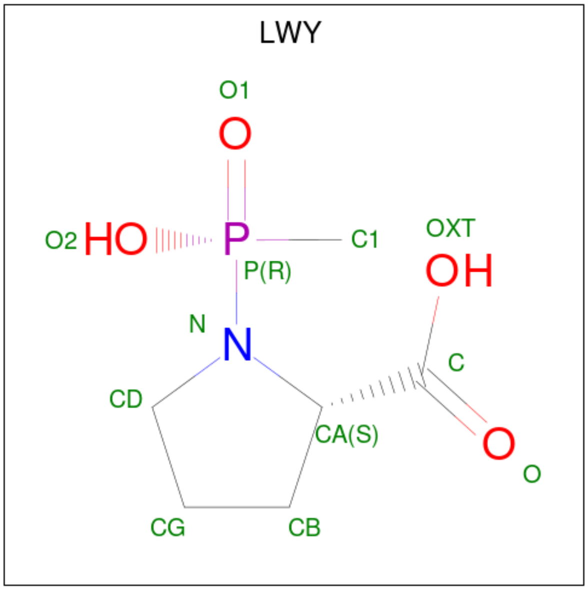
- Molecule 1 is a protein called PROLIDASE.

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 (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is 1-[(R)-hydroxy(methyl)phosphoryl]-L-proline (three-letter code: LWY) (formula: $C_6H_{12}NO_4P$).



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

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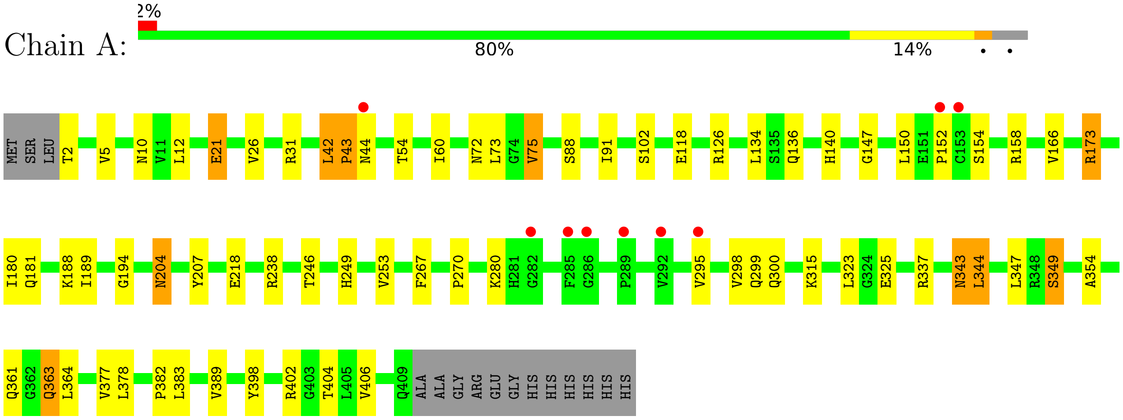
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	O	1	Total C N O P 12 6 1 4 1	0	0
3	P	1	Total C N O P 12 6 1 4 1	0	0

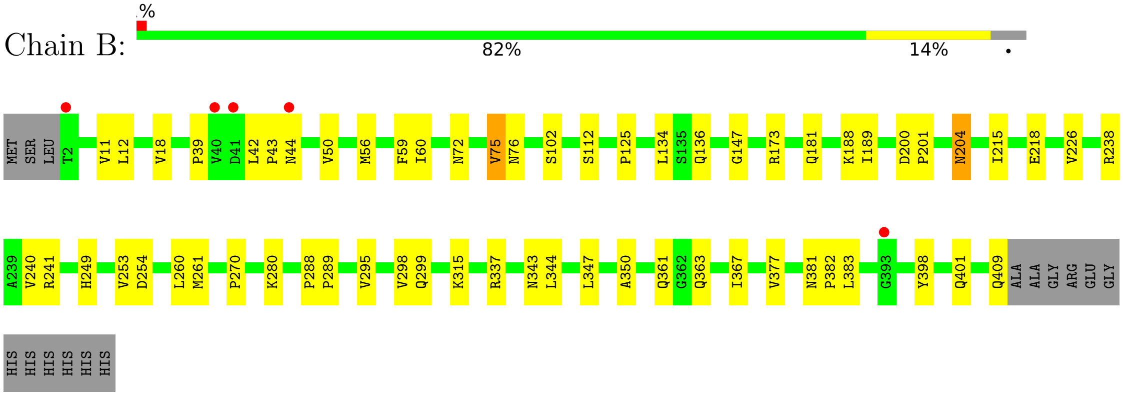
3 Residue-property plots ⓘ

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.

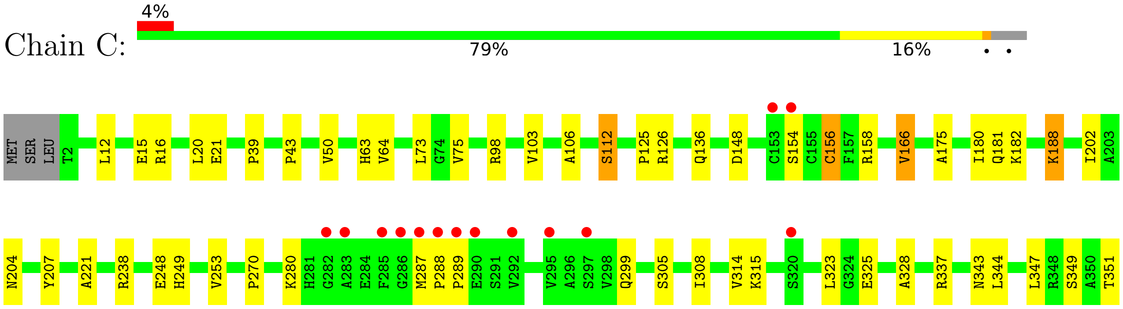
- Molecule 1: PROLIDASE



- Molecule 1: PROLIDASE

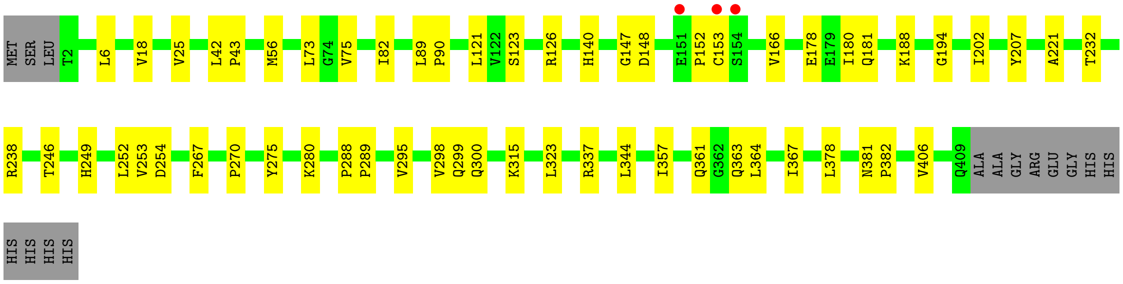


- Molecule 1: PROLIDASE



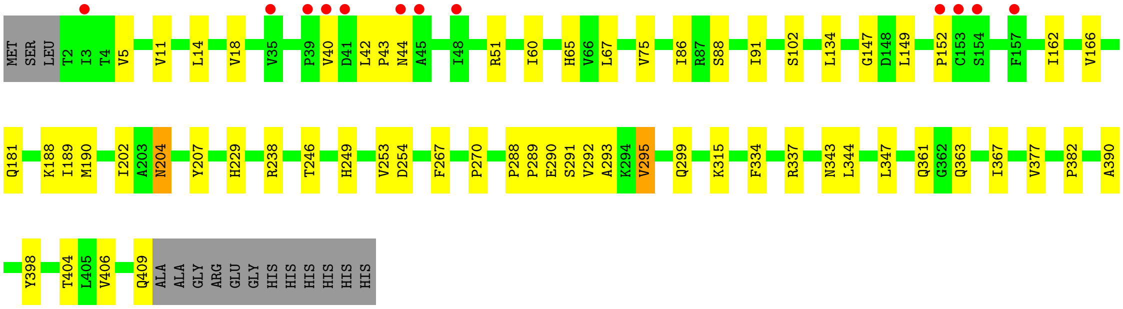
- Molecule 1: PROLIDASE

Chain D:



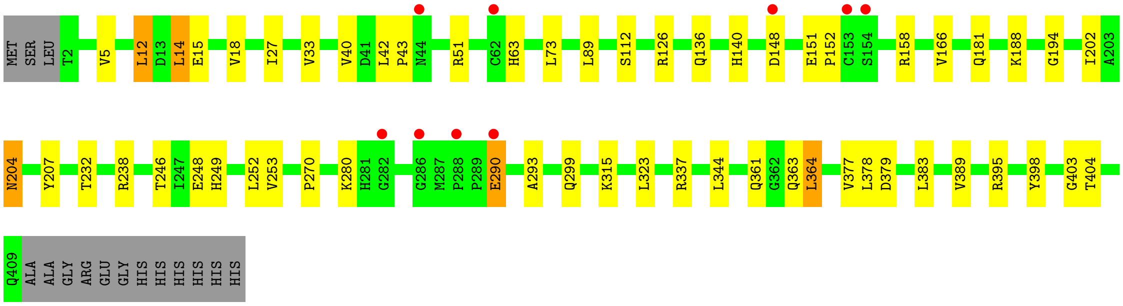
- Molecule 1: PROLIDASE

Chain E:



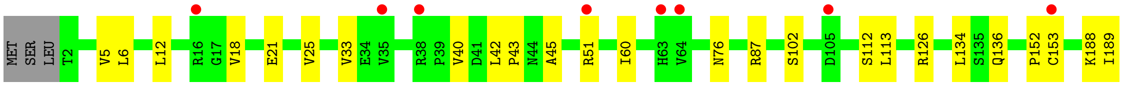
- Molecule 1: PROLIDASE

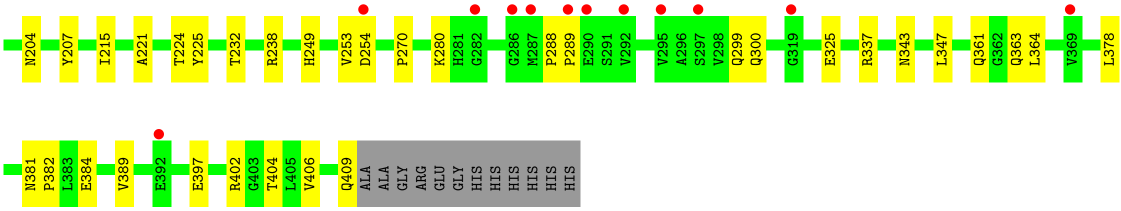
Chain F:



- Molecule 1: PROLIDASE

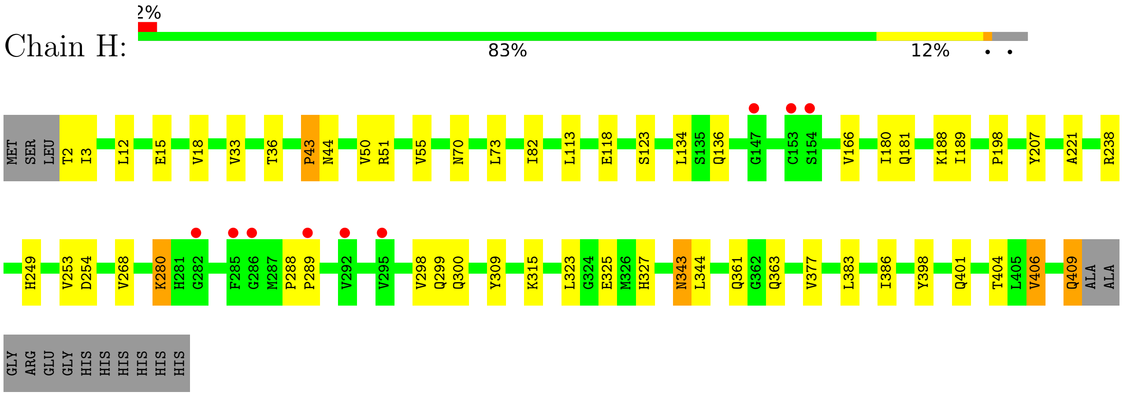
Chain G:





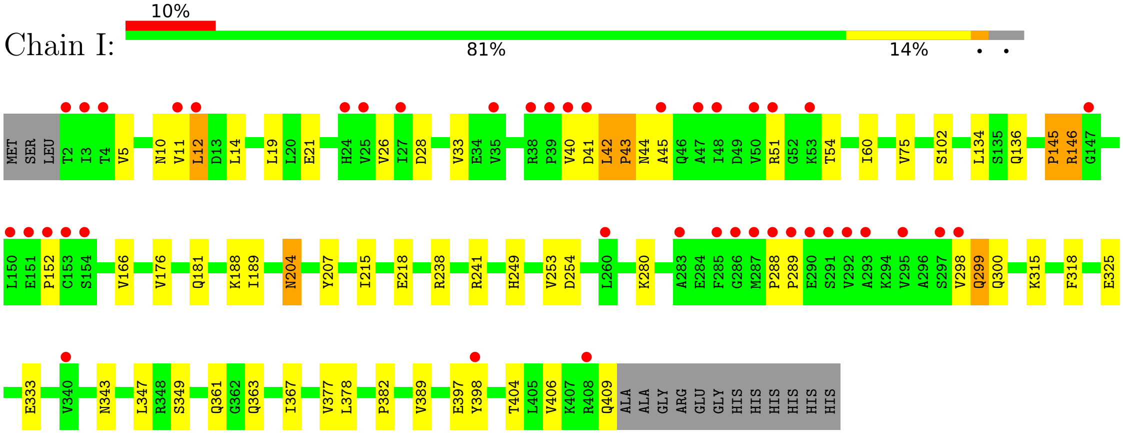
- Molecule 1: PROLIDASE

Chain H:



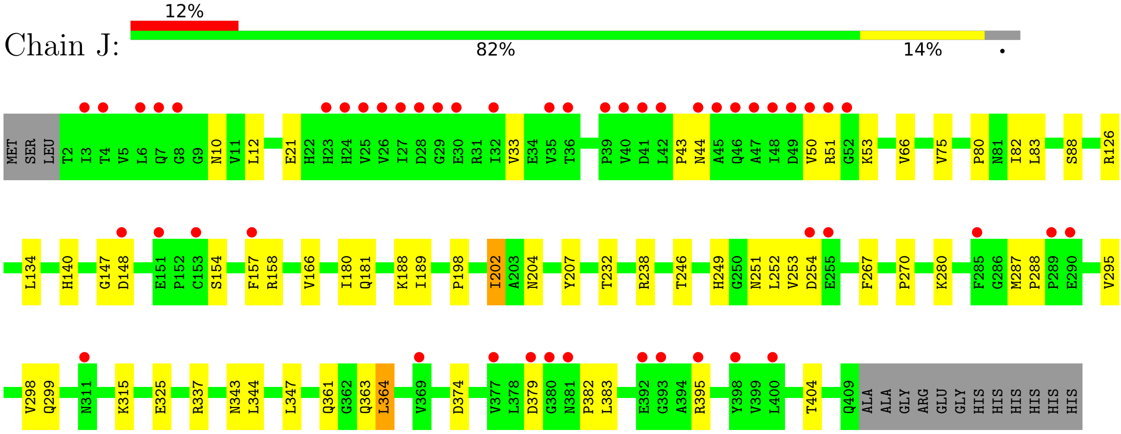
- Molecule 1: PROLIDASE

Chain I:

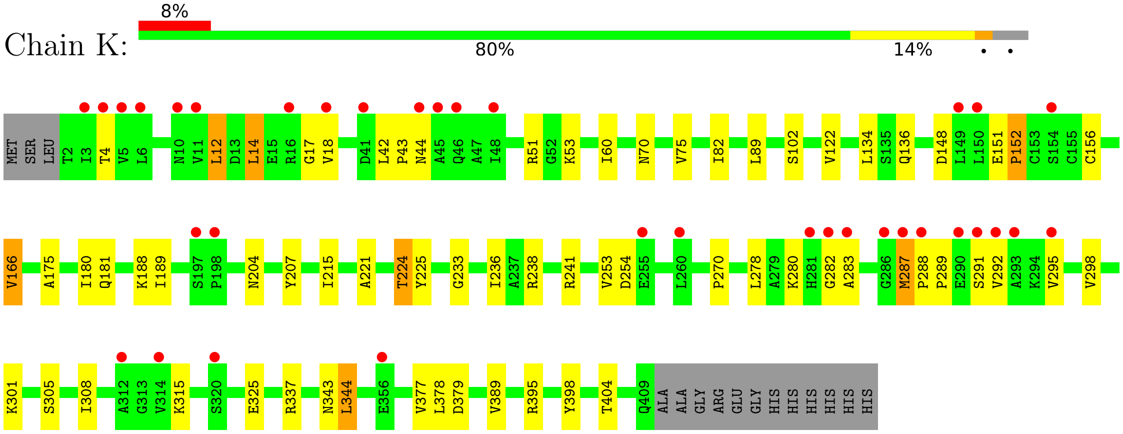


- Molecule 1: PROLIDASE

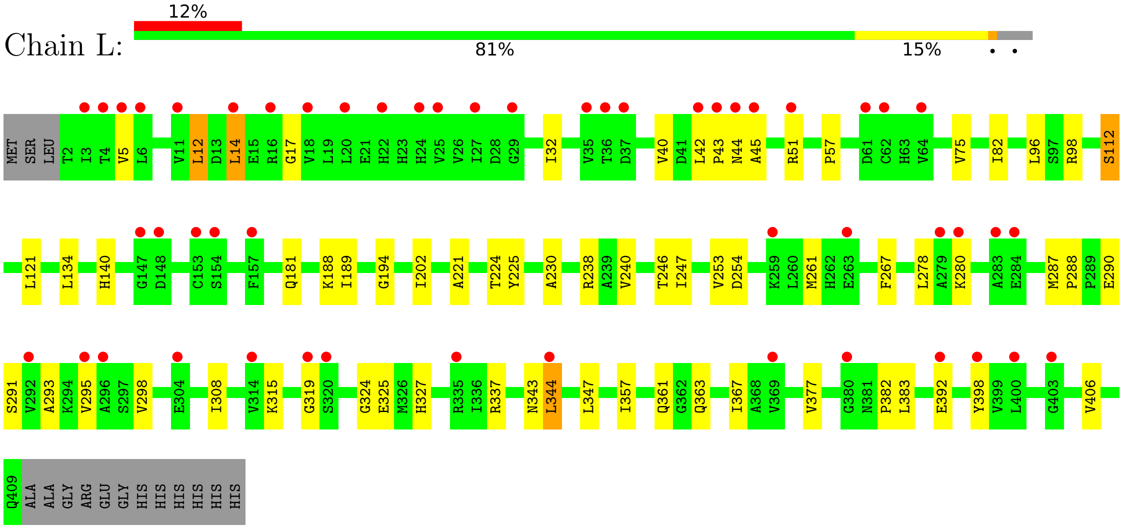
Chain J:



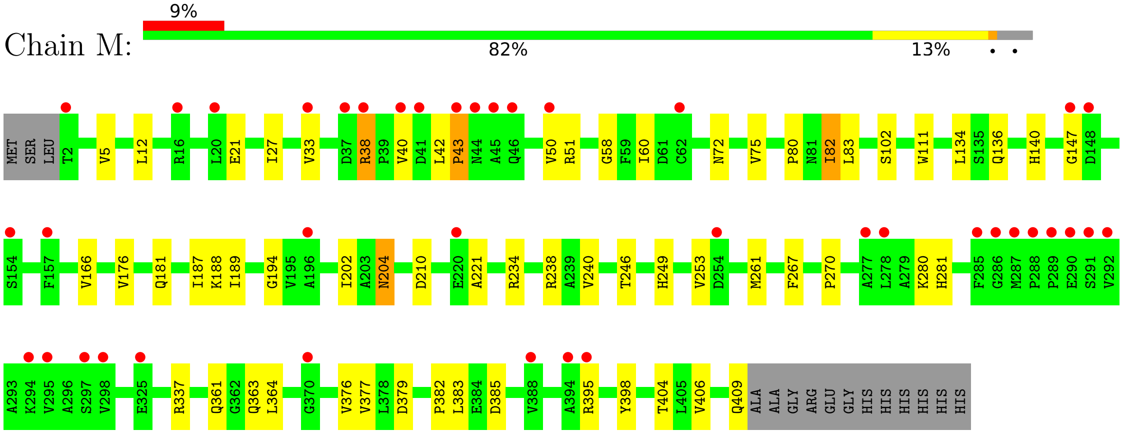
- Molecule 1: PROLIDASE



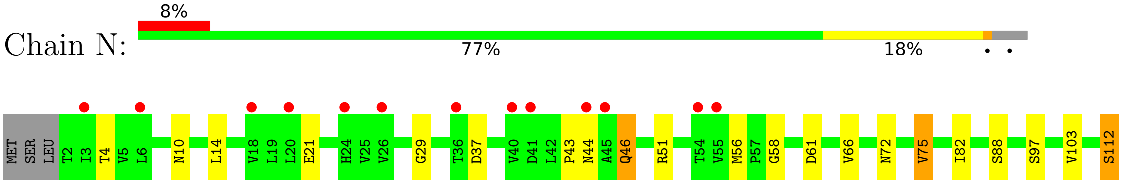
- Molecule 1: PROLIDASE

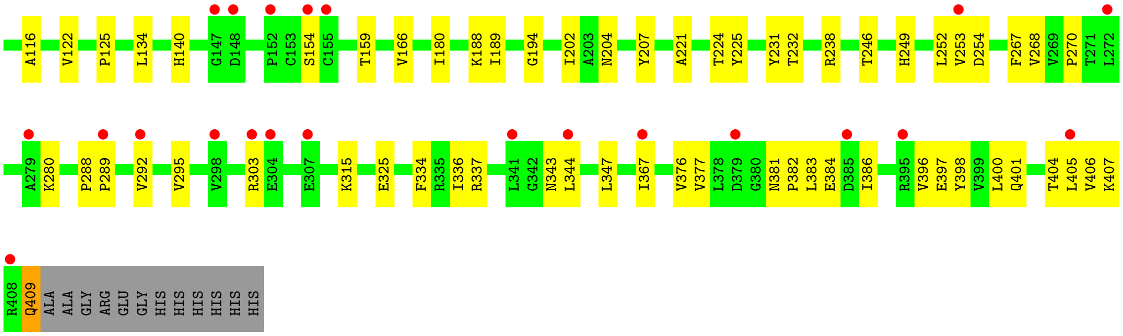


- Molecule 1: PROLIDASE



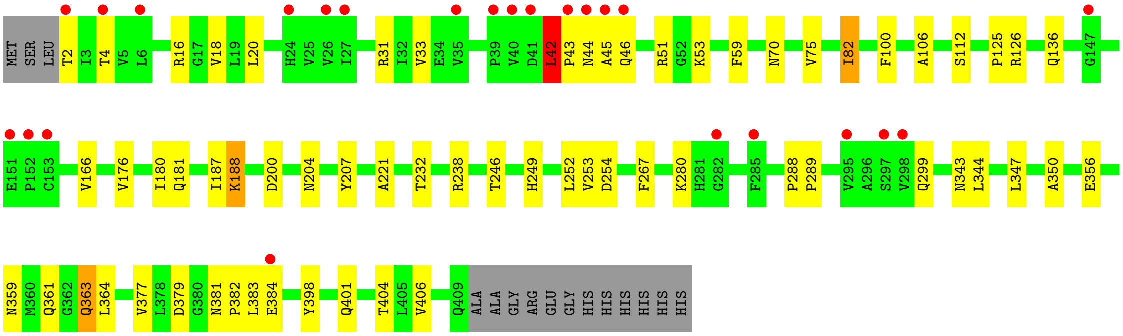
- Molecule 1: PROLIDASE





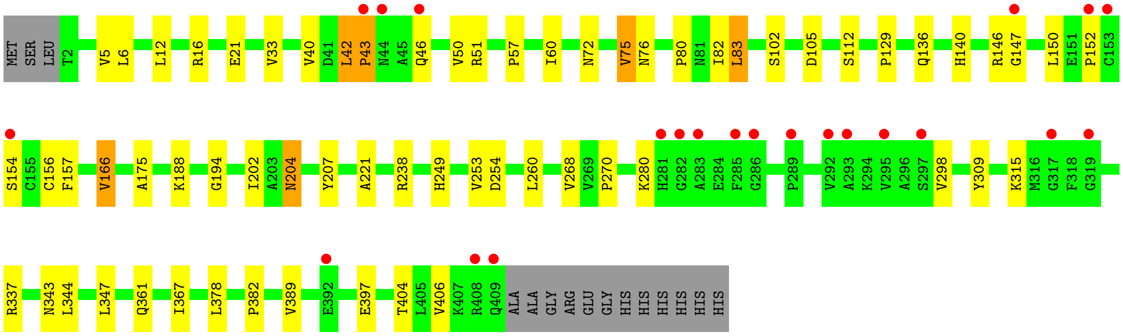
- Molecule 1: PROLIDASE

Chain O:



- Molecule 1: PROLIDASE

Chain P:



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 40.07 – 2.81	Depositor EDS
% Data completeness (in resolution range)	89.9 (40.00-2.81) 89.9 (40.07-2.81)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 (3.02%)	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)	0.31 , 54.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	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.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: KCX, ZN, LWY

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	0.35	0/3064	0.56	0/4156
1	B	0.35	0/3064	0.57	0/4156
1	C	0.35	0/3064	0.57	0/4156
1	D	0.36	0/3064	0.56	0/4156
1	E	0.37	0/3064	0.56	0/4156
1	F	0.35	0/3064	0.56	0/4156
1	G	0.35	0/3064	0.57	0/4156
1	H	0.36	0/3064	0.58	0/4156
1	I	0.36	0/3064	0.56	1/4156 (0.0%)
1	J	0.36	0/3064	0.57	0/4156
1	K	0.36	0/3064	0.56	0/4156
1	L	0.36	0/3064	0.56	0/4156
1	M	0.37	0/3064	0.56	0/4156
1	N	0.36	0/3064	0.57	0/4156
1	O	0.35	0/3064	0.56	1/4156 (0.0%)
1	P	0.35	0/3064	0.58	0/4156
All	All	0.36	0/49024	0.57	2/66496 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	O	42	LEU	CA-CB-CG	5.83	128.71	115.30
1	I	42	LEU	CA-CB-CG	5.10	127.04	115.30

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	3037	34	0
1	B	3033	0	3037	20	0
1	C	3033	0	3037	25	0
1	D	3033	0	3037	19	0
1	E	3033	0	3037	19	0
1	F	3033	0	3037	19	0
1	G	3033	0	3037	21	0
1	H	3033	0	3037	16	0
1	I	3033	0	3037	21	0
1	J	3033	0	3037	18	0
1	K	3033	0	3037	27	0
1	L	3033	0	3037	31	0
1	M	3033	0	3037	22	0
1	N	3033	0	3037	29	0
1	O	3033	0	3037	22	0
1	P	3033	0	3037	19	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	48752	343	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 (343) 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:L:287:MET:HG3	1:L:288:PRO:HD2	1.34	1.07
1:K:278:LEU:HD22	1:K:287:MET:HE3	1.42	1.01
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	1.56	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:J:347:LEU:HD11	1:J:382:PRO:HB2	1.75	0.68
1:K:278:LEU:CD2	1:K:287:MET:CE	2.71	0.67
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:K:278:LEU:CD2	1:K:287:MET:HE1	2.32	0.60
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: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: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: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: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: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:P:57:PRO:HG3	1:P:367:ILE:HG13	1.92	0.52
1:F:290:GLU:CD	1:F:290:GLU:H	2.09	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:L:224:THR:OG1	1:L:225:TYR:N	2.43	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
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: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:H:134:LEU:HB2	1:H:189:ILE:HG22	1.96	0.48
1:L:134:LEU:HB2	1:L:189:ILE:HG22	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:K:287:MET:HB2	1:K:287:MET:HE2	1.40	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: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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:L:278:LEU:HD22	1:L:287:MET:CE	2.45	0.46
1:C:156:CYS:SG	1:C:182:LYS:NZ	2.89	0.46
1:D:89:LEU:HB2	1:D:90:PRO:HD3	1.98	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: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:O:126:ARG:HH11	1:O:364:LEU:HD11	1.82	0.45
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:O	1:A:344:LEU:CD2	2.66	0.44
1:G:381:ASN:HA	1:G:382:PRO:HD2	1.82	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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: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:F:290:GLU:O	1:F:293:ALA:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:282:GLY:O	1:K:287:MET:HB3	2.19	0.43
1:L:278:LEU:CD1	1:L:287:MET:HE1	2.39	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:A:344:LEU:CD2	1:A:344:LEU:C	2.87	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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:A:42:LEU:HA	1:A:43:PRO:HD3	1.86	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 ⓘ

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	405/423 (96%)	385 (95%)	15 (4%)	5 (1%)	13	37
1	B	405/423 (96%)	381 (94%)	20 (5%)	4 (1%)	15	42
1	C	405/423 (96%)	380 (94%)	21 (5%)	4 (1%)	15	42
1	D	405/423 (96%)	379 (94%)	21 (5%)	5 (1%)	13	37
1	E	405/423 (96%)	380 (94%)	20 (5%)	5 (1%)	13	37
1	F	405/423 (96%)	379 (94%)	23 (6%)	3 (1%)	22	51
1	G	405/423 (96%)	375 (93%)	26 (6%)	4 (1%)	15	42
1	H	405/423 (96%)	383 (95%)	18 (4%)	4 (1%)	15	42
1	I	405/423 (96%)	377 (93%)	23 (6%)	5 (1%)	13	37
1	J	405/423 (96%)	374 (92%)	26 (6%)	5 (1%)	13	37
1	K	405/423 (96%)	378 (93%)	24 (6%)	3 (1%)	22	51
1	L	405/423 (96%)	377 (93%)	27 (7%)	1 (0%)	47	76
1	M	405/423 (96%)	383 (95%)	19 (5%)	3 (1%)	22	51
1	N	405/423 (96%)	371 (92%)	30 (7%)	4 (1%)	15	42
1	O	405/423 (96%)	375 (93%)	27 (7%)	3 (1%)	22	51
1	P	405/423 (96%)	375 (93%)	25 (6%)	5 (1%)	13	37
All	All	6480/6768 (96%)	6052 (93%)	365 (6%)	63 (1%)	15	42

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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%)	286 (91%)	28 (9%)	9	27
1	B	314/325 (97%)	289 (92%)	25 (8%)	12	32
1	C	314/325 (97%)	283 (90%)	31 (10%)	8	22
1	D	314/325 (97%)	294 (94%)	20 (6%)	17	44
1	E	314/325 (97%)	290 (92%)	24 (8%)	13	35
1	F	314/325 (97%)	287 (91%)	27 (9%)	10	29
1	G	314/325 (97%)	293 (93%)	21 (7%)	16	41
1	H	314/325 (97%)	283 (90%)	31 (10%)	8	22
1	I	314/325 (97%)	285 (91%)	29 (9%)	9	26
1	J	314/325 (97%)	286 (91%)	28 (9%)	9	27
1	K	314/325 (97%)	282 (90%)	32 (10%)	7	21
1	L	314/325 (97%)	291 (93%)	23 (7%)	14	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	M	314/325 (97%)	288 (92%)	26 (8%)	11	31
1	N	314/325 (97%)	286 (91%)	28 (9%)	9	27
1	O	314/325 (97%)	288 (92%)	26 (8%)	11	31
1	P	314/325 (97%)	284 (90%)	30 (10%)	8	24
All	All	5024/5200 (97%)	4595 (92%)	429 (8%)	10	30

All (429) 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	75	VAL
1	A	136	GLN
1	A	150	LEU
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	295	VAL
1	A	298	VAL
1	A	315	LYS
1	A	325	GLU
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	404	THR
1	A	406	VAL
1	B	12	LEU
1	B	18	VAL
1	B	42	LEU
1	B	44	ASN

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Mol	Chain	Res	Type
1	B	50	VAL
1	B	75	VAL
1	B	76	ASN
1	B	112	SER
1	B	136	GLN
1	B	181	GLN
1	B	204	ASN
1	B	238	ARG
1	B	253	VAL
1	B	254	ASP
1	B	280	LYS
1	B	295	VAL
1	B	298	VAL
1	B	299	GLN
1	B	315	LYS
1	B	343	ASN
1	B	344	LEU
1	B	361	GLN
1	B	363	GLN
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

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Mol	Chain	Res	Type
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	392	GLU
1	C	404	THR
1	C	406	VAL
1	D	18	VAL
1	D	42	LEU
1	D	75	VAL
1	D	123	SER
1	D	148	ASP
1	D	153	CYS
1	D	166	VAL
1	D	180	ILE
1	D	181	GLN
1	D	238	ARG
1	D	253	VAL
1	D	254	ASP
1	D	280	LYS
1	D	295	VAL
1	D	315	LYS
1	D	344	LEU
1	D	361	GLN
1	D	363	GLN
1	D	378	LEU
1	D	406	VAL
1	E	14	LEU
1	E	18	VAL
1	E	42	LEU
1	E	44	ASN
1	E	51	ARG
1	E	67	LEU
1	E	75	VAL
1	E	166	VAL
1	E	181	GLN
1	E	202	ILE
1	E	204	ASN
1	E	238	ARG

