



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 30, 2017 – 10:46 PM EDT

PDB ID : 5C76  
Title : ATP-driven lipid-linked oligosaccharide flippase PglK in apo-inward facing state (2)  
Authors : Perez, C.; Gerber, S.; Locher, K.P.  
Deposited on : unknown  
Resolution : 3.94 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030345

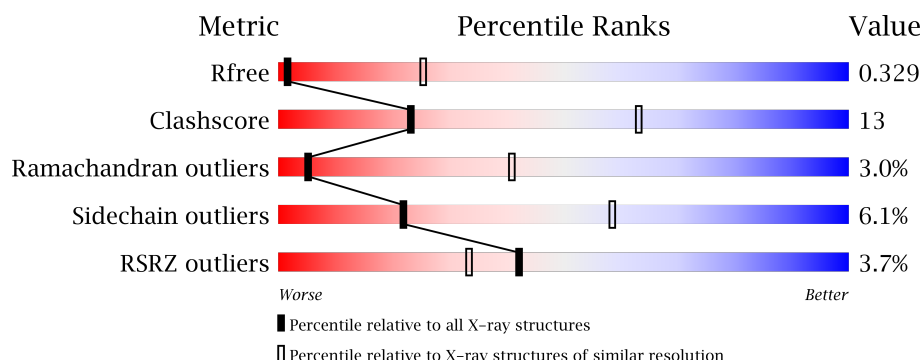
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.94 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))
$R_{free}$	100719	1021 (4.28-3.60)
Clashscore	112137	1117 (4.28-3.60)
Ramachandran outliers	110173	1076 (4.28-3.60)
Sidechain outliers	110143	1067 (4.28-3.60)
RSRZ outliers	101464	1034 (4.28-3.60)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	564	<div> <div>2%</div> <div>64%</div> <div>33%</div> <div>.</div> </div>
1	B	564	<div> <div>4%</div> <div>65%</div> <div>32%</div> <div>..</div> </div>
1	C	564	<div> <div>4%</div> <div>65%</div> <div>31%</div> <div>.</div> </div>
1	D	564	<div> <div>5%</div> <div>67%</div> <div>30%</div> <div>.</div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 18228 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 WlaB protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	564	Total	C	N	O	S	0	0	0
			4557	3000	732	811	14			
1	B	564	Total	C	N	O	S	0	0	0
			4557	3000	732	811	14			
1	C	564	Total	C	N	O	S	0	0	0
			4557	3000	732	811	14			
1	D	564	Total	C	N	O	S	0	0	0
			4557	3000	732	811	14			

