



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 08:35 AM GMT

PDB ID : 3N2C
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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

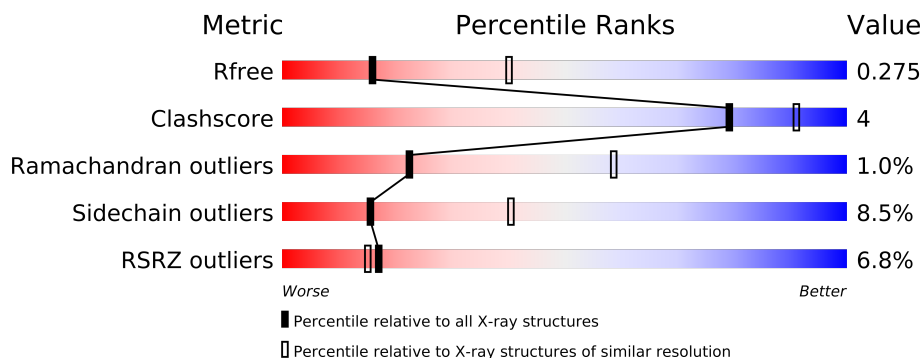
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	1963 (2.84-2.80)
Clashscore	79885	2478 (2.84-2.80)
Ramachandran outliers	78287	2429 (2.84-2.80)
Sidechain outliers	78261	2431 (2.84-2.80)
RSRZ outliers	66119	1966 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	423	
1	B	423	
1	C	423	
1	D	423	
1	E	423	
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	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
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 hydrogen and 0 are deuterium.

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.

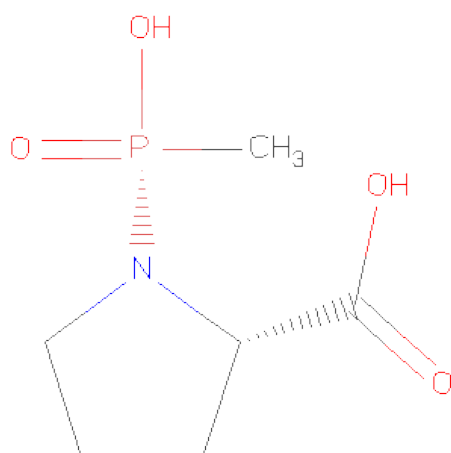
- Molecule 1 is a protein called PROLIDASE.

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	P	2	Total 2	Zn 2	0	0
2	G	2	Total 2	Zn 2	0	0
2	J	2	Total 2	Zn 2	0	0
2	D	2	Total 2	Zn 2	0	0
2	K	2	Total 2	Zn 2	0	0
2	E	2	Total 2	Zn 2	0	0
2	H	2	Total 2	Zn 2	0	0
2	B	2	Total 2	Zn 2	0	0
2	I	2	Total 2	Zn 2	0	0
2	C	2	Total 2	Zn 2	0	0
2	A	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	L	2	Total 2	Zn 2	0	0
2	F	2	Total 2	Zn 2	0	0
2	M	2	Total 2	Zn 2	0	0

- Molecule 3 is 1-[(R)-HYDROXY(METHYL)PHOSPHORYL]-L-PROLINE (three-letter code: 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		

Continued on next page...

Continued from previous page...

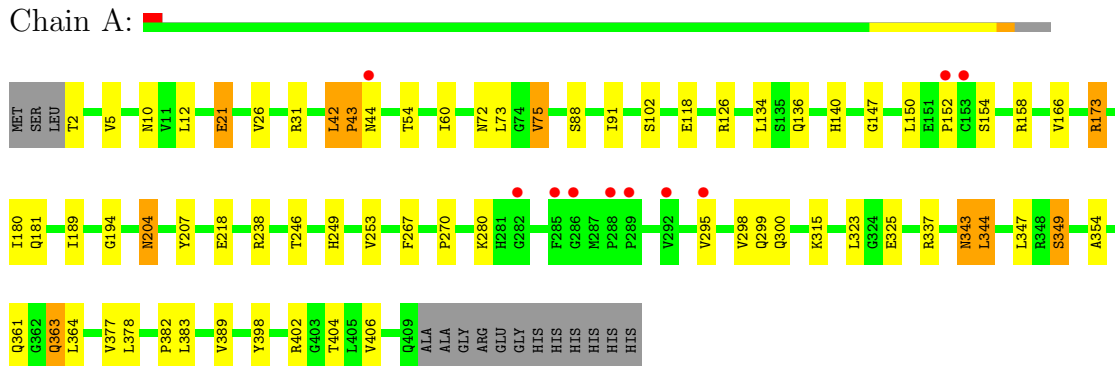
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	O	1	Total	C	N	O	P	0	0
			12	6	1	4	1		
3	P	1	Total	C	N	O	P	0	0
			12	6	1	4	1		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

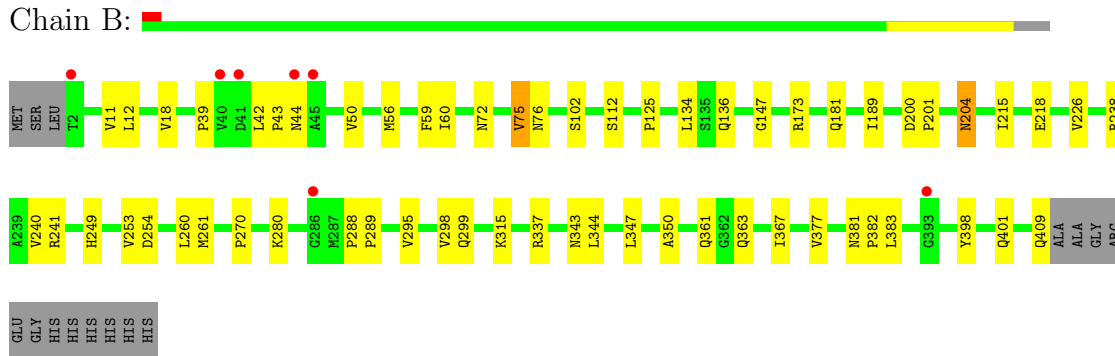
• Molecule 1: PROLIDASE

Chain A:



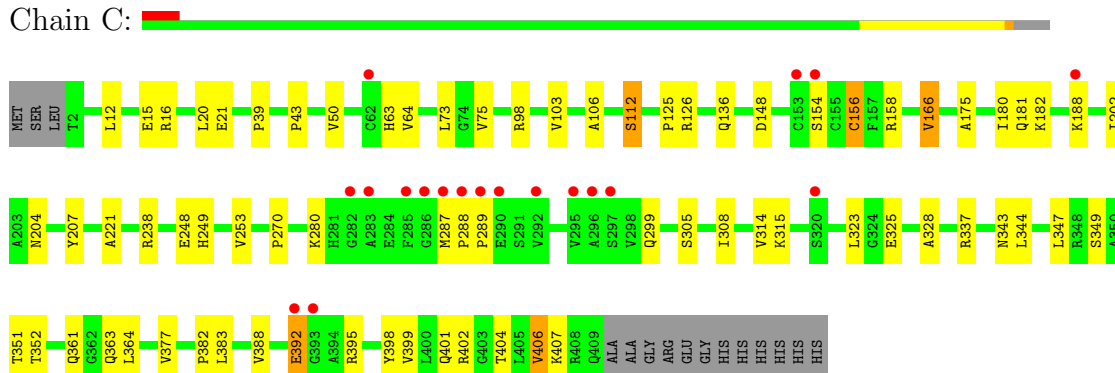
• Molecule 1: PROLIDASE

Chain B:



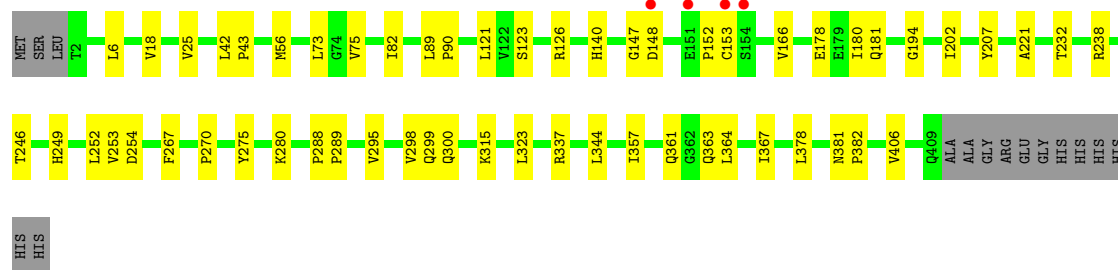
• Molecule 1: PROLIDASE

Chain C:



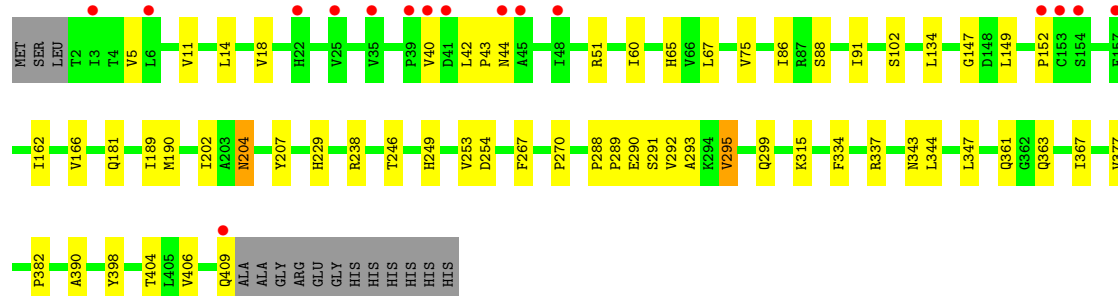
- Molecule 1: PROLIDASE

Chain D:



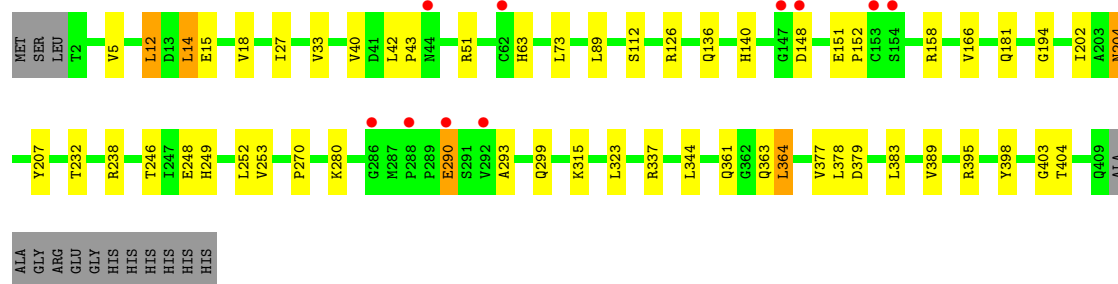
- Molecule 1: PROLIDASE

Chain E:



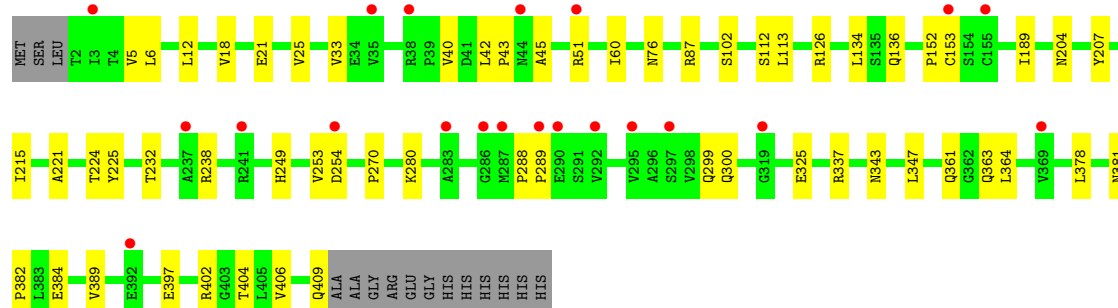
- Molecule 1: PROLIDASE

Chain F:



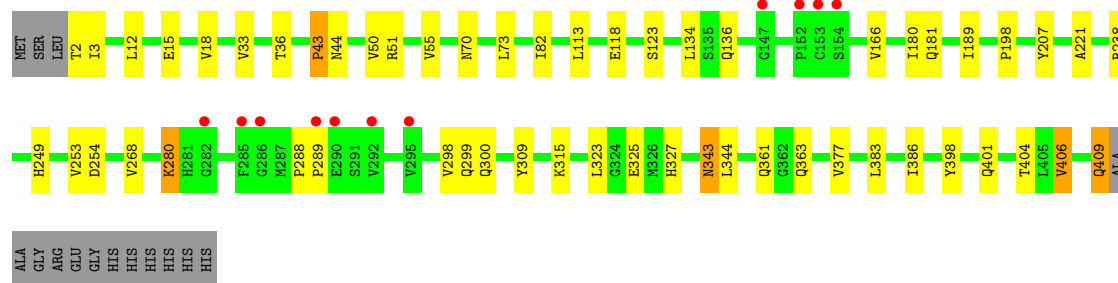
- Molecule 1: PROLIDASE

Chain G:



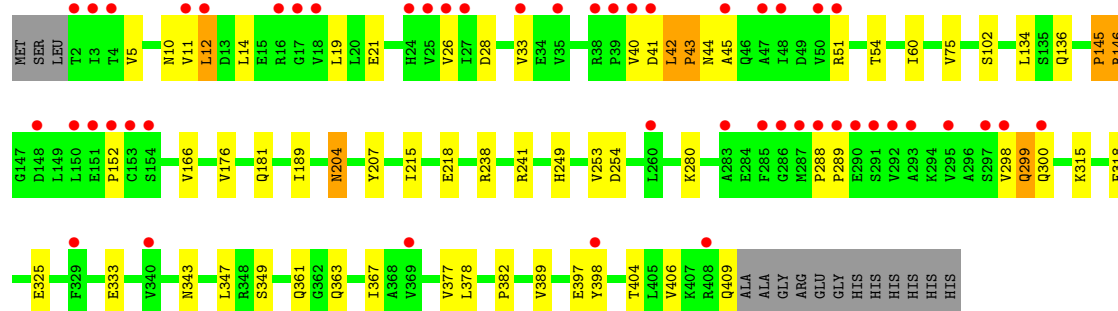
- Molecule 1: PROLIDASE

Chain H:



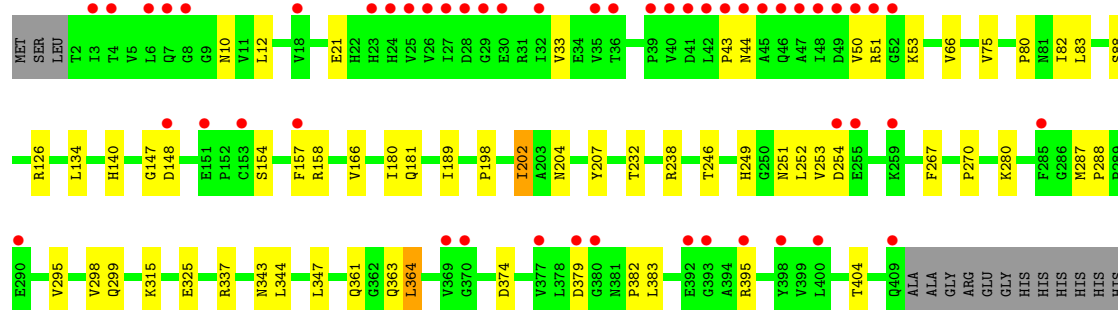
- Molecule 1: PROLIDASE

Chain I:



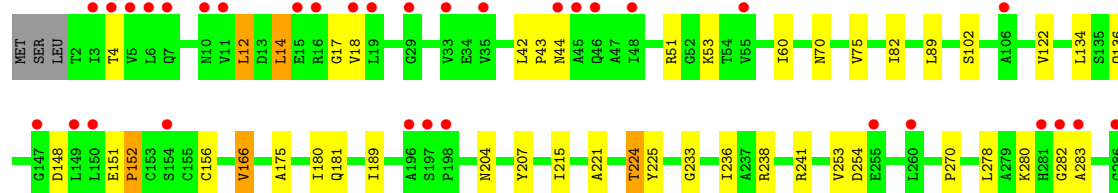
- Molecule 1: PROLIDASE

Chain J:



- Molecule 1: PROLIDASE

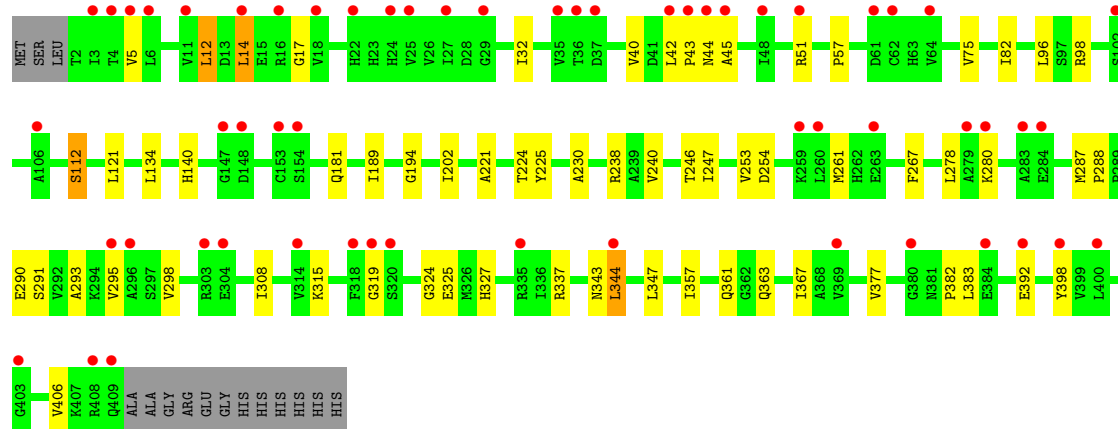
Chain K:





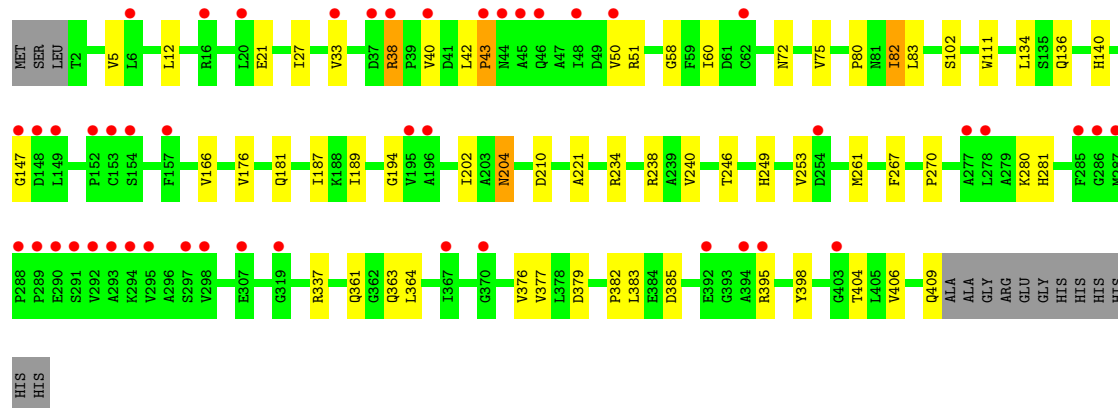
• Molecule 1: PROLIDASE

Chain L:



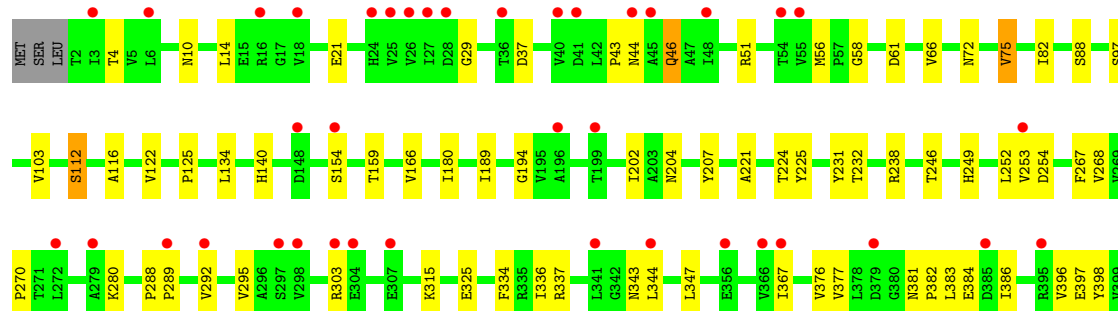
• Molecule 1: PROLIDASE

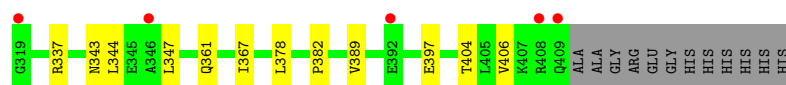
Chain M:



• Molecule 1: PROLIDASE

Chain N:





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
$\langle I/\sigma(I) \rangle$ ¹	1.02 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.220 , 0.273 0.230 , 0.275	Depositor DCC
R_{free} test set	5054 reflections (3.11%)	DCC
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 , 38.6	EDS
Estimated twinning fraction	0.014 for -k,-h,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 167449 reflections	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.

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	0.35	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(°)	Ideal(°)
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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	12	0	10	0	0
3	E	12	0	10	0	0
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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

All (343) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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:H	1:A:343:ASN:ND2	1.50	0.97
1:K:278:LEU:HD22	1:K:287:MET:CE	2.01	0.89
1:A:343:ASN:H	1:A:343:ASN:HD22	1.07	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:N	1:A:343:ASN:HD22	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(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:K:60:ILE:HG12	1:K:102:SER:HB2	1.85	0.58
1:I:42:LEU:HB2	1:I:45:ALA:HB3	1.84	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:G:381:ASN:HD22	1:G:384:GLU:HG2	1.72	0.55
1:E:377:VAL:HB	1:E:398:TYR:HB2	1.88	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:G:378:LEU:HD21	1:G:389:VAL:HG22	1.90	0.54
1:B:204:ASN:HB2	1:H:221:ALA:O	2.08	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:O:4:THR:HG23	1:O:46:GLN:HB3	1.91	0.53
1:B:173:ARG:HG2	1:B:218:GLU:HG3	1.89	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
1:N:154:SER:HB3	1:P:150:LEU:HD21	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:O:347:LEU:HD11	1:O:382:PRO:HB2	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: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:C:98:ARG:HD3	1:C:392:GLU:HG2	1.93	0.49
1:B:134:LEU:HB2	1:B:189:ILE:HG22	1.94	0.49
1:K:134:LEU:HB2	1:K:189:ILE:HG22	1.92	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:A:134:LEU:HB2	1:A:189:ILE:HG22	1.94	0.49
1:K:288:PRO:O	1:K:291:SER:HB2	2.11	0.49
1:B:11:VAL:HG13	1:B:367:ILE:HD12	1.93	0.49
1:K:377:VAL:HB	1:K:398:TYR:HB2	1.94	0.49
1:B:241:ARG:HG3	1:B:260:LEU:HD21	1.95	0.49
1:I:134:LEU:HB2	1:I:189:ILE:HG22	1.94	0.49
1:F:73:LEU:HD21	1:F:323:LEU:HD22	1.95	0.49
1:K:12:LEU:HD22	1:K:14:LEU:HG	1.95	0.49
1:N:56:MET:HA	1:N:367:ILE:HD11	1.95	0.48
1:M:60:ILE:HG12	1:M:102:SER:HB2	1.94	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: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:O:356:GLU:HA	1:O:361:GLN:HG2	1.95	0.48
1:B:60:ILE:HA	1:B:102:SER:O	2.13	0.48
1:O:59:PHE:HB3	1:O:350:ALA:HB1	1.94	0.48
1:J:379:ASP:HB3	1:J:395:ARG:HB3	1.96	0.48
1:L:134:LEU:HB2	1:L:189:ILE:HG22	1.96	0.48
1:H:134:LEU:HB2	1:H:189:ILE:HG22	1.96	0.48
1:J:246:THR:HG22	1:J:267:PHE:HB2	1.95	0.48
1:P:60:ILE:HG12	1:P:102:SER:HB2	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:M:82:ILE:HG23	1:N:112:SER:HB2	1.96	0.48
1:I:378:LEU:HD21	1:I:389:VAL:HG22	1.96	0.48
1:K:287:MET:HB2	1:K:287:MET:HE2	1.40	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:A:60:ILE:HG12	1:A:102:SER:HB2	1.95	0.47
1:N:125:PRO:HA	1:N:401:GLN:HE22	1.79	0.47
1:I:377:VAL:HB	1:I:398:TYR:HB2	1.96	0.47
1:A:140:HIS:NE2	3:A:427:LWY:O1	2.47	0.47
1:J:126:ARG:HH11	1:J:364:LEU:HD11	1.80	0.47
1:F:379:ASP:HB3	1:F:395:ARG:HB3	1.96	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: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:D:73:LEU:HD21	1:D:323:LEU:HD22	1.97	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:G:60:ILE:HG12	1:G:102:SER:HB2	1.96	0.47
1:D:178:GLU:HG2	1:E:149:LEU:HD13	1.96	0.47
1:C:106:ALA:HB1	1:C:188:KCX:HZ	1.79	0.47
1:O:31:ARG:HH22	1:O:363:GLN:HG3	1.80	0.47
1:K:166:VAL:HG11	1:K:175:ALA:HB2	1.97	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:D:221:ALA:O	1:E:204:ASN:HB2	2.15	0.47
1:B:240:VAL:HG21	1:B:261:MET:HG2	1.98	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:L:5:VAL:HG11	1:L:40:VAL:HG21	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: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:E:288:PRO:HA	1:E:289:PRO:HD3	1.75	0.46
1:A:88:SER:HA	1:A:91:ILE:HD12	1.97	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:M:221:ALA:O	1:P:204:ASN:HB2	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:12:LEU:HD22	1:F:14:LEU:HG	1.98	0.46
1:L:278:LEU:HD22	1:L:287:MET:CE	2.45	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:L:377:VAL:HB	1:L:398:TYR:HB2	1.97	0.46
1:D:89:LEU:HB2	1:D:90:PRO:HD3	1.98	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:L:240:VAL:HG21	1:L:261:MET:HG2	1.98	0.45
1:C:112:SER:HB2	1:H:82:ILE:HB	1.97	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:E:5:VAL:HG11	1:E:40:VAL:HG21	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:P:80:PRO:HB2	1:P:83:LEU:HB2	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:E:86:ILE:HD12	1:F:89:LEU:HD11	1.98	0.45
1:B:72:ASN:HB3	1:B:75:VAL:HG12	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:N:246:THR:HG22	1:N:267:PHE:HB2	2.00	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:G:381:ASN:HA	1:G:382:PRO:HD2	1.82	0.44
1:A:344:LEU:CD2	1:A:344:LEU:O	2.66	0.44
1:G:126:ARG:HH11	1:G:364:LEU:HD21	1.82	0.44
1:E:292:VAL:O	1:E:295:VAL:HG12	2.17	0.44
1:H:50:VAL:O	1:H:50:VAL:HG12	2.17	0.44
1:N:72:ASN:HB3	1:N:75:VAL:HG12	2.00	0.44
1:A:140:HIS:CE1	1:A:194:GLY:HA3	2.52	0.44
1:P:154:SER:HA	1:P:157:PHE:HB2	1.99	0.44
1:J:287:MET:HA	1:J:288:PRO:HD2	1.81	0.44
1:N:61:ASP:HB3	1:N:103:VAL:HG12	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:M:379:ASP:HB3	1:M:395:ARG:HB3	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:I:5:VAL:HG22	1:I:26:VAL:HA	1.99	0.43
1:A:126:ARG:HH11	1:A:364:LEU:HD21	1.83	0.43
1:D:82:ILE:HG21	1:G:113:LEU:HG	2.00	0.43
1:O:246:THR:HG22	1:O:267:PHE:HB2	2.00	0.43
1:C:63:HIS:ND1	1:C:248:GLU:OE1	2.50	0.43
1:I:42:LEU:HA	1:I:43:PRO:HD3	1.78	0.43
1:B:60:ILE:HG12	1:B:102:SER:HB2	2.00	0.43
1:A:349:SER:O	1:A:354:ALA:HB2	2.18	0.43
1:M:80:PRO:HB2	1:M:83:LEU:HB2	2.01	0.43
1:O:59:PHE:HB2	1:O:100:PHE:CD1	2.53	0.43
1:H:280:LYS:HB2	1:H:280:LYS:HE3	1.93	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:O:176:VAL:HG13	1:O:187:ILE:HG13	2.01	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: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:J:154:SER:HA	1:J:157:PHE:HB2	2.00	0.43
1:A:73:LEU:HD21	1:A:323:LEU:HD22	2.01	0.43
1:L:57:PRO:HG3	1:L:367:ILE:HG13	2.01	0.43
1:C:288:PRO:HA	1:C:289:PRO:HD3	1.83	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:L:288:PRO:HG2	1:L:291:SER:OG	2.19	0.43
1:L:140:HIS:CE1	1:L:194:GLY:HA3	2.54	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:D:299:GLN:HG3	1:D:300:GLN:HE21	1.84	0.43
1:L:278:LEU:CD1	1:L:287:MET:HE1	2.39	0.43
1:K:282:GLY:O	1:K:287:MET:HB3	2.19	0.43
1:F:290:GLU:O	1:F:293:ALA:HB3	2.19	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:N:97:SER:HA	1:N:407:LYS:HG3	2.00	0.42
1:C:73:LEU:HD21	1:C:323:LEU:HD22	2.01	0.42
1:N:232:THR:HA	1:N:252:LEU:HB2	2.01	0.42
1:F:126:ARG:HH11	1:F:364:LEU:HD11	1.84	0.42
1:N:270:PRO:O	1:N:337:ARG:NH2	2.53	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:A:299:GLN:HG3	1:A:300:GLN:HE21	1.84	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:M:111:TRP:CD2	1:P:146:ARG:HG2	2.55	0.42
1:D:232:THR:HA	1:D:252:LEU:HB2	2.02	0.42
1:N:194:GLY:HA2	1:N:231:TYR:HE2	1.85	0.42
1:H:299:GLN:HG3	1:H:300:GLN:HE21	1.83	0.42
1:A:10:ASN:HA	1:A:21:GLU:HA	2.01	0.42
1:N:303:ARG:HH21	1:N:336:ILE:HG12	1.85	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: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:I:11:VAL:HG13	1:I:367:ILE:HD12	2.01	0.42
1:M:5:VAL:HG21	1:M:40:VAL:HG21	2.01	0.42
1:D:140:HIS:CE1	1:D:194:GLY:HA3	2.55	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: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:H:113:LEU:HD23	1:H:113:LEU:HA	1.94	0.41
1:O:125:PRO:HA	1:O:401:GLN:HE22	1.84	0.41
1:N:334:PHE:HB3	1:N:386:ILE:HD11	2.02	0.41
1:L:290:GLU:O	1:L:293:ALA:HB3	2.20	0.41
1:B:270:PRO:O	1:B:337:ARG:NH2	2.52	0.41
1:B:200:ASP:HA	1:B:201:PRO:HD3	1.89	0.41
1:G:397:GLU:HA	1:G:409:GLN:HB2	2.02	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:D:246:THR:HG21	1:D:357:ILE:HG23	2.03	0.41
1:L:32:ILE:HD13	1:L:367:ILE:HG23	2.03	0.41
1:C:287:MET:HA	1:C:288:PRO:HD2	1.89	0.41
1:E:190:MET:HA	1:E:229:HIS:HB3	2.01	0.41
1:L:221:ALA:O	1:M:204:ASN:HB2	2.20	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: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:L:324:GLY:O	1:L:327:HIS:ND1	2.48	0.41
1:I:145:PRO:HB2	1:I:146:ARG:H	1.67	0.41
1:N:66:VAL:HG12	1:N:88:SER:HB2	2.03	0.41
1:L:96:LEU:HD21	1:L:406:VAL:HG11	2.02	0.41
1:M:38:ARG:H	1:M:38:ARG:HG2	1.62	0.41
1:C:401:GLN:HB2	1:C:406:VAL:HG21	2.03	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:B:288:PRO:HA	1:B:289:PRO:HD3	1.88	0.41
1:K:151:GLU:HA	1:K:152:PRO:HD3	1.94	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:378:LEU:HD21	1:K:389:VAL:HG22	2.02	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:C:154:SER:O	1:C:158:ARG:HG2	2.21	0.41
1:K:89:LEU:HD22	1:K:122:VAL:HG11	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:I:288:PRO:HA	1:I:289:PRO:HD3	1.77	0.41
1:G:6:LEU:HB2	1:G:25:VAL:HB	2.03	0.41
1:A:5:VAL:HG22	1:A:26:VAL:HG13	2.01	0.41
1:J:53:LYS:HB2	1:J:53:LYS:HE3	1.83	0.41
1:I:60:ILE:HG12	1:I:102:SER:HB2	2.03	0.41
1:L:12:LEU:HD22	1:L:14:LEU:HG	2.03	0.41
1:K:288:PRO:HA	1:K:289:PRO:HD3	1.89	0.41
1:I:40:VAL:HG13	1:I:42:LEU:HD22	2.02	0.41
1:B:215:ILE:HG22	1:B:226:VAL:HG21	2.02	0.41
1:A:154:SER:O	1:A:158:ARG:HG2	2.21	0.41
1:L:246:THR:HG21	1:L:357:ILE:HG23	2.02	0.41
1:D:126:ARG:HH11	1:D:364:LEU:HD21	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:A:72:ASN:HB3	1:A:75:VAL:HG12	2.02	0.41
1:C:126:ARG:HH11	1:C:364:LEU:HD21	1.86	0.41
1:O:359:ASN:HD22	1:O:361:GLN:HE21	1.67	0.41
1:C:125:PRO:HA	1:C:401:GLN:HE22	1.86	0.41
1:C:166:VAL:HG11	1:C:175:ALA: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:F:232:THR:HA	1:F:252:LEU:HB2	2.03	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:M:72:ASN:HB3	1:M:75:VAL:HG12	2.03	0.40
1:D:381:ASN:HA	1:D:382:PRO:HD2	1.90	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:C:64:VAL:HG21	1:C:103:VAL:HB	2.03	0.40
1:E:290:GLU:O	1:E:293:ALA:HB3	2.20	0.40
1:A:270:PRO:HD2	1:A:337:ARG:HH22	1.86	0.40
1:I:176:VAL:HG11	1:I:218:GLU:HB3	2.04	0.40
1:M:140:HIS:CE1	1:M:194:GLY:HA3	2.56	0.40
1:K:283:ALA:HB2	1:K:292:VAL:HG21	2.03	0.40
1:A:42:LEU:HA	1:A:43:PRO:HD3	1.86	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%)	19 53