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Mol	Chain	Res	Type
1	E	253	VAL
1	E	254	ASP
1	E	295	VAL
1	E	299	GLN
1	E	315	LYS
1	E	343	ASN
1	E	344	LEU
1	E	361	GLN
1	E	363	GLN
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	33	VAL
1	F	42	LEU
1	F	51	ARG
1	F	112	SER
1	F	136	GLN
1	F	148	ASP
1	F	166	VAL
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	299	GLN
1	F	315	LYS
1	F	344	LEU
1	F	361	GLN
1	F	363	GLN
1	F	364	LEU
1	F	383	LEU
1	F	404	THR
1	G	12	LEU
1	G	18	VAL
1	G	21	GLU

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Mol	Chain	Res	Type
1	G	33	VAL
1	G	51	ARG
1	G	76	ASN
1	G	112	SER
1	G	136	GLN
1	G	153	CYS
1	G	204	ASN
1	G	232	THR
1	G	238	ARG
1	G	253	VAL
1	G	254	ASP
1	G	280	LYS
1	G	325	GLU
1	G	343	ASN
1	G	361	GLN
1	G	363	GLN
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	33	VAL
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	238	ARG
1	H	253	VAL
1	H	254	ASP
1	H	280	LYS
1	H	298	VAL
1	H	315	LYS
1	H	325	GLU
1	H	327	HIS
1	H	343	ASN

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Mol	Chain	Res	Type
1	H	344	LEU
1	H	361	GLN
1	H	363	GLN
1	H	383	LEU
1	H	404	THR
1	H	406	VAL
1	H	409	GLN
1	I	12	LEU
1	I	28	ASP
1	I	33	VAL
1	I	41	ASP
1	I	44	ASN
1	I	51	ARG
1	I	75	VAL
1	I	136	GLN
1	I	146	ARG
1	I	166	VAL
1	I	181	GLN
1	I	204	ASN
1	I	238	ARG
1	I	241	ARG
1	I	253	VAL
1	I	254	ASP
1	I	280	LYS
1	I	298	VAL
1	I	299	GLN
1	I	315	LYS
1	I	325	GLU
1	I	343	ASN
1	I	349	SER
1	I	361	GLN
1	I	363	GLN
1	I	397	GLU
1	I	404	THR
1	I	406	VAL
1	I	409	GLN
1	J	12	LEU
1	J	33	VAL
1	J	44	ASN
1	J	50	VAL
1	J	51	ARG
1	J	75	VAL

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Mol	Chain	Res	Type
1	J	82	ILE
1	J	148	ASP
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	254	ASP
1	J	280	LYS
1	J	295	VAL
1	J	299	GLN
1	J	315	LYS
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	374	ASP
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	42	LEU
1	K	44	ASN
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	204	ASN
1	K	224	THR
1	K	238	ARG
1	K	241	ARG

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Mol	Chain	Res	Type
1	K	253	VAL
1	K	254	ASP
1	K	280	LYS
1	K	287	MET
1	K	295	VAL
1	K	298	VAL
1	K	301	LYS
1	K	315	LYS
1	K	325	GLU
1	K	343	ASN
1	K	344	LEU
1	K	404	THR
1	L	12	LEU
1	L	14	LEU
1	L	44	ASN
1	L	51	ARG
1	L	75	VAL
1	L	82	ILE
1	L	112	SER
1	L	121	LEU
1	L	181	GLN
1	L	202	ILE
1	L	238	ARG
1	L	253	VAL
1	L	254	ASP
1	L	280	LYS
1	L	295	VAL
1	L	298	VAL
1	L	315	LYS
1	L	325	GLU
1	L	343	ASN
1	L	344	LEU
1	L	361	GLN
1	L	363	GLN
1	L	383	LEU
1	M	12	LEU
1	M	21	GLU
1	M	27	ILE
1	M	33	VAL
1	M	38	ARG
1	M	50	VAL
1	M	51	ARG

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Mol	Chain	Res	Type
1	M	82	ILE
1	M	136	GLN
1	M	166	VAL
1	M	181	GLN
1	M	202	ILE
1	M	204	ASN
1	M	210	ASP
1	M	234	ARG
1	M	238	ARG
1	M	253	VAL
1	M	280	LYS
1	M	281	HIS
1	M	361	GLN
1	M	363	GLN
1	M	364	LEU
1	M	383	LEU
1	M	404	THR
1	M	406	VAL
1	M	409	GLN
1	N	14	LEU
1	N	37	ASP
1	N	44	ASN
1	N	46	GLN
1	N	51	ARG
1	N	75	VAL
1	N	82	ILE
1	N	112	SER
1	N	159	THR
1	N	166	VAL
1	N	180	ILE
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	315	LYS
1	N	325	GLU
1	N	343	ASN
1	N	344	LEU

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Mol	Chain	Res	Type
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	33	VAL
1	O	42	LEU
1	O	44	ASN
1	O	51	ARG
1	O	70	ASN
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	254	ASP
1	O	280	LYS
1	O	299	GLN
1	O	343	ASN
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
1	P	46	GLN
1	P	51	ARG
1	P	75	VAL
1	P	76	ASN
1	P	82	ILE
1	P	83	LEU

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Mol	Chain	Res	Type
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	254	ASP
1	P	260	LEU
1	P	280	LYS
1	P	298	VAL
1	P	315	LYS
1	P	343	ASN
1	P	344	LEU
1	P	361	GLN
1	P	397	GLU
1	P	404	THR
1	P	406	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (81) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	299	GLN
1	A	300	GLN
1	A	343	ASN
1	A	359	ASN
1	A	361	GLN
1	A	363	GLN
1	B	10	ASN
1	B	299	GLN
1	B	401	GLN
1	B	409	GLN
1	C	46	GLN
1	C	299	GLN
1	C	300	GLN
1	C	359	ASN
1	C	409	GLN
1	D	10	ASN
1	D	44	ASN
1	D	299	GLN

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Mol	Chain	Res	Type
1	D	300	GLN
1	D	361	GLN
1	D	363	GLN
1	E	10	ASN
1	E	299	GLN
1	E	359	ASN
1	E	361	GLN
1	F	10	ASN
1	F	44	ASN
1	F	299	GLN
1	F	361	GLN
1	G	44	ASN
1	G	299	GLN
1	G	300	GLN
1	G	361	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	359	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
1	J	251	ASN
1	J	299	GLN
1	J	343	ASN
1	J	363	GLN
1	K	10	ASN
1	K	299	GLN
1	K	300	GLN
1	K	409	GLN
1	L	10	ASN
1	L	44	ASN
1	L	299	GLN
1	L	361	GLN
1	M	299	GLN
1	M	300	GLN

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Mol	Chain	Res	Type
1	M	361	GLN
1	N	10	ASN
1	N	44	ASN
1	N	299	GLN
1	N	300	GLN
1	N	401	GLN
1	O	10	ASN
1	O	44	ASN
1	O	206	GLN
1	O	223	ASN
1	O	299	GLN
1	O	300	GLN
1	O	359	ASN
1	O	363	GLN
1	O	401	GLN
1	P	10	ASN
1	P	44	ASN
1	P	46	GLN
1	P	299	GLN
1	P	300	GLN

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	J	188	2,1	9,11,12	0.85	0	5,12,14	1.19	1 (20%)
1	KCX	L	188	2,1	9,11,12	0.91	0	5,12,14	1.15	1 (20%)
1	KCX	M	188	2,1	9,11,12	0.83	0	5,12,14	1.22	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
1	KCX	G	188	2,1	9,11,12	0.90	0	5,12,14	1.23	1 (20%)
1	KCX	H	188	2,1	9,11,12	0.87	0	5,12,14	1.21	1 (20%)
1	KCX	O	188	2,1	9,11,12	0.87	0	5,12,14	1.29	1 (20%)
1	KCX	K	188	2,1	9,11,12	0.80	0	5,12,14	1.14	1 (20%)
1	KCX	D	188	2,1	9,11,12	0.87	0	5,12,14	1.13	1 (20%)
1	KCX	B	188	2,1	9,11,12	0.87	0	5,12,14	1.19	1 (20%)
1	KCX	F	188	2,1	9,11,12	0.84	0	5,12,14	1.12	1 (20%)
1	KCX	P	188	2,1	9,11,12	0.82	0	5,12,14	1.07	1 (20%)
1	KCX	I	188	2,1	9,11,12	0.86	0	5,12,14	1.28	1 (20%)
1	KCX	E	188	2,1	9,11,12	0.83	0	5,12,14	1.21	1 (20%)
1	KCX	A	188	2,1	9,11,12	0.84	0	5,12,14	1.57	1 (20%)
1	KCX	N	188	2,1	9,11,12	0.89	0	5,12,14	1.17	1 (20%)
1	KCX	C	188	2,1	9,11,12	0.82	0	5,12,14	1.32	1 (20%)