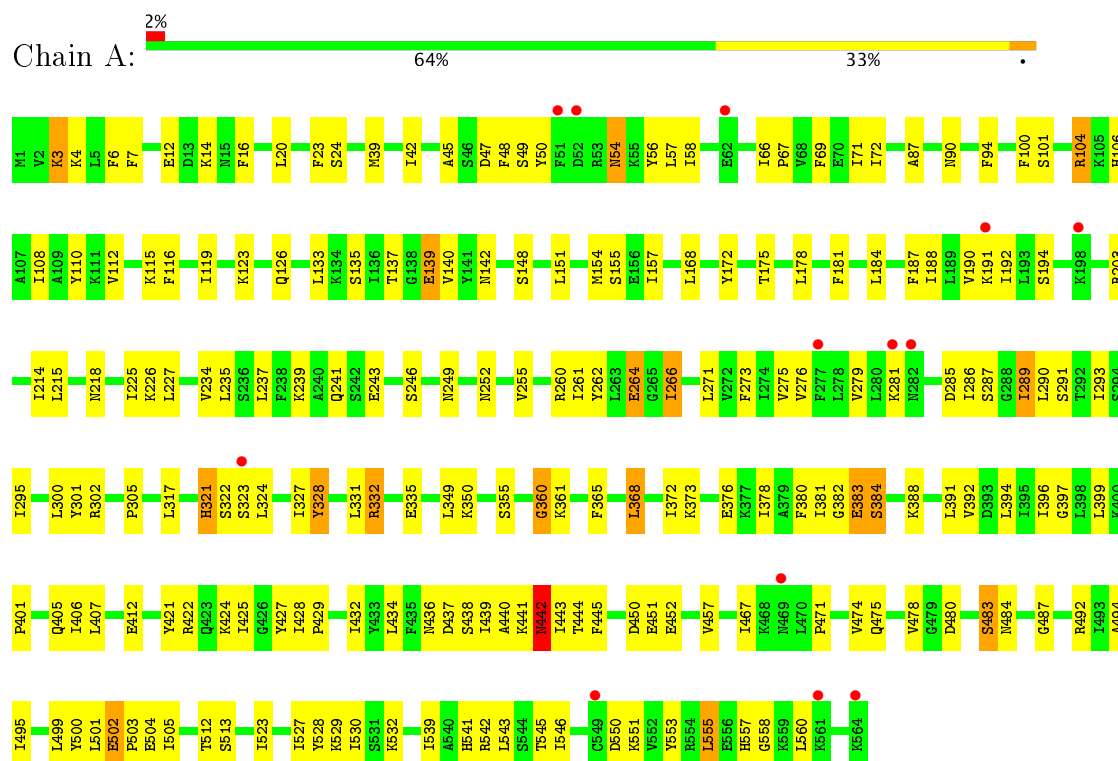
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	VAL	LEU	conflict	UNP O86150
A	105	LYS	TYR	conflict	UNP O86150
A	510	GLN	GLU	conflict	UNP O86150
B	2	VAL	LEU	conflict	UNP O86150
B	105	LYS	TYR	conflict	UNP O86150
B	510	GLN	GLU	conflict	UNP O86150
C	2	VAL	LEU	conflict	UNP O86150
C	105	LYS	TYR	conflict	UNP O86150
C	510	GLN	GLU	conflict	UNP O86150
D	2	VAL	LEU	conflict	UNP O86150
D	105	LYS	TYR	conflict	UNP O86150
D	510	GLN	GLU	conflict	UNP O86150

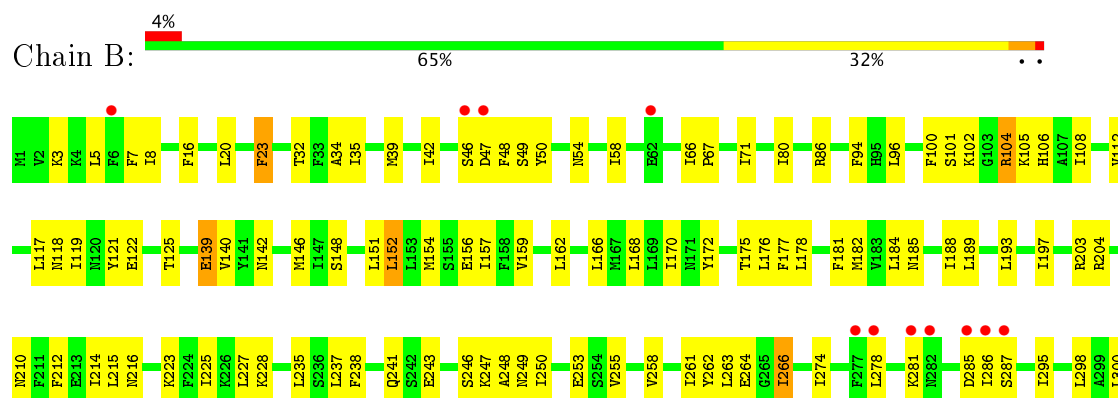
### 3 Residue-property plots

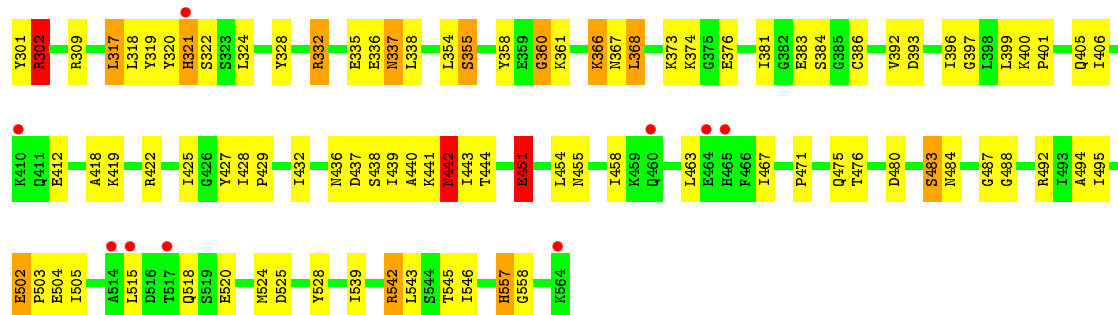
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: WlaB protein