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	405/423 (96%)	381 (94%)	20 (5%)	4 (1%)	22	59
1	C	405/423 (96%)	380 (94%)	21 (5%)	4 (1%)	22	59
1	D	405/423 (96%)	379 (94%)	21 (5%)	5 (1%)	19	53
1	E	405/423 (96%)	380 (94%)	20 (5%)	5 (1%)	19	53
1	F	405/423 (96%)	379 (94%)	23 (6%)	3 (1%)	30	68
1	G	405/423 (96%)	375 (93%)	26 (6%)	4 (1%)	22	59
1	H	405/423 (96%)	383 (95%)	18 (4%)	4 (1%)	22	59
1	I	405/423 (96%)	377 (93%)	23 (6%)	5 (1%)	19	53
1	J	405/423 (96%)	374 (92%)	26 (6%)	5 (1%)	19	53
1	K	405/423 (96%)	378 (93%)	24 (6%)	3 (1%)	30	68
1	L	405/423 (96%)	377 (93%)	27 (7%)	1 (0%)	56	88
1	M	405/423 (96%)	383 (95%)	19 (5%)	3 (1%)	30	68
1	N	405/423 (96%)	371 (92%)	30 (7%)	4 (1%)	22	59
1	O	405/423 (96%)	375 (93%)	27 (7%)	3 (1%)	30	68
1	P	405/423 (96%)	375 (93%)	25 (6%)	5 (1%)	19	53
All	All	6480/6768 (96%)	6052 (93%)	365 (6%)	63 (1%)	22	59

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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%)	14	38
1	B	314/325 (97%)	289 (92%)	25 (8%)	17	44
1	C	314/325 (97%)	283 (90%)	31 (10%)	11	31
1	D	314/325 (97%)	294 (94%)	20 (6%)	25	57
1	E	314/325 (97%)	290 (92%)	24 (8%)	19	46
1	F	314/325 (97%)	287 (91%)	27 (9%)	15	40
1	G	314/325 (97%)	293 (93%)	21 (7%)	23	55
1	H	314/325 (97%)	283 (90%)	31 (10%)	11	31
1	I	314/325 (97%)	285 (91%)	29 (9%)	13	36
1	J	314/325 (97%)	286 (91%)	28 (9%)	14	38
1	K	314/325 (97%)	282 (90%)	32 (10%)	11	29
1	L	314/325 (97%)	291 (93%)	23 (7%)	20	49
1	M	314/325 (97%)	288 (92%)	26 (8%)	16	42
1	N	314/325 (97%)	286 (91%)	28 (9%)	14	38
1	O	314/325 (97%)	288 (92%)	26 (8%)	16	42
1	P	314/325 (97%)	284 (90%)	30 (10%)	12	33
All	All	5024/5200 (97%)	4595 (92%)	429 (8%)	15	40

All (429) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	12	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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