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	J	188	2,1	-	1/9/10/12	-
1	KCX	L	188	2,1	-	0/9/10/12	-
1	KCX	M	188	2,1	-	0/9/10/12	-
1	KCX	G	188	2,1	-	1/9/10/12	-
1	KCX	H	188	2,1	-	1/9/10/12	-
1	KCX	O	188	2,1	-	0/9/10/12	-
1	KCX	K	188	2,1	-	0/9/10/12	-
1	KCX	D	188	2,1	-	0/9/10/12	-
1	KCX	B	188	2,1	-	0/9/10/12	-
1	KCX	F	188	2,1	-	0/9/10/12	-
1	KCX	P	188	2,1	-	0/9/10/12	-
1	KCX	I	188	2,1	-	1/9/10/12	-
1	KCX	E	188	2,1	-	0/9/10/12	-
1	KCX	A	188	2,1	-	0/9/10/12	-
1	KCX	N	188	2,1	-	1/9/10/12	-
1	KCX	C	188	2,1	-	0/9/10/12	-

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	188	KCX	OQ1-CX-NZ	-3.21	119.99	124.96
1	I	188	KCX	OQ1-CX-NZ	-2.72	120.74	124.96
1	C	188	KCX	OQ1-CX-NZ	-2.70	120.77	124.96
1	O	188	KCX	OQ1-CX-NZ	-2.68	120.80	124.96
1	G	188	KCX	OQ1-CX-NZ	-2.64	120.87	124.96
1	E	188	KCX	OQ1-CX-NZ	-2.63	120.89	124.96
1	J	188	KCX	OQ1-CX-NZ	-2.59	120.94	124.96
1	M	188	KCX	OQ1-CX-NZ	-2.58	120.96	124.96
1	H	188	KCX	OQ1-CX-NZ	-2.55	121.01	124.96
1	B	188	KCX	OQ1-CX-NZ	-2.52	121.05	124.96
1	N	188	KCX	OQ1-CX-NZ	-2.51	121.06	124.96
1	L	188	KCX	OQ1-CX-NZ	-2.45	121.16	124.96
1	K	188	KCX	OQ1-CX-NZ	-2.43	121.19	124.96
1	F	188	KCX	OQ1-CX-NZ	-2.37	121.28	124.96
1	D	188	KCX	OQ1-CX-NZ	-2.31	121.37	124.96
1	P	188	KCX	OQ1-CX-NZ	-2.26	121.45	124.96

There are no chirality outliers.

All (5) 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	I	188	KCX	CG-CD-CE-NZ
1	G	188	KCX	CG-CD-CE-NZ
1	H	188	KCX	CG-CD-CE-NZ

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	O	188	KCX	1	0
1	C	188	KCX	1	0

5.5 Carbohydrates (i)

There are no monosaccharides 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	O	427	2	9,12,12	1.06	1 (11%)	9,18,18	1.06	0
3	LWY	L	427	2	9,12,12	1.06	1 (11%)	9,18,18	1.11	0
3	LWY	J	427	2	9,12,12	1.07	1 (11%)	9,18,18	1.02	0
3	LWY	H	427	2	9,12,12	1.08	1 (11%)	9,18,18	0.96	0
3	LWY	B	427	2	9,12,12	1.01	1 (11%)	9,18,18	1.18	0
3	LWY	G	427	2	9,12,12	1.09	1 (11%)	9,18,18	1.02	0
3	LWY	F	427	2	9,12,12	1.07	1 (11%)	9,18,18	1.00	0
3	LWY	M	427	2	9,12,12	1.07	1 (11%)	9,18,18	1.04	0
3	LWY	P	427	2	9,12,12	1.09	1 (11%)	9,18,18	0.89	0
3	LWY	K	427	2	9,12,12	1.07	1 (11%)	9,18,18	0.91	0
3	LWY	D	427	2	9,12,12	1.10	1 (11%)	9,18,18	0.96	0
3	LWY	A	427	2	9,12,12	1.06	1 (11%)	9,18,18	1.04	0
3	LWY	N	427	2	9,12,12	1.04	1 (11%)	9,18,18	1.01	0
3	LWY	C	427	2	9,12,12	1.06	1 (11%)	9,18,18	1.01	0
3	LWY	I	427	2	9,12,12	1.02	0	9,18,18	1.10	0
3	LWY	E	427	2	9,12,12	1.08	1 (11%)	9,18,18	1.00	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	O	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	J	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	B	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	F	427	2	-	0/4/20/20	0/1/1/1
3	LWY	M	427	2	-	0/4/20/20	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LWY	P	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	D	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	N	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	I	427	2	-	0/4/20/20	0/1/1/1
3	LWY	E	427	2	-	0/4/20/20	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	427	LWY	P-O2	-2.17	1.50	1.56
3	E	427	LWY	P-O2	-2.12	1.51	1.56
3	F	427	LWY	P-O2	-2.12	1.51	1.56
3	G	427	LWY	P-O2	-2.11	1.51	1.56
3	A	427	LWY	P-O2	-2.09	1.51	1.56
3	H	427	LWY	P-O2	-2.09	1.51	1.56
3	B	427	LWY	P-O2	-2.08	1.51	1.56
3	J	427	LWY	P-O2	-2.08	1.51	1.56
3	O	427	LWY	P-O2	-2.07	1.51	1.56
3	M	427	LWY	P-O2	-2.06	1.51	1.56
3	L	427	LWY	P-O2	-2.05	1.51	1.56
3	K	427	LWY	P-O2	-2.03	1.51	1.56
3	D	427	LWY	P-O2	-2.03	1.51	1.56
3	C	427	LWY	P-O2	-2.02	1.51	1.56
3	N	427	LWY	P-O2	-2.01	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	L	427	LWY	1	0
3	J	427	LWY	1	0
3	M	427	LWY	1	0
3	A	427	LWY	2	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	-0.07	9 (2%)	62	52	50, 78, 119, 133	0
1	B	407/423 (96%)	-0.14	5 (1%)	79	73	32, 67, 107, 137	0
1	C	407/423 (96%)	0.04	16 (3%)	39	29	48, 73, 114, 142	0
1	D	407/423 (96%)	-0.22	3 (0%)	87	84	42, 63, 97, 154	0
1	E	407/423 (96%)	-0.04	12 (2%)	51	41	42, 70, 112, 142	0
1	F	407/423 (96%)	-0.04	9 (2%)	62	52	49, 73, 113, 134	0
1	G	407/423 (96%)	0.18	20 (4%)	29	20	48, 81, 118, 145	0
1	H	407/423 (96%)	-0.13	9 (2%)	62	52	39, 64, 107, 140	0
1	I	407/423 (96%)	0.39	42 (10%)	6	3	58, 94, 134, 150	0
1	J	407/423 (96%)	0.47	49 (12%)	4	2	64, 96, 140, 154	0
1	K	407/423 (96%)	0.43	35 (8%)	10	5	59, 99, 137, 153	0
1	L	407/423 (96%)	0.56	51 (12%)	3	2	67, 106, 136, 150	0
1	M	407/423 (96%)	0.38	40 (9%)	7	4	52, 96, 132, 155	0
1	N	407/423 (96%)	0.41	35 (8%)	10	5	51, 97, 134, 160	0
1	O	407/423 (96%)	0.19	24 (5%)	22	14	40, 86, 126, 154	0
1	P	407/423 (96%)	0.11	22 (5%)	25	17	45, 76, 121, 142	0
All	All	6512/6768 (96%)	0.16	381 (5%)	22	14	32, 82, 128, 160	0

All (381) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	18	VAL	8.4
1	M	289	PRO	7.2
1	J	44	ASN	6.5
1	N	45	ALA	6.2
1	J	45	ALA	6.2