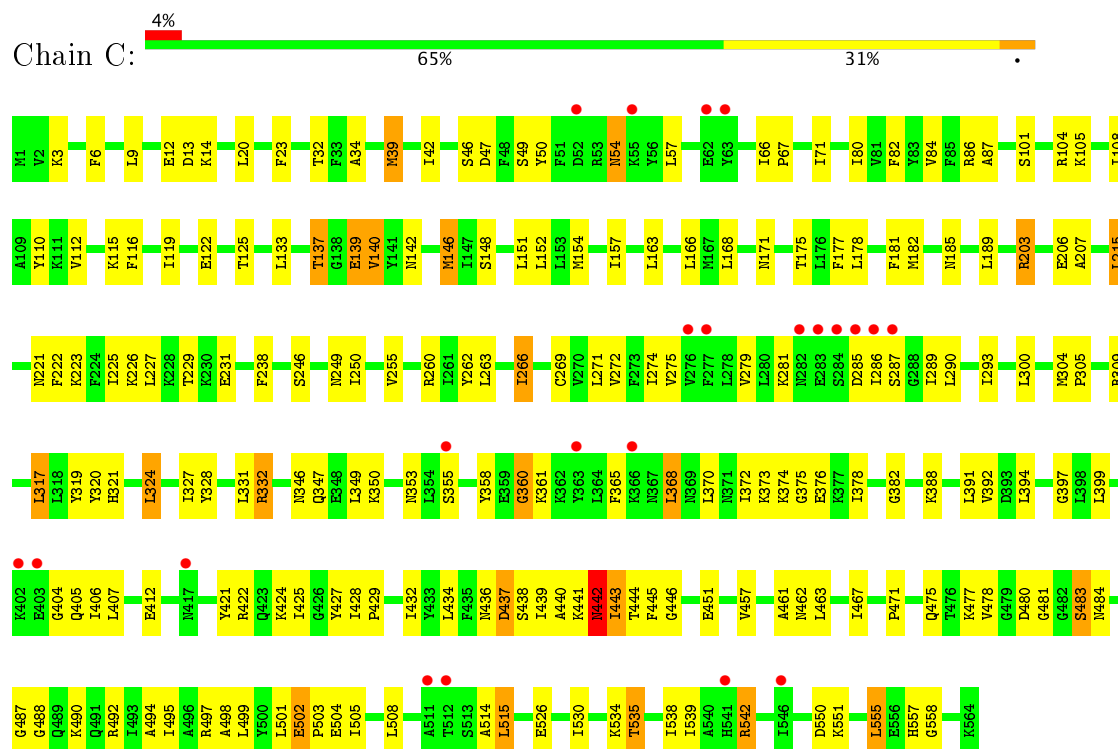


#### • Molecule 1: WlaB protein

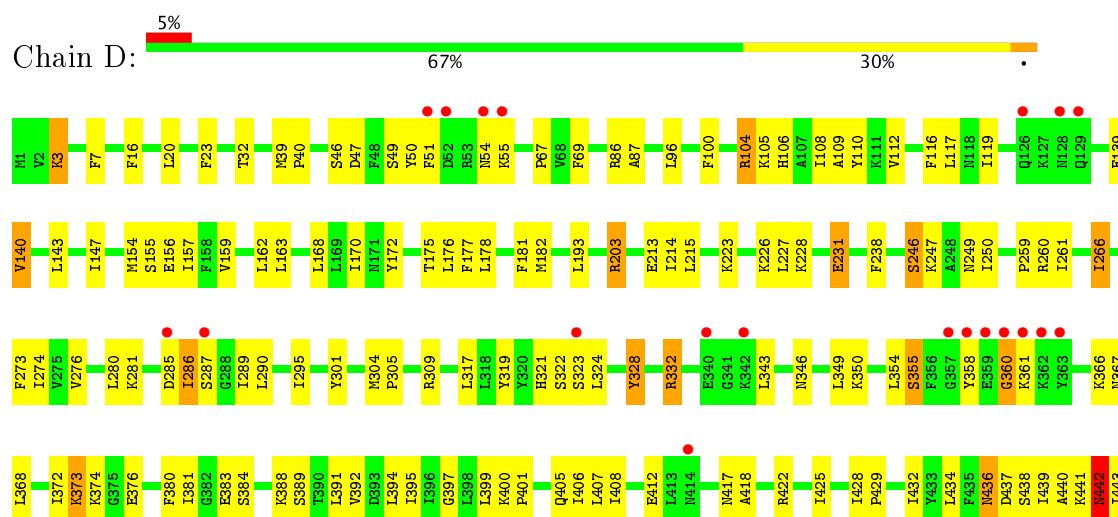




• Molecule 1: WlaB protein



• Molecule 1: WlaB protein





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.41Å 183.33Å 136.26Å 90.00° 106.70° 90.00°	Depositor
Resolution (Å)	29.82 – 3.94 29.82 – 3.94	Depositor EDS
% Data completeness (in resolution range)	86.2 (29.82-3.94) 86.3 (29.82-3.94)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.83 (at 3.98Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.275 , 0.329 0.274 , 0.329	Depositor DCC
$R_{free}$ test set	1693 reflections (5.06%)	DCC
Wilson B-factor (Å <sup>2</sup> )	166.3	Xtriage
Anisotropy	0.011	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.24 , 111.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	18228	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	208.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

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	0.29	0/4641	0.50	0/6246
1	B	0.28	0/4641	0.49	1/6246 (0.0%)
1	C	0.28	0/4641	0.48	0/6246
1	D	0.27	0/4641	0.47	0/6246
All	All	0.28	0/18564	0.48	1/24984 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	302	ARG	NE-CZ-NH2	5.11	122.86	120.30

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	4557	0	4764	141	0
1	B	4557	0	4764	130	0
1	C	4557	0	4764	131	0
1	D	4557	0	4764	128	0
All	All	18228	0	19056	476	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 13.