Some 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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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 chains 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	A	188	1,2	11,11,12	5.43	2 (18%)	10,12,14	1.74	3 (30%)
1	KCX	B	188	1,2	11,11,12	5.25	2 (18%)	10,12,14	1.64	4 (40%)
1	KCX	C	188	1,2	11,11,12	5.48	2 (18%)	10,12,14	1.40	2 (20%)
1	KCX	D	188	1,2	11,11,12	5.36	2 (18%)	10,12,14	1.26	2 (20%)
1	KCX	E	188	1,2	11,11,12	5.26	2 (18%)	10,12,14	1.53	4 (40%)
1	KCX	F	188	1,2	11,11,12	5.42	2 (18%)	10,12,14	1.55	4 (40%)
1	KCX	G	188	1,2	11,11,12	5.36	2 (18%)	10,12,14	1.33	2 (20%)
1	KCX	H	188	1,2	11,11,12	5.41	2 (18%)	10,12,14	1.41	3 (30%)
1	KCX	I	188	1,2	11,11,12	5.47	2 (18%)	10,12,14	1.52	3 (30%)
1	KCX	J	188	1,2	11,11,12	5.45	2 (18%)	10,12,14	1.42	3 (30%)
1	KCX	K	188	1,2	11,11,12	5.26	2 (18%)	10,12,14	1.50	3 (30%)
1	KCX	L	188	1,2	11,11,12	5.43	2 (18%)	10,12,14	1.35	3 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	KCX	M	188	1,2	11,11,12	5.41	2 (18%)	10,12,14	1.41	2 (20%)
1	KCX	N	188	1,2	11,11,12	5.29	2 (18%)	10,12,14	1.52	4 (40%)
1	KCX	O	188	1,2	11,11,12	5.41	2 (18%)	10,12,14	1.48	3 (30%)
1	KCX	P	188	1,2	11,11,12	5.51	2 (18%)	10,12,14	1.75	4 (40%)

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	A	188	1,2	-	0/8/10/12	0/0/0/0
1	KCX	B	188	1,2	-	0/8/10/12	0/0/0/0
1	KCX	C	188	1,2	-	0/8/10/12	0/0/0/0
1	KCX	D	188	1,2	-	0/8/10/12	0/0/0/0
1	KCX	E	188	1,2	-	0/8/10/12	0/0/0/0
1	KCX	F	188	1,2	-	0/8/10/12	0/0/0/0
1	KCX	G	188	1,2	-	0/8/10/12	0/0/0/0
1	KCX	H	188	1,2	-	0/8/10/12	0/0/0/0
1	KCX	I	188	1,2	-	0/8/10/12	0/0/0/0
1	KCX	J	188	1,2	-	0/8/10/12	0/0/0/0
1	KCX	K	188	1,2	-	0/8/10/12	0/0/0/0
1	KCX	L	188	1,2	-	0/8/10/12	0/0/0/0
1	KCX	M	188	1,2	-	0/8/10/12	0/0/0/0
1	KCX	N	188	1,2	-	0/8/10/12	0/0/0/0
1	KCX	O	188	1,2	-	0/8/10/12	0/0/0/0
1	KCX	P	188	1,2	-	0/8/10/12	0/0/0/0

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	188	KCX	O-C	17.97	1.23	1.11
1	C	188	KCX	O-C	17.81	1.23	1.11
1	I	188	KCX	O-C	17.76	1.23	1.11
1	A	188	KCX	O-C	17.70	1.23	1.11
1	J	188	KCX	O-C	17.65	1.23	1.11
1	F	188	KCX	O-C	17.63	1.23	1.11
1	O	188	KCX	O-C	17.63	1.23	1.11
1	L	188	KCX	O-C	17.61	1.23	1.11
1	H	188	KCX	O-C	17.59	1.23	1.11
1	M	188	KCX	O-C	17.51	1.23	1.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	188	KCX	O-C	17.46	1.23	1.11
1	G	188	KCX	O-C	17.41	1.23	1.11
1	K	188	KCX	O-C	17.14	1.23	1.11
1	N	188	KCX	O-C	17.14	1.23	1.11
1	E	188	KCX	O-C	17.10	1.23	1.11
1	B	188	KCX	O-C	17.10	1.23	1.11
1	M	188	KCX	CA-C	2.94	1.53	1.48
1	C	188	KCX	CA-C	2.92	1.53	1.48
1	J	188	KCX	CA-C	2.91	1.53	1.48
1	I	188	KCX	CA-C	2.86	1.53	1.48
1	L	188	KCX	CA-C	2.79	1.53	1.48
1	N	188	KCX	CA-C	2.68	1.53	1.48
1	P	188	KCX	CA-C	2.66	1.53	1.48
1	H	188	KCX	CA-C	2.55	1.53	1.48
1	G	188	KCX	CA-C	2.53	1.53	1.48
1	F	188	KCX	CA-C	2.49	1.52	1.48
1	A	188	KCX	CA-C	2.47	1.52	1.48
1	E	188	KCX	CA-C	2.46	1.52	1.48
1	K	188	KCX	CA-C	2.42	1.52	1.48
1	B	188	KCX	CA-C	2.36	1.52	1.48
1	O	188	KCX	CA-C	2.35	1.52	1.48
1	D	188	KCX	CA-C	2.29	1.52	1.48

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	188	KCX	C-CA-N	-3.76	110.07	113.83
1	A	188	KCX	OQ1-CX-NZ	-2.98	119.99	124.94
1	A	188	KCX	OQ2-CX-NZ	2.97	120.03	116.33
1	B	188	KCX	C-CA-N	-2.86	110.97	113.83
1	K	188	KCX	C-CA-N	-2.85	110.98	113.83
1	F	188	KCX	C-CA-N	-2.81	111.02	113.83
1	A	188	KCX	C-CA-N	-2.75	111.08	113.83
1	N	188	KCX	C-CA-N	-2.66	111.17	113.83
1	O	188	KCX	C-CA-N	-2.66	111.17	113.83
1	B	188	KCX	OQ2-CX-NZ	2.64	119.61	116.33
1	I	188	KCX	C-CA-N	-2.58	111.26	113.83
1	E	188	KCX	OQ2-CX-NZ	2.56	119.52	116.33
1	I	188	KCX	OQ1-CX-NZ	-2.53	120.74	124.94
1	C	188	KCX	OQ1-CX-NZ	-2.51	120.77	124.94
1	H	188	KCX	OQ2-CX-NZ	2.50	119.45	116.33
1	O	188	KCX	OQ1-CX-NZ	-2.49	120.80	124.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	188	KCX	OQ1-CX-NZ	-2.45	120.87	124.94
1	E	188	KCX	OQ1-CX-NZ	-2.44	120.89	124.94
1	L	188	KCX	OQ2-CX-NZ	2.42	119.34	116.33
1	I	188	KCX	OQ2-CX-NZ	2.41	119.33	116.33
1	J	188	KCX	OQ1-CX-NZ	-2.40	120.94	124.94
1	P	188	KCX	OQ2-CX-NZ	2.40	119.31	116.33
1	M	188	KCX	OQ1-CX-NZ	-2.39	120.96	124.94
1	C	188	KCX	OQ2-CX-NZ	2.37	119.28	116.33
1	N	188	KCX	OQ2-CX-NZ	2.36	119.27	116.33
1	H	188	KCX	OQ1-CX-NZ	-2.36	121.01	124.94
1	M	188	KCX	OQ2-CX-NZ	2.36	119.27	116.33
1	P	188	KCX	OQ2-CX-OQ1	-2.35	119.23	122.17
1	B	188	KCX	OQ1-CX-NZ	-2.34	121.05	124.94
1	E	188	KCX	C-CA-N	-2.34	111.49	113.83
1	F	188	KCX	OQ2-CX-NZ	2.33	119.24	116.33
1	N	188	KCX	OQ1-CX-NZ	-2.33	121.06	124.94
1	J	188	KCX	OQ2-CX-NZ	2.27	119.16	116.33
1	L	188	KCX	OQ1-CX-NZ	-2.27	121.16	124.94
1	J	188	KCX	C-CA-N	-2.27	111.56	113.83
1	B	188	KCX	OQ2-CX-OQ1	-2.27	119.34	122.17
1	K	188	KCX	OQ1-CX-NZ	-2.25	121.19	124.94
1	G	188	KCX	OQ2-CX-NZ	2.22	119.09	116.33
1	F	188	KCX	OQ1-CX-NZ	-2.20	121.28	124.94
1	F	188	KCX	OQ2-CX-OQ1	-2.15	119.48	122.17
1	D	188	KCX	OQ1-CX-NZ	-2.14	121.37	124.94
1	L	188	KCX	OQ2-CX-OQ1	-2.14	119.49	122.17
1	K	188	KCX	OQ2-CX-NZ	2.14	118.99	116.33
1	O	188	KCX	OQ2-CX-NZ	2.14	118.99	116.33
1	H	188	KCX	OQ2-CX-OQ1	-2.11	119.54	122.17
1	P	188	KCX	OQ1-CX-NZ	-2.10	121.45	124.94
1	E	188	KCX	OQ2-CX-OQ1	-2.07	119.58	122.17
1	D	188	KCX	OQ2-CX-NZ	2.05	118.88	116.33
1	N	188	KCX	OQ2-CX-OQ1	-2.00	119.67	122.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	A	427	2	12,12,12	1.62	4 (33%)	18,18,18	1.19	1 (5%)
3	LWY	B	427	2	12,12,12	1.73	4 (33%)	18,18,18	1.13	1 (5%)
3	LWY	C	427	2	12,12,12	1.66	3 (25%)	18,18,18	1.14	1 (5%)
3	LWY	D	427	2	12,12,12	1.64	3 (25%)	18,18,18	1.12	2 (11%)
3	LWY	E	427	2	12,12,12	1.69	4 (33%)	18,18,18	1.06	0
3	LWY	F	427	2	12,12,12	1.67	4 (33%)	18,18,18	1.09	0
3	LWY	G	427	2	12,12,12	1.64	4 (33%)	18,18,18	1.11	1 (5%)
3	LWY	H	427	2	12,12,12	1.58	4 (33%)	18,18,18	1.07	1 (5%)
3	LWY	I	427	2	12,12,12	1.69	3 (25%)	18,18,18	1.20	2 (11%)
3	LWY	J	427	2	12,12,12	1.66	4 (33%)	18,18,18	1.17	3 (16%)
3	LWY	K	427	2	12,12,12	1.61	3 (25%)	18,18,18	1.03	0
3	LWY	L	427	2	12,12,12	1.74	3 (25%)	18,18,18	1.20	2 (11%)
3	LWY	M	427	2	12,12,12	1.65	4 (33%)	18,18,18	1.14	2 (11%)
3	LWY	N	427	2	12,12,12	1.64	3 (25%)	18,18,18	1.17	2 (11%)
3	LWY	O	427	2	12,12,12	1.72	4 (33%)	18,18,18	1.13	0
3	LWY	P	427	2	12,12,12	1.67	4 (33%)	18,18,18	0.97	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	A	427	2	-	0/6/20/20	0/1/1/1
3	LWY	B	427	2	-	0/6/20/20	0/1/1/1
3	LWY	C	427	2	-	0/6/20/20	0/1/1/1
3	LWY	D	427	2	-	0/6/20/20	0/1/1/1
3	LWY	E	427	2	-	0/6/20/20	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LWY	F	427	2	-	0/6/20/20	0/1/1/1
3	LWY	G	427	2	-	0/6/20/20	0/1/1/1
3	LWY	H	427	2	-	0/6/20/20	0/1/1/1
3	LWY	I	427	2	-	0/6/20/20	0/1/1/1
3	LWY	J	427	2	-	0/6/20/20	0/1/1/1
3	LWY	K	427	2	-	0/6/20/20	0/1/1/1
3	LWY	L	427	2	-	0/6/20/20	0/1/1/1
3	LWY	M	427	2	-	0/6/20/20	0/1/1/1
3	LWY	N	427	2	-	0/6/20/20	0/1/1/1
3	LWY	O	427	2	-	0/6/20/20	0/1/1/1
3	LWY	P	427	2	-	0/6/20/20	0/1/1/1