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Mol	Chain	Res	Type	RSRZ
1	E	44	ASN	6.2
1	M	297	SER	6.1
1	C	287	MET	6.0
1	P	289	PRO	5.9
1	O	44	ASN	5.9
1	K	292	VAL	5.8
1	I	153	CYS	5.4
1	G	153	CYS	5.4
1	M	298	VAL	5.2
1	J	392	GLU	5.1
1	J	27	ILE	5.1
1	N	44	ASN	5.0
1	I	40	VAL	5.0
1	M	196	ALA	5.0
1	D	154	SER	4.9
1	P	147	GLY	4.9
1	I	287	MET	4.8
1	J	25	VAL	4.7
1	J	398	TYR	4.7
1	H	286	GLY	4.7
1	J	41	ASP	4.6
1	I	286	GLY	4.6
1	L	45	ALA	4.6
1	M	44	ASN	4.5
1	J	24	HIS	4.5
1	K	45	ALA	4.5
1	C	288	PRO	4.4
1	M	285	PHE	4.4
1	J	35	VAL	4.4
1	N	55	VAL	4.4
1	K	44	ASN	4.4
1	I	41	ASP	4.3
1	H	285	PHE	4.3
1	M	394	ALA	4.2
1	J	395	ARG	4.2
1	C	290	GLU	4.2
1	K	287	MET	4.2
1	G	392	GLU	4.1
1	P	153	CYS	4.1
1	E	153	CYS	4.1
1	J	3	ILE	4.1
1	M	45	ALA	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	41	ASP	4.0
1	L	153	CYS	4.0
1	J	40	VAL	4.0
1	M	40	VAL	4.0
1	L	44	ASN	4.0
1	A	44	ASN	4.0
1	F	286	GLY	3.9
1	J	47	ALA	3.9
1	C	153	CYS	3.9
1	N	385	ASP	3.9
1	I	2	THR	3.9
1	N	6	LEU	3.8
1	K	286	GLY	3.8
1	O	147	GLY	3.8
1	I	12	LEU	3.8
1	K	16	ARG	3.8
1	I	27	ILE	3.8
1	M	291	SER	3.8
1	I	39	PRO	3.7
1	E	40	VAL	3.7
1	J	23	HIS	3.7
1	L	392	GLU	3.7
1	L	62	CYS	3.7
1	E	39	PRO	3.7
1	L	148	ASP	3.7
1	F	290	GLU	3.6
1	I	154	SER	3.6
1	I	283	ALA	3.6
1	I	48	ILE	3.6
1	C	289	PRO	3.6
1	M	288	PRO	3.6
1	N	148	ASP	3.6
1	I	408	ARG	3.6
1	C	292	VAL	3.6
1	H	292	VAL	3.6
1	P	292	VAL	3.6
1	I	24	HIS	3.6
1	L	279	ALA	3.5
1	K	198	PRO	3.5
1	E	41	ASP	3.5
1	C	392	GLU	3.5
1	N	289	PRO	3.5

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Mol	Chain	Res	Type	RSRZ
1	G	287	MET	3.5
1	E	154	SER	3.5
1	N	41	ASP	3.5
1	L	43	PRO	3.5
1	K	291	SER	3.4
1	N	292	VAL	3.4
1	J	46	GLN	3.4
1	K	3	ILE	3.4
1	O	285	PHE	3.4
1	H	282	GLY	3.3
1	K	314	VAL	3.3
1	N	307	GLU	3.3
1	J	153	CYS	3.3
1	O	6	LEU	3.3
1	M	370	GLY	3.3
1	J	285	PHE	3.3
1	P	154	SER	3.3
1	P	408	ARG	3.3
1	L	27	ILE	3.3
1	G	289	PRO	3.3
1	J	7	GLN	3.3
1	H	153	CYS	3.3
1	N	298	VAL	3.2
1	O	153	CYS	3.2
1	C	285	PHE	3.2
1	I	289	PRO	3.2
1	N	24	HIS	3.2
1	C	283	ALA	3.2
1	L	296	ALA	3.2
1	M	292	VAL	3.2
1	J	29	GLY	3.2
1	M	286	GLY	3.2
1	O	41	ASP	3.2
1	I	35	VAL	3.2
1	I	340	VAL	3.2
1	I	291	SER	3.2
1	I	292	VAL	3.1
1	K	6	LEU	3.1
1	O	298	VAL	3.1
1	C	286	GLY	3.1
1	C	393	GLY	3.1
1	J	380	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	H	154	SER	3.1
1	L	42	LEU	3.1
1	N	344	LEU	3.1
1	O	27	ILE	3.1
1	L	400	LEU	3.1
1	J	42	LEU	3.1
1	B	44	ASN	3.1
1	P	285	PHE	3.1
1	O	297	SER	3.1
1	J	6	LEU	3.1
1	L	154	SER	3.1
1	P	293	ALA	3.1
1	F	154	SER	3.1
1	L	147	GLY	3.1
1	G	295	VAL	3.1
1	I	25	VAL	3.1
1	M	157	PHE	3.0
1	N	253	VAL	3.0
1	D	153	CYS	3.0
1	N	405	LEU	3.0
1	P	281	HIS	3.0
1	G	35	VAL	3.0
1	G	38	ARG	3.0
1	K	290	GLU	3.0
1	L	398	TYR	3.0
1	N	154	SER	3.0
1	G	51	ARG	2.9
1	I	50	VAL	2.9
1	K	255	GLU	2.9
1	C	320	SER	2.9
1	N	3	ILE	2.9
1	F	153	CYS	2.9
1	J	39	PRO	2.9
1	M	37	ASP	2.9
1	N	379	ASP	2.9
1	L	4	THR	2.9
1	B	40	VAL	2.9
1	I	45	ALA	2.9
1	M	43	PRO	2.9
1	I	295	VAL	2.9
1	N	279	ALA	2.9
1	O	24	HIS	2.9