All (476) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:520:GLU:OE1	1:B:542:ARG:NH1	2.09	0.85
1:B:503:PRO:HB2	1:B:504:GLU:HG2	1.61	0.82
1:A:425:ILE:HG22	1:A:505:ILE:HB	1.62	0.81
1:C:503:PRO:HB2	1:C:504:GLU:HG2	1.62	0.81
1:C:203:ARG:HH11	1:C:206:GLU:HB3	1.45	0.81
1:D:425:ILE:HG22	1:D:505:ILE:HB	1.61	0.81
1:B:168:LEU:HA	1:B:175:THR:HG21	1.63	0.81
1:A:502:GLU:HB2	1:A:503:PRO:HD3	1.66	0.78
1:A:503:PRO:HB2	1:A:504:GLU:HG2	1.65	0.78
1:C:139:GLU:HB3	1:C:324:LEU:HB3	1.64	0.78
1:D:100:PHE:HA	1:D:104:ARG:HH21	1.50	0.77
1:A:139:GLU:OE2	1:A:324:LEU:HD12	1.86	0.76
1:D:503:PRO:HB2	1:D:504:GLU:HG2	1.67	0.76
1:A:218:ASN:HD21	1:A:237:LEU:HD11	1.50	0.76
1:A:168:LEU:HA	1:A:175:THR:HG21	1.66	0.76
1:C:492:ARG:NH1	1:C:526:GLU:OE1	2.19	0.75
1:B:425:ILE:HG22	1:B:505:ILE:HB	1.68	0.74
1:A:438:SER:O	1:A:440:ALA:N	2.21	0.74
1:B:39:MET:HB2	1:B:295:ILE:HD11	1.70	0.73
1:D:392:VAL:HG21	1:D:539:ILE:HG12	1.71	0.73
1:C:483:SER:OG	1:C:484:ASN:N	2.23	0.72
1:C:502:GLU:HB2	1:C:503:PRO:HD3	1.71	0.72
1:D:502:GLU:HB2	1:D:503:PRO:HD3	1.72	0.72
1:A:501:LEU:HD11	1:D:228:LYS:HZ1	1.55	0.71
1:B:502:GLU:HB2	1:B:503:PRO:HD3	1.71	0.71
1:A:442:ASN:O	1:A:444:THR:N	2.23	0.71
1:D:442:ASN:O	1:D:444:THR:N	2.25	0.70
1:A:483:SER:OG	1:A:484:ASN:N	2.23	0.70
1:C:392:VAL:HG21	1:C:539:ILE:HG12	1.74	0.70
1:B:483:SER:OG	1:B:484:ASN:N	2.21	0.69
1:B:400:LYS:NZ	1:D:516:ASP:HB2	2.08	0.69
1:B:392:VAL:HG21	1:B:539:ILE:HG12	1.75	0.68
1:C:438:SER:O	1:C:440:ALA:N	2.26	0.68
1:A:429:PRO:HG2	1:A:432:ILE:HG22	1.74	0.68
1:B:425:ILE:HD11	1:C:227:LEU:HD22	1.76	0.68
1:A:45:ALA:HA	1:A:72:ILE:HD12	1.77	0.67
1:D:483:SER:OG	1:D:484:ASN:N	2.21	0.67
1:A:392:VAL:HG21	1:A:539:ILE:HG12	1.76	0.66
1:B:360:GLY:H	1:B:361:LYS:HD2	1.61	0.66
1:C:39:MET:SD	1:C:39:MET:N	2.68	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:388:LYS:NZ	1:D:541:HIS:HA	2.11	0.66
1:C:429:PRO:HG2	1:C:432:ILE:HG22	1.78	0.66
1:B:212:PHE:O	1:B:216:ASN:ND2	2.26	0.66