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	427	LWY	P-N	3.75	1.69	1.63
3	B	427	LWY	P-N	3.74	1.69	1.63
3	O	427	LWY	P-N	3.63	1.68	1.63
3	I	427	LWY	P-N	3.52	1.68	1.63
3	E	427	LWY	P-N	3.36	1.68	1.63
3	F	427	LWY	P-N	3.34	1.68	1.63
3	N	427	LWY	P-N	3.30	1.68	1.63
3	J	427	LWY	P-N	3.29	1.68	1.63
3	P	427	LWY	P-N	3.26	1.68	1.63
3	C	427	LWY	P-N	3.24	1.68	1.63
3	M	427	LWY	P-N	3.11	1.68	1.63
3	D	427	LWY	P-N	3.09	1.68	1.63
3	G	427	LWY	P-N	2.93	1.67	1.63
3	K	427	LWY	P-N	2.89	1.67	1.63
3	A	427	LWY	P-N	2.87	1.67	1.63
3	G	427	LWY	P-O1	2.83	1.61	1.48
3	E	427	LWY	P-O1	2.83	1.61	1.48
3	O	427	LWY	P-O1	2.82	1.61	1.48
3	H	427	LWY	P-N	2.81	1.67	1.63
3	P	427	LWY	P-O1	2.81	1.61	1.48
3	B	427	LWY	P-O1	2.80	1.61	1.48
3	K	427	LWY	P-O1	2.79	1.61	1.48
3	M	427	LWY	P-O1	2.77	1.61	1.48
3	C	427	LWY	P-O1	2.76	1.61	1.48
3	D	427	LWY	P-O1	2.76	1.61	1.48
3	H	427	LWY	P-O1	2.74	1.61	1.48
3	F	427	LWY	P-O1	2.74	1.61	1.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	427	LWY	P-O1	2.72	1.61	1.48
3	L	427	LWY	P-O1	2.72	1.61	1.48
3	A	427	LWY	P-O1	2.71	1.60	1.48
3	J	427	LWY	P-O1	2.71	1.60	1.48
3	I	427	LWY	P-O1	2.70	1.60	1.48
3	A	427	LWY	P-C1	-2.68	1.71	1.79
3	I	427	LWY	P-C1	-2.59	1.71	1.79
3	C	427	LWY	P-C1	-2.56	1.71	1.79
3	M	427	LWY	P-C1	-2.53	1.71	1.79
3	G	427	LWY	P-C1	-2.53	1.71	1.79
3	J	427	LWY	P-C1	-2.50	1.72	1.79
3	K	427	LWY	P-C1	-2.50	1.72	1.79
3	D	427	LWY	P-C1	-2.48	1.72	1.79
3	F	427	LWY	P-C1	-2.48	1.72	1.79
3	L	427	LWY	P-C1	-2.48	1.72	1.79
3	E	427	LWY	P-C1	-2.47	1.72	1.79
3	B	427	LWY	P-C1	-2.47	1.72	1.79
3	P	427	LWY	P-C1	-2.43	1.72	1.79
3	N	427	LWY	P-C1	-2.42	1.72	1.79
3	H	427	LWY	P-C1	-2.42	1.72	1.79
3	O	427	LWY	P-C1	-2.41	1.72	1.79
3	P	427	LWY	P-O2	-2.12	1.50	1.56
3	F	427	LWY	P-O2	-2.07	1.51	1.56
3	E	427	LWY	P-O2	-2.07	1.51	1.56
3	G	427	LWY	P-O2	-2.06	1.51	1.56
3	A	427	LWY	P-O2	-2.04	1.51	1.56
3	H	427	LWY	P-O2	-2.04	1.51	1.56
3	J	427	LWY	P-O2	-2.03	1.51	1.56
3	B	427	LWY	P-O2	-2.03	1.51	1.56
3	O	427	LWY	P-O2	-2.02	1.51	1.56
3	M	427	LWY	P-O2	-2.01	1.51	1.56

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	427	LWY	O2-P-N	2.44	109.10	105.31
3	D	427	LWY	O1-P-C1	-2.33	105.76	112.49
3	I	427	LWY	O1-P-C1	-2.29	105.89	112.49
3	N	427	LWY	O2-P-N	2.28	108.85	105.31
3	J	427	LWY	O2-P-N	2.27	108.83	105.31
3	H	427	LWY	CD-N-CA	2.25	114.48	109.24
3	I	427	LWY	O2-P-N	2.25	108.81	105.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	427	LWY	CD-N-CA	2.22	114.40	109.24
3	C	427	LWY	CD-N-CA	2.18	114.32	109.24
3	D	427	LWY	CD-N-CA	2.16	114.27	109.24
3	M	427	LWY	O1-P-C1	-2.11	106.41	112.49
3	G	427	LWY	CD-N-CA	2.10	114.12	109.24
3	J	427	LWY	O1-P-C1	-2.09	106.46	112.49
3	M	427	LWY	CD-N-CA	2.06	114.03	109.24
3	N	427	LWY	O1-P-C1	-2.05	106.56	112.49
3	B	427	LWY	O1-P-C1	-2.05	106.56	112.49
3	J	427	LWY	CD-N-CA	2.04	113.98	109.24
3	L	427	LWY	O1-P-C1	-2.01	106.68	112.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	408/423 (96%)	-0.01	10 (2%) 54 55	50, 78, 119, 133	0
1	B	408/423 (96%)	-0.11	7 (1%) 67 67	32, 67, 107, 137	0
1	C	408/423 (96%)	0.10	19 (4%) 30 30	48, 73, 114, 142	0
1	D	408/423 (96%)	-0.21	4 (0%) 79 80	42, 63, 97, 154	0
1	E	408/423 (96%)	-0.01	16 (3%) 37 37	42, 70, 112, 142	0
1	F	408/423 (96%)	-0.01	10 (2%) 54 55	49, 73, 113, 134	0
1	G	408/423 (96%)	0.23	21 (5%) 27 27	48, 81, 118, 145	0
1	H	408/423 (96%)	-0.12	11 (2%) 52 53	39, 64, 107, 140	0
1	I	408/423 (96%)	0.40	49 (12%) 5 4	58, 94, 134, 150	0
1	J	408/423 (96%)	0.52	51 (12%) 5 4	64, 96, 140, 154	0
1	K	408/423 (96%)	0.52	45 (11%) 6 5	59, 99, 137, 153	0
1	L	408/423 (96%)	0.62	57 (13%) 3 3	67, 106, 136, 150	0
1	M	408/423 (96%)	0.47	47 (11%) 5 4	52, 96, 132, 155	0
1	N	408/423 (96%)	0.46	41 (10%) 8 6	51, 97, 134, 160	0
1	O	408/423 (96%)	0.24	30 (7%) 14 12	40, 86, 126, 154	0
1	P	408/423 (96%)	0.14	25 (6%) 21 20	45, 76, 121, 142	0
All	All	6528/6768 (96%)	0.20	443 (6%) 17 15	32, 82, 128, 160	0