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Mol	Chain	Res	Type	RSRZ
1	J	48	ILE	2.9
1	C	297	SER	2.9
1	E	157	PHE	2.9
1	I	285	PHE	2.9
1	N	304	GLU	2.9
1	K	295	VAL	2.9
1	K	4	THR	2.8
1	K	282	GLY	2.8
1	M	294	LYS	2.8
1	I	260	LEU	2.8
1	J	36	THR	2.8
1	L	61	ASP	2.8
1	K	149	LEU	2.8
1	I	151	GLU	2.8
1	L	51	ARG	2.8
1	O	39	PRO	2.8
1	J	50	VAL	2.8
1	M	147	GLY	2.8
1	F	148	ASP	2.8
1	I	152	PRO	2.8
1	K	197	SER	2.8
1	G	292	VAL	2.8
1	L	16	ARG	2.8
1	L	18	VAL	2.8
1	M	278	LEU	2.8
1	K	283	ALA	2.8
1	O	45	ALA	2.8
1	E	3	ILE	2.7
1	L	314	VAL	2.7
1	J	52	GLY	2.7
1	M	290	GLU	2.7
1	J	30	GLU	2.7
1	E	45	ALA	2.7
1	C	282	GLY	2.7
1	L	6	LEU	2.7
1	N	18	VAL	2.7
1	I	290	GLU	2.7
1	L	304	GLU	2.7
1	N	54	THR	2.7
1	M	295	VAL	2.7
1	I	293	ALA	2.7
1	N	26	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	L	403	GLY	2.7
1	F	62	CYS	2.7
1	P	286	GLY	2.7
1	M	277	ALA	2.7
1	A	292	VAL	2.6
1	J	4	THR	2.6
1	O	4	THR	2.6
1	E	152	PRO	2.6
1	L	295	VAL	2.6
1	O	282	GLY	2.6
1	L	25	VAL	2.6
1	I	150	LEU	2.6
1	L	14	LEU	2.6
1	A	286	GLY	2.6
1	J	254	ASP	2.6
1	M	395	ARG	2.6
1	I	3	ILE	2.6
1	M	16	ARG	2.6
1	K	46	GLN	2.6
1	P	409	GLN	2.6
1	A	282	GLY	2.6
1	N	155	CYS	2.6
1	L	259	LYS	2.6
1	M	287	MET	2.6
1	J	8	GLY	2.6
1	L	319	GLY	2.6
1	G	369	VAL	2.6
1	L	5	VAL	2.6
1	M	220	GLU	2.6
1	I	38	ARG	2.6
1	I	51	ARG	2.5
1	K	150	LEU	2.5
1	C	154	SER	2.5
1	O	2	THR	2.5
1	J	369	VAL	2.5
1	M	148	ASP	2.5
1	P	392	GLU	2.5
1	H	147	GLY	2.5
1	I	297	SER	2.5
1	J	49	ASP	2.5
1	L	344	LEU	2.5
1	P	283	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	K	260	LEU	2.5
1	P	43	PRO	2.5
1	K	312	ALA	2.5
1	N	303	ARG	2.4
1	J	393	GLY	2.4
1	M	154	SER	2.4
1	N	40	VAL	2.4
1	K	281	HIS	2.4
1	J	157	PHE	2.4
1	K	293	ALA	2.4
1	G	290	GLU	2.4
1	O	151	GLU	2.4
1	J	32	ILE	2.4
1	A	152	PRO	2.4
1	K	288	PRO	2.4
1	A	153	CYS	2.4
1	D	151	GLU	2.4
1	A	285	PHE	2.4
1	N	152	PRO	2.4
1	P	282	GLY	2.4
1	H	289	PRO	2.4
1	O	152	PRO	2.4
1	L	24	HIS	2.4
1	M	62	CYS	2.4
1	M	38	ARG	2.4
1	J	151	GLU	2.4
1	P	295	VAL	2.4
1	K	41	ASP	2.4
1	L	3	ILE	2.4
1	P	44	ASN	2.3
1	L	380	GLY	2.3
1	J	26	VAL	2.3
1	J	51	ARG	2.3
1	L	29	GLY	2.3
1	L	64	VAL	2.3
1	J	255	GLU	2.3
1	N	341	LEU	2.3
1	N	395	ARG	2.3
1	J	148	ASP	2.3
1	J	400	LEU	2.3
1	G	16	ARG	2.3
1	O	35	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	P	152	PRO	2.3
1	I	53	LYS	2.3
1	P	319	GLY	2.3
1	J	381	ASN	2.2
1	L	320	SER	2.2
1	G	286	GLY	2.2
1	K	10	ASN	2.2
1	O	295	VAL	2.2
1	L	22	HIS	2.2
1	L	36	THR	2.2
1	M	20	LEU	2.2
1	L	35	VAL	2.2
1	O	26	VAL	2.2
1	G	254	ASP	2.2
1	M	254	ASP	2.2
1	F	282	GLY	2.2
1	L	263	GLU	2.2
1	M	41	ASP	2.2
1	E	48	ILE	2.2
1	N	408	ARG	2.2
1	L	11	VAL	2.2
1	L	292	VAL	2.2
1	L	37	ASP	2.2
1	L	335	ARG	2.2
1	N	272	LEU	2.2
1	K	154	SER	2.2
1	L	157	PHE	2.2
1	K	11	VAL	2.2
1	N	367	ILE	2.2
1	B	2	THR	2.2
1	I	288	PRO	2.2
1	L	280	LYS	2.2
1	I	47	ALA	2.2
1	F	288	PRO	2.2
1	M	2	THR	2.2
1	N	36	THR	2.2
1	M	33	VAL	2.2
1	L	20	LEU	2.1
1	N	20	LEU	2.1
1	G	63	HIS	2.1
1	A	295	VAL	2.1
1	B	393	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	O	384	GLU	2.1
1	L	284	GLU	2.1
1	M	46	GLN	2.1
1	G	282	GLY	2.1
1	G	319	GLY	2.1
1	K	320	SER	2.1
1	I	4	THR	2.1
1	G	105	ASP	2.1
1	J	28	ASP	2.1
1	A	289	PRO	2.1
1	G	297	SER	2.1
1	I	298	VAL	2.1
1	J	290	GLU	2.1
1	K	48	ILE	2.1
1	J	377	VAL	2.1
1	K	5	VAL	2.1
1	M	50	VAL	2.1
1	J	379	ASP	2.1
1	M	388	VAL	2.1
1	O	43	PRO	2.1
1	P	317	GLY	2.1
1	E	35	VAL	2.1
1	K	356	GLU	2.1
1	M	325	GLU	2.0
1	G	64	VAL	2.0
1	I	11	VAL	2.0
1	J	311	ASN	2.0
1	P	46	GLN	2.0
1	P	297	SER	2.0
1	I	398	TYR	2.0
1	N	147	GLY	2.0
1	C	295	VAL	2.0
1	O	40	VAL	2.0
1	J	289	PRO	2.0
1	H	295	VAL	2.0
1	O	46	GLN	2.0
1	I	147	GLY	2.0
1	L	283	ALA	2.0
1	L	369	VAL	2.0
1	F	44	ASN	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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	KCX	C	188	12/13	0.93	0.26	48,63,78,85	0
1	KCX	H	188	12/13	0.94	0.21	51,59,94,107	0
1	KCX	L	188	12/13	0.94	0.26	76,91,120,127	0
1	KCX	D	188	12/13	0.95	0.18	48,54,72,82	0
1	KCX	B	188	12/13	0.95	0.19	41,46,88,89	0
1	KCX	K	188	12/13	0.95	0.25	75,89,99,100	0
1	KCX	A	188	12/13	0.95	0.18	64,77,107,111	0
1	KCX	O	188	12/13	0.95	0.14	41,61,79,94	0
1	KCX	J	188	12/13	0.96	0.19	62,79,108,108	0
1	KCX	N	188	12/13	0.96	0.18	68,78,133,140	0
1	KCX	I	188	12/13	0.96	0.15	61,74,110,111	0
1	KCX	F	188	12/13	0.97	0.23	52,61,115,124	0
1	KCX	M	188	12/13	0.97	0.15	67,75,92,103	0
1	KCX	G	188	12/13	0.97	0.21	55,64,92,97	0
1	KCX	E	188	12/13	0.97	0.14	48,52,78,86	0
1	KCX	P	188	12/13	0.97	0.19	52,64,90,93	0

6.3 Carbohydrates ⓘ

There are no monosaccharides 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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ZN	K	425	1/1	0.92	0.15	125,125,125,125	0
2	ZN	M	425	1/1	0.93	0.10	114,114,114,114	0
3	LWY	K	427	12/12	0.95	0.23	127,133,135,135	0
3	LWY	L	427	12/12	0.95	0.15	101,111,114,115	0
3	LWY	G	427	12/12	0.96	0.20	85,91,95,97	0
2	ZN	M	426	1/1	0.96	0.10	103,103,103,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	LWY	C	427	12/12	0.96	0.20	89,94,98,100	0
3	LWY	M	427	12/12	0.96	0.21	103,113,116,116	0
3	LWY	B	427	12/12	0.97	0.13	73,77,81,83	0
2	ZN	C	425	1/1	0.97	0.17	90,90,90,90	0
2	ZN	K	426	1/1	0.97	0.09	110,110,110,110	0
2	ZN	E	426	1/1	0.97	0.12	84,84,84,84	0
2	ZN	H	425	1/1	0.97	0.14	89,89,89,89	0
3	LWY	A	427	12/12	0.97	0.16	95,103,107,108	0
3	LWY	O	427	12/12	0.97	0.14	81,90,93,95	0
2	ZN	O	425	1/1	0.98	0.12	92,92,92,92	0
2	ZN	P	426	1/1	0.98	0.12	94,94,94,94	0
2	ZN	I	426	1/1	0.98	0.07	115,115,115,115	0
2	ZN	J	425	1/1	0.98	0.14	102,102,102,102	0
2	ZN	J	426	1/1	0.98	0.13	101,101,101,101	0
3	LWY	D	427	12/12	0.98	0.16	63,71,80,81	0
3	LWY	E	427	12/12	0.98	0.17	81,88,90,90	0
3	LWY	F	427	12/12	0.98	0.16	97,98,101,106	0
2	ZN	A	425	1/1	0.98	0.10	86,86,86,86	0
3	LWY	H	427	12/12	0.98	0.14	77,81,88,88	0
3	LWY	I	427	12/12	0.98	0.14	102,106,112,113	0
3	LWY	J	427	12/12	0.98	0.15	90,105,106,107	0
2	ZN	D	425	1/1	0.98	0.16	73,73,73,73	0
2	ZN	L	425	1/1	0.98	0.15	102,102,102,102	0
2	ZN	A	426	1/1	0.98	0.10	99,99,99,99	0
3	LWY	N	427	12/12	0.98	0.19	109,111,112,115	0
2	ZN	B	426	1/1	0.98	0.10	84,84,84,84	0
3	LWY	P	427	12/12	0.98	0.13	74,87,89,92	0
2	ZN	G	426	1/1	0.99	0.15	95,95,95,95	0
2	ZN	L	426	1/1	0.99	0.10	108,108,108,108	0
2	ZN	B	425	1/1	0.99	0.12	78,78,78,78	0
2	ZN	H	426	1/1	0.99	0.12	92,92,92,92	0
2	ZN	N	426	1/1	0.99	0.11	95,95,95,95	0
2	ZN	I	425	1/1	0.99	0.08	100,100,100,100	0
2	ZN	P	425	1/1	0.99	0.13	87,87,87,87	0
2	ZN	D	426	1/1	0.99	0.11	72,72,72,72	0
2	ZN	E	425	1/1	0.99	0.16	79,79,79,79	0
2	ZN	C	426	1/1	0.99	0.16	91,91,91,91	0
2	ZN	F	425	1/1	0.99	0.17	96,96,96,96	0
2	ZN	G	425	1/1	0.99	0.15	84,84,84,84	0
2	ZN	F	426	1/1	1.00	0.16	89,89,89,89	0
2	ZN	N	425	1/1	1.00	0.12	90,90,90,90	0
2	ZN	O	426	1/1	1.00	0.13	93,93,93,93	0

6.5 Other polymers ⓘ

There are no such residues in this entry.