1:A:442:ASN:O	1:A:445:PHE:N	2.26	0.65
1:D:438:SER:O	1:D:440:ALA:N	2.29	0.65
1:C:397:GLY:HA3	1:C:422:ARG:HD2	1.78	0.65
1:A:501:LEU:HD11	1:D:228:LYS:NZ	2.12	0.64
1:D:112:VAL:HG22	1:D:332:ARG:HH22	1.62	0.64
1:A:261:ILE:HG22	1:D:87:ALA:HA	1.78	0.64
1:B:47:ASP:HB3	1:C:286:ILE:HG12	1.80	0.63
1:A:227:LEU:HD22	1:D:425:ILE:HD11	1.80	0.63
1:B:228:LYS:HG2	1:C:501:LEU:HD21	1.80	0.63
1:C:349:LEU:HB2	1:C:372:ILE:HB	1.79	0.63
1:A:66:ILE:HD12	1:A:71:ILE:HG23	1.79	0.63
1:B:438:SER:O	1:B:440:ALA:N	2.32	0.63
1:B:358:TYR:HB2	1:B:361:LYS:HD3	1.81	0.63
1:D:451:GLU:O	1:D:455:ASN:ND2	2.29	0.63
1:B:520:GLU:CD	1:B:542:ARG:HH12	2.02	0.62
1:B:400:LYS:HZ1	1:D:516:ASP:HB2	1.64	0.62
1:A:262:TYR:O	1:A:266:ILE:HG22	1.99	0.62
1:C:425:ILE:HG22	1:C:505:ILE:HB	1.79	0.62
1:D:429:PRO:HG2	1:D:432:ILE:HG22	1.80	0.62
1:B:264:GLU:HB3	1:C:86:ARG:HH12	1.64	0.61
1:B:105:LYS:HD2	1:B:140:VAL:HG12	1.82	0.61
1:C:203:ARG:HH11	1:C:206:GLU:CB	2.13	0.61
1:C:181:PHE:CE2	1:C:266:ILE:HD11	2.36	0.60
1:B:204:ARG:HA	1:B:248:ALA:HB1	1.84	0.60
1:D:349:LEU:HB2	1:D:372:ILE:HB	1.82	0.60
1:C:434:LEU:HB2	1:C:481:GLY:HA2	1.84	0.60
1:D:139:GLU:OE2	1:D:324:LEU:HD12	2.02	0.60
1:B:451:GLU:O	1:B:455:ASN:ND2	2.31	0.60
1:A:178:LEU:HD13	1:A:300:LEU:HD11	1.84	0.60
1:B:442:ASN:O	1:B:444:THR:N	2.35	0.60
1:B:528:TYR:OH	1:B:545:THR:O	2.14	0.59
1:A:287:SER:HB2	1:D:286:ILE:HG22	1.85	0.59
1:D:332:ARG:HB3	1:D:332:ARG:NH1	2.17	0.59
1:D:388:LYS:HZ2	1:D:541:HIS:HA	1.66	0.59
1:C:168:LEU:HA	1:C:175:THR:HG21	1.82	0.59
1:C:358:TYR:HB2	1:C:361:LYS:HD3	1.85	0.59
1:D:492:ARG:NH1	1:D:523:ILE:HG12	2.17	0.59
1:B:178:LEU:HD13	1:B:300:LEU:HD11	1.83	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:477:LYS:O	1:C:484:ASN:ND2	2.37	0.58
1:A:441:LYS:HA	1:A:442:ASN:O	2.04	0.58
1:A:39:MET:HB2	1:A:295:ILE:HD11	1.86	0.58
1:A:317:LEU:O	1:A:321:HIS:NE2	2.36	0.58
1:C:105:LYS:HD2	1:C:140:VAL:HB	1.84	0.58
1:A:100:PHE:HA	1:A:104:ARG:HH21	1.67	0.57