All (443) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	18	VAL	8.2
1	M	289	PRO	7.8
1	J	44	ASN	7.1
1	J	45	ALA	6.7
1	K	292	VAL	6.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	N	45	ALA	6.5
1	O	44	ASN	6.5
1	E	44	ASN	6.4
1	C	287	MET	6.1
1	M	298	VAL	6.1
1	J	398	TYR	6.0
1	M	196	ALA	5.4
1	N	55	VAL	5.2
1	J	27	ILE	5.2
1	L	45	ALA	5.2
1	J	35	VAL	5.1
1	I	40	VAL	5.1
1	P	147	GLY	5.0
1	G	153	CYS	5.0
1	D	154	SER	5.0
1	N	44	ASN	4.9
1	H	285	PHE	4.9
1	P	289	PRO	4.8
1	K	45	ALA	4.8
1	J	3	ILE	4.8
1	I	287	MET	4.7
1	K	287	MET	4.7
1	J	25	VAL	4.7
1	A	44	ASN	4.6
1	M	297	SER	4.6
1	I	286	GLY	4.6
1	K	286	GLY	4.6
1	M	44	ASN	4.6
1	C	153	CYS	4.5
1	L	153	CYS	4.5
1	J	47	ALA	4.5
1	L	44	ASN	4.5
1	M	40	VAL	4.5
1	J	41	ASP	4.5
1	I	2	THR	4.4
1	I	153	CYS	4.4
1	M	394	ALA	4.4
1	N	148	ASP	4.4
1	G	392	GLU	4.3
1	K	16	ARG	4.2
1	L	62	CYS	4.2
1	I	41	ASP	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	39	PRO	4.1
1	K	6	LEU	4.1
1	J	392	GLU	4.1
1	M	288	PRO	4.1
1	I	27	ILE	4.1
1	M	285	PHE	4.1
1	M	295	VAL	4.0
1	B	40	VAL	4.0
1	H	286	GLY	4.0
1	N	6	LEU	4.0
1	K	44	ASN	4.0
1	C	288	PRO	4.0
1	B	44	ASN	3.9
1	J	395	ARG	3.9
1	K	291	SER	3.9
1	P	292	VAL	3.9
1	I	408	ARG	3.9
1	C	292	VAL	3.9
1	M	45	ALA	3.9
1	I	12	LEU	3.8
1	L	400	LEU	3.8
1	I	39	PRO	3.8
1	E	153	CYS	3.8
1	C	290	GLU	3.8
1	F	286	GLY	3.8
1	J	40	VAL	3.8
1	K	198	PRO	3.7
1	J	24	HIS	3.7
1	J	46	GLN	3.7
1	K	314	VAL	3.7
1	B	41	ASP	3.7
1	E	41	ASP	3.6
1	C	392	GLU	3.6
1	J	48	ILE	3.6
1	L	392	GLU	3.6
1	P	285	PHE	3.5
1	I	283	ALA	3.5
1	L	51	ARG	3.5
1	L	43	PRO	3.5
1	K	3	ILE	3.5
1	L	148	ASP	3.5
1	I	48	ILE	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	O	27	ILE	3.5
1	G	295	VAL	3.5
1	G	287	MET	3.5
1	O	6	LEU	3.5
1	I	154	SER	3.4
1	M	43	PRO	3.4
1	C	285	PHE	3.4
1	C	320	SER	3.4
1	H	153	CYS	3.4
1	J	6	LEU	3.4
1	E	40	VAL	3.4
1	I	35	VAL	3.4
1	O	147	GLY	3.4
1	L	61	ASP	3.4
1	L	319	GLY	3.3
1	N	18	VAL	3.3
1	L	279	ALA	3.3
1	N	26	VAL	3.3
1	N	292	VAL	3.3
1	N	307	GLU	3.3
1	J	380	GLY	3.3
1	N	379	ASP	3.3
1	P	283	ALA	3.3
1	P	293	ALA	3.3
1	M	290	GLU	3.3
1	G	51	ARG	3.3
1	P	408	ARG	3.3
1	N	298	VAL	3.3
1	F	290	GLU	3.3
1	G	289	PRO	3.2
1	G	35	VAL	3.2
1	O	298	VAL	3.2
1	C	283	ALA	3.2
1	F	153	CYS	3.2
1	M	286	GLY	3.2
1	E	154	SER	3.2
1	J	7	GLN	3.2
1	I	285	PHE	3.2
1	J	153	CYS	3.2
1	I	340	VAL	3.2
1	M	148	ASP	3.2
1	O	45	ALA	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	N	3	ILE	3.2
1	L	314	VAL	3.2
1	I	152	PRO	3.1
1	I	25	VAL	3.1
1	N	41	ASP	3.1
1	P	154	SER	3.1
1	M	278	LEU	3.1
1	N	289	PRO	3.1
1	L	25	VAL	3.1
1	H	292	VAL	3.1
1	C	393	GLY	3.1
1	P	286	GLY	3.1
1	I	24	HIS	3.1
1	L	27	ILE	3.1
1	C	289	PRO	3.1
1	K	312	ALA	3.1
1	L	296	ALA	3.1
1	O	35	VAL	3.1
1	G	38	ARG	3.0
1	L	147	GLY	3.0
1	N	344	LEU	3.0
1	K	255	GLU	3.0
1	K	283	ALA	3.0
1	L	16	ARG	3.0
1	N	367	ILE	3.0
1	A	292	VAL	3.0
1	J	148	ASP	3.0
1	M	292	VAL	3.0
1	N	405	LEU	3.0
1	O	285	PHE	3.0
1	N	54	THR	3.0
1	L	154	SER	3.0
1	C	295	VAL	3.0
1	I	292	VAL	3.0
1	K	46	GLN	3.0
1	G	292	VAL	3.0
1	J	285	PHE	3.0
1	N	253	VAL	3.0
1	M	62	CYS	3.0
1	P	153	CYS	3.0
1	O	39	PRO	2.9
1	E	157	PHE	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	O	153	CYS	2.9
1	B	286	GLY	2.9
1	G	297	SER	2.9
1	I	151	GLU	2.9
1	J	39	PRO	2.9
1	N	385	ASP	2.9
1	L	14	LEU	2.9
1	L	398	TYR	2.9
1	M	291	SER	2.9
1	F	147	GLY	2.9
1	O	24	HIS	2.9
1	I	150	LEU	2.9
1	K	149	LEU	2.9
1	G	286	GLY	2.9
1	L	403	GLY	2.9
1	J	4	THR	2.9
1	M	38	ARG	2.9
1	J	369	VAL	2.9
1	K	154	SER	2.8
1	D	153	CYS	2.8
1	F	148	ASP	2.8
1	M	37	ASP	2.8
1	I	288	PRO	2.8
1	L	5	VAL	2.8
1	N	40	VAL	2.8
1	M	46	GLN	2.8
1	I	3	ILE	2.8
1	L	4	THR	2.8
1	A	288	PRO	2.8
1	L	295	VAL	2.8
1	J	151	GLU	2.8
1	P	392	GLU	2.8
1	I	38	ARG	2.8
1	F	44	ASN	2.8
1	I	291	SER	2.8
1	M	294	LYS	2.8
1	O	151	GLU	2.8
1	F	288	PRO	2.8
1	K	4	THR	2.8
1	J	29	GLY	2.8
1	M	370	GLY	2.8
1	E	45	ALA	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	L	304	GLU	2.7
1	K	5	VAL	2.7
1	O	297	SER	2.7
1	L	6	LEU	2.7
1	L	369	VAL	2.7
1	N	154	SER	2.7
1	J	43	PRO	2.7
1	I	293	ALA	2.7
1	J	52	GLY	2.7
1	E	48	ILE	2.7
1	J	32	ILE	2.7
1	K	288	PRO	2.7
1	I	16	ARG	2.7
1	C	297	SER	2.7
1	I	11	VAL	2.7
1	M	287	MET	2.7
1	N	303	ARG	2.7
1	P	281	HIS	2.7
1	J	42	LEU	2.7
1	K	11	VAL	2.7
1	M	147	GLY	2.7
1	I	45	ALA	2.7
1	L	35	VAL	2.7
1	F	154	SER	2.7
1	G	3	ILE	2.6
1	L	48	ILE	2.6
1	C	154	SER	2.6
1	O	41	ASP	2.6
1	K	150	LEU	2.6
1	M	16	ARG	2.6
1	I	18	VAL	2.6
1	J	393	GLY	2.6
1	B	393	GLY	2.6
1	C	282	GLY	2.6
1	O	282	GLY	2.6
1	G	369	VAL	2.6
1	I	295	VAL	2.6
1	N	304	GLU	2.6
1	O	4	THR	2.6
1	A	286	GLY	2.6
1	E	3	ILE	2.6
1	I	329	PHE	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	J	30	GLU	2.6
1	O	152	PRO	2.6
1	B	2	THR	2.6
1	N	24	HIS	2.6
1	A	285	PHE	2.6
1	N	279	ALA	2.5
1	N	16	ARG	2.5
1	A	295	VAL	2.5
1	I	290	GLU	2.5
1	K	290	GLU	2.5
1	P	295	VAL	2.5
1	H	282	GLY	2.5
1	M	20	LEU	2.5
1	A	153	CYS	2.5
1	N	395	ARG	2.5
1	G	44	ASN	2.5
1	J	50	VAL	2.5
1	I	289	PRO	2.5
1	L	24	HIS	2.5
1	L	18	VAL	2.5
1	L	64	VAL	2.5
1	M	395	ARG	2.5
1	G	290	GLU	2.5
1	K	293	ALA	2.5
1	M	293	ALA	2.5
1	K	10	ASN	2.5
1	J	18	VAL	2.5
1	I	260	LEU	2.5
1	I	47	ALA	2.5
1	P	44	ASN	2.5
1	K	281	HIS	2.5
1	D	151	GLU	2.5
1	M	157	PHE	2.4
1	M	254	ASP	2.4
1	L	320	SER	2.4
1	C	286	GLY	2.4
1	L	3	ILE	2.4
1	P	282	GLY	2.4
1	P	319	GLY	2.4
1	L	42	LEU	2.4
1	N	36	THR	2.4
1	E	35	VAL	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	J	23	HIS	2.4
1	K	398	TYR	2.4
1	P	297	SER	2.4
1	L	11	VAL	2.4
1	O	43	PRO	2.4
1	L	303	ARG	2.4
1	A	282	GLY	2.4
1	K	282	GLY	2.4
1	N	408	ARG	2.4
1	F	292	VAL	2.4
1	K	295	VAL	2.4
1	K	366	VAL	2.4
1	O	46	GLN	2.4
1	K	147	GLY	2.4
1	J	36	THR	2.4
1	K	197	SER	2.4
1	J	290	GLU	2.4
1	L	344	LEU	2.3
1	L	36	THR	2.3
1	O	2	THR	2.3
1	P	409	GLN	2.3
1	M	403	GLY	2.3
1	J	254	ASP	2.3
1	F	62	CYS	2.3
1	M	153	CYS	2.3
1	M	6	LEU	2.3
1	G	237	ALA	2.3
1	G	241	ARG	2.3
1	O	279	ALA	2.3
1	O	26	VAL	2.3
1	L	259	LYS	2.3
1	L	318	PHE	2.3
1	H	152	PRO	2.3
1	N	272	LEU	2.3
1	L	409	GLN	2.3
1	M	50	VAL	2.3
1	N	48	ILE	2.3
1	K	33	VAL	2.3
1	H	154	SER	2.3
1	L	280	LYS	2.3
1	L	106	ALA	2.3
1	N	199	THR	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	K	7	GLN	2.3
1	A	289	PRO	2.3
1	H	147	GLY	2.3
1	L	380	GLY	2.3
1	M	33	VAL	2.3
1	O	40	VAL	2.3
1	L	29	GLY	2.2
1	P	43	PRO	2.2
1	C	62	CYS	2.2
1	I	50	VAL	2.2
1	M	195	VAL	2.2
1	J	28	ASP	2.2
1	L	22	HIS	2.2
1	K	29	GLY	2.2
1	B	45	ALA	2.2
1	J	377	VAL	2.2
1	K	55	VAL	2.2
1	I	4	THR	2.2
1	M	152	PRO	2.2
1	I	26	VAL	2.2
1	J	259	LYS	2.2
1	J	400	LEU	2.2
1	L	37	ASP	2.2
1	P	317	GLY	2.2
1	I	33	VAL	2.2
1	N	341	LEU	2.2
1	I	369	VAL	2.2
1	H	295	VAL	2.2
1	K	106	ALA	2.2
1	L	335	ARG	2.2
1	O	155	CYS	2.2
1	L	263	GLU	2.2
1	I	17	GLY	2.2
1	M	48	ILE	2.2
1	L	102	SER	2.2
1	M	154	SER	2.2
1	A	152	PRO	2.2
1	I	298	VAL	2.2
1	M	277	ALA	2.2
1	M	392	GLU	2.2
1	J	370	GLY	2.2
1	M	319	GLY	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	J	26	VAL	2.1
1	N	25	VAL	2.1
1	J	379	ASP	2.1
1	I	300	GLN	2.1
1	N	356	GLU	2.1
1	E	152	PRO	2.1
1	J	8	GLY	2.1
1	O	157	PHE	2.1
1	O	224	THR	2.1
1	E	25	VAL	2.1
1	M	149	LEU	2.1
1	G	319	GLY	2.1
1	J	49	ASP	2.1
1	P	346	ALA	2.1
1	I	398	TYR	2.1
1	O	304	GLU	2.1
1	O	384	GLU	2.1
1	J	157	PHE	2.1
1	H	289	PRO	2.1
1	K	260	LEU	2.1
1	N	366	VAL	2.1
1	O	295	VAL	2.1
1	G	283	ALA	2.1
1	J	51	ARG	2.1
1	C	188	KCX	2.1
1	I	297	SER	2.1
1	P	38	ARG	2.1
1	L	284	GLU	2.1
1	M	367	ILE	2.1
1	J	409	GLN	2.1
1	N	297	SER	2.1
1	I	148	ASP	2.1
1	M	307	GLU	2.1
1	G	155	CYS	2.1
1	G	254	ASP	2.0
1	E	409	GLN	2.0
1	L	408	ARG	2.0
1	J	255	GLU	2.0
1	K	15	GLU	2.0
1	K	19	LEU	2.0
1	P	288	PRO	2.0
1	E	22	HIS	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	L	260	LEU	2.0
1	I	51	ARG	2.0
1	N	27	ILE	2.0
1	P	271	THR	2.0
1	K	356	GLU	2.0
1	L	384	GLU	2.0
1	O	398	TYR	2.0
1	D	148	ASP	2.0
1	N	28	ASP	2.0
1	K	35	VAL	2.0
1	P	152	PRO	2.0
1	H	290	GLU	2.0
1	K	48	ILE	2.0
1	C	296	ALA	2.0
1	K	196	ALA	2.0
1	L	283	ALA	2.0
1	N	196	ALA	2.0
1	E	6	LEU	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	KCX	C	188	12/13	0.26	0.73	48,63,78,85	0
1	KCX	K	188	12/13	0.25	0.53	75,89,99,100	0
1	KCX	H	188	12/13	0.21	0.40	51,59,94,107	0
1	KCX	L	188	12/13	0.24	0.32	76,91,120,127	0
1	KCX	B	188	12/13	0.17	0.32	41,46,88,89	0
1	KCX	A	188	12/13	0.20	0.00	64,77,107,111	0
1	KCX	J	188	12/13	0.19	-0.08	62,79,108,108	0
1	KCX	D	188	12/13	0.18	-0.27	48,54,72,82	0
1	KCX	N	188	12/13	0.17	-0.34	68,78,133,140	0
1	KCX	F	188	12/13	0.21	-0.58	52,61,115,124	0
1	KCX	P	188	12/13	0.18	-0.61	52,64,90,93	0
1	KCX	O	188	12/13	0.15	-1.03	41,61,79,94	0
1	KCX	G	188	12/13	0.20	-1.17	55,64,92,97	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	KCX	M	188	12/13	0.14	-1.36	67,75,92,103	0
1	KCX	E	188	12/13	0.14	-1.57	48,52,78,86	0
1	KCX	I	188	12/13	0.15	-1.74	61,74,110,111	0