1:A:264:GLU:N	1:A:264:GLU:OE2	2.37	0.57
1:D:285:ASP:O	1:D:287:SER:N	2.36	0.57
1:D:381:ILE:HD11	1:D:546:ILE:HD13	1.87	0.57
1:D:109:ALA:HB2	1:D:140:VAL:HG11	1.86	0.57
1:A:290:LEU:HD13	1:D:290:LEU:HB3	1.86	0.56
1:D:170:ILE:HD13	1:D:295:ILE:HG21	1.87	0.56
1:D:3:LYS:H	1:D:3:LYS:HD3	1.71	0.56
1:A:428:ILE:HD13	1:A:495:ILE:HG12	1.88	0.56
1:D:405:GLN:NE2	1:D:412:GLU:OE1	2.37	0.56
1:A:321:HIS:CG	1:A:322:SER:H	2.23	0.56
1:B:20:LEU:HB3	1:B:151:LEU:HD13	1.87	0.56
1:C:391:LEU:HD12	1:C:555:LEU:HD13	1.86	0.56
1:A:54:ASN:HB3	1:A:57:LEU:HB2	1.87	0.56
1:B:524:MET:HG3	1:B:545:THR:HG22	1.86	0.56
1:D:355:SER:OG	1:D:367:ASN:N	2.35	0.56
1:D:193:LEU:HD13	1:D:259:PRO:HG3	1.86	0.56
1:B:355:SER:OG	1:B:367:ASN:N	2.32	0.56
1:C:457:VAL:O	1:C:461:ALA:N	2.35	0.56
1:C:557:HIS:ND1	1:C:557:HIS:O	2.38	0.55
1:B:39:MET:HA	1:B:42:ILE:HG22	1.88	0.55
1:A:39:MET:HA	1:A:42:ILE:HG22	1.88	0.55
1:A:360:GLY:H	1:A:361:LYS:HD2	1.71	0.55
1:B:108:ILE:O	1:B:112:VAL:HG23	2.06	0.55
1:C:181:PHE:HE2	1:C:266:ILE:HD11	1.72	0.55
1:A:383:GLU:OE1	1:B:557:HIS:N	2.30	0.55
1:C:6:PHE:HD1	1:C:14:LYS:HG2	1.71	0.55
1:A:20:LEU:HB3	1:A:151:LEU:HD13	1.89	0.55
1:A:512:THR:HG22	1:A:541:HIS:CE1	2.42	0.55
1:C:441:LYS:HE2	1:C:446:GLY:HA2	1.88	0.54
1:A:478:VAL:O	1:A:483:SER:OG	2.25	0.54
1:C:178:LEU:O	1:C:182:MET:HB2	2.08	0.54
1:C:440:ALA:O	1:C:444:THR:N	2.28	0.54
1:A:427:TYR:HE2	1:A:429:PRO:HB3	1.71	0.54
1:B:285:ASP:O	1:B:287:SER:N	2.40	0.54
1:A:225:ILE:HG21	1:D:117:LEU:HD22	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:223:LYS:O	1:D:227:LEU:HD13	2.07	0.54
1:D:478:VAL:O	1:D:483:SER:OG	2.26	0.54
1:D:492:ARG:HH12	1:D:523:ILE:HG12	1.72	0.54
1:A:94:PHE:CE2	1:D:260:ARG:NH1	2.77	0.53
1:A:135:SER:HA	1:A:139:GLU:HG2	1.90	0.53
1:B:159:VAL:HG11	1:B:302:ARG:NH2	2.24	0.53
1:C:397:GLY:C	1:C:422:ARG:HH11	2.12	0.53
1:B:184:LEU:O	1:B:188:ILE:HG13	2.09	0.53
1:C:108:ILE:O	1:C:112:VAL:HG23	2.09	0.53
1:C:424:LYS:HB2	1:C:504:GLU:HG3	1.90	0.53