6.3 Carbohydrates

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	LWY	K	427	12/12	0.22	0.13	127,133,135,135	0
3	LWY	A	427	12/12	0.17	-0.10	95,103,107,108	0
3	LWY	M	427	12/12	0.21	-0.16	103,113,116,116	0
3	LWY	E	427	12/12	0.17	-0.16	81,88,90,90	0
3	LWY	C	427	12/12	0.19	-0.26	89,94,98,100	0
3	LWY	N	427	12/12	0.18	-0.30	109,111,112,115	0
3	LWY	G	427	12/12	0.20	-0.35	85,91,95,97	0
2	ZN	N	426	1/1	0.12	-0.52	95,95,95,95	0
3	LWY	D	427	12/12	0.15	-0.65	63,71,80,81	0
3	LWY	L	427	12/12	0.15	-0.67	101,111,114,115	0
3	LWY	J	427	12/12	0.14	-0.68	90,105,106,107	0
2	ZN	D	425	1/1	0.16	-0.75	73,73,73,73	0
3	LWY	F	427	12/12	0.15	-0.91	97,98,101,106	0
2	ZN	K	425	1/1	0.15	-1.08	125,125,125,125	0
2	ZN	O	426	1/1	0.14	-1.11	93,93,93,93	0
3	LWY	H	427	12/12	0.14	-1.11	77,81,88,88	0
2	ZN	C	426	1/1	0.17	-1.15	91,91,91,91	0
2	ZN	F	426	1/1	0.16	-1.17	89,89,89,89	0
2	ZN	L	425	1/1	0.15	-1.20	102,102,102,102	0
3	LWY	P	427	12/12	0.14	-1.21	74,87,89,92	0
2	ZN	E	426	1/1	0.14	-1.26	84,84,84,84	0
3	LWY	B	427	12/12	0.12	-1.27	73,77,81,83	0
2	ZN	L	426	1/1	0.10	-1.30	108,108,108,108	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	ZN	J	426	1/1	0.14	-1.36	101,101,101,101	0
2	ZN	P	426	1/1	0.14	-1.41	94,94,94,94	0
2	ZN	G	426	1/1	0.14	-1.42	95,95,95,95	0
2	ZN	N	425	1/1	0.13	-1.49	90,90,90,90	0
3	LWY	O	427	12/12	0.13	-1.53	81,90,93,95	0
2	ZN	M	426	1/1	0.12	-1.56	103,103,103,103	0
2	ZN	H	425	1/1	0.16	-1.61	89,89,89,89	0
2	ZN	F	425	1/1	0.17	-1.61	96,96,96,96	0
2	ZN	K	426	1/1	0.12	-1.62	110,110,110,110	0
3	LWY	I	427	12/12	0.13	-1.65	102,106,112,113	0
2	ZN	H	426	1/1	0.13	-1.66	92,92,92,92	0
2	ZN	O	425	1/1	0.14	-1.84	92,92,92,92	0
2	ZN	A	426	1/1	0.12	-1.91	99,99,99,99	0
2	ZN	P	425	1/1	0.14	-1.92	87,87,87,87	0
2	ZN	D	426	1/1	0.13	-1.97	72,72,72,72	0
2	ZN	G	425	1/1	0.16	-2.01	84,84,84,84	0
2	ZN	B	426	1/1	0.10	-2.05	84,84,84,84	0
2	ZN	B	425	1/1	0.12	-2.14	78,78,78,78	0
2	ZN	E	425	1/1	0.16	-2.28	79,79,79,79	0
2	ZN	J	425	1/1	0.14	-2.56	102,102,102,102	0
2	ZN	M	425	1/1	0.12	-2.80	114,114,114,114	0
2	ZN	A	425	1/1	0.12	-3.09	86,86,86,86	0
2	ZN	I	426	1/1	0.09	-3.26	115,115,115,115	0
2	ZN	I	425	1/1	0.10	-3.36	100,100,100,100	0
2	ZN	C	425	1/1	0.18	-3.48	90,90,90,90	0

6.5 Other polymers ⓘ

There are no such residues in this entry.