1:A:381:ILE:HD11	1:A:546:ILE:HD13	1.90	0.53
1:A:321:HIS:CG	1:A:322:SER:N	2.77	0.53
1:B:381:ILE:HD11	1:B:546:ILE:HD13	1.91	0.53
1:D:273:PHE:HA	1:D:276:VAL:HG22	1.91	0.53
1:D:441:LYS:HA	1:D:442:ASN:O	2.09	0.53
1:B:264:GLU:HB3	1:C:86:ARG:NH1	2.24	0.53
1:A:290:LEU:HB3	1:D:290:LEU:HD13	1.91	0.53
1:B:557:HIS:O	1:B:557:HIS:ND1	2.42	0.52
1:C:332:ARG:NH1	1:C:332:ARG:HB3	2.23	0.52
1:B:429:PRO:HG2	1:B:432:ILE:HG22	1.89	0.52
1:A:384:SER:H	1:A:388:LYS:HE2	1.75	0.52
1:C:405:GLN:NE2	1:C:412:GLU:OE1	2.41	0.52
1:A:214:ILE:HG12	1:A:241:GLN:HG2	1.92	0.52
1:A:286:ILE:HG22	1:D:287:SER:HB2	1.91	0.52
1:A:427:TYR:CE2	1:A:429:PRO:HB3	2.44	0.52
1:A:424:LYS:HB2	1:A:504:GLU:HG3	1.90	0.52
1:C:49:SER:OG	1:C:50:TYR:N	2.40	0.52
1:C:360:GLY:H	1:C:361:LYS:HD2	1.74	0.52
1:B:227:LEU:HD22	1:C:425:ILE:HD11	1.92	0.52
1:D:477:LYS:O	1:D:484:ASN:ND2	2.42	0.52
1:A:24:SER:HB3	1:A:155:SER:HB2	1.91	0.52
1:C:178:LEU:HD13	1:C:300:LEU:HD11	1.90	0.52
1:B:432:ILE:HG21	1:B:494:ALA:HB2	1.92	0.51
1:C:285:ASP:O	1:C:287:SER:N	2.43	0.51
1:A:154:MET:O	1:A:157:ILE:HG13	2.11	0.51
1:A:553:TYR:HB3	1:A:560:LEU:HG	1.92	0.51
1:A:3:LYS:H	1:A:3:LYS:HD3	1.76	0.51
1:B:49:SER:OG	1:B:50:TYR:N	2.42	0.51
1:D:32:THR:HG22	1:D:163:LEU:HG	1.92	0.51
1:B:393:ASP:OD1	1:C:223:LYS:NZ	2.37	0.51
1:D:178:LEU:O	1:D:182:MET:HB2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:ASN:O	1:B:214:ILE:HG12	2.10	0.50
1:D:527:ILE:HA	1:D:530:ILE:HG12	1.92	0.50
1:A:285:ASP:O	1:A:287:SER:N	2.42	0.50
1:B:427:TYR:HE2	1:B:429:PRO:HB3	1.75	0.50
1:C:378:ILE:HG22	1:C:551:LYS:HB2	1.92	0.50
1:A:184:LEU:O	1:A:188:ILE:HG13	2.10	0.50
1:A:328:TYR:HD1	1:A:332:ARG:HD2	1.77	0.50
1:B:46:SER:OG	1:C:286:ILE:O	2.27	0.50
1:B:154:MET:O	1:B:157:ILE:HG13	2.11	0.50
1:C:350:LYS:HB3	1:C:407:LEU:HB2	1.94	0.50
1:A:373:LYS:HB2	1:A:376:GLU:HG3	1.94	0.50
1:A:502:GLU:HB2	1:A:503:PRO:CD	2.39	0.50
1:D:557:HIS:ND1	1:D:557:HIS:O	2.44	0.50
1:C:101:SER:HB3	1:C:148:SER:OG	2.12	0.50
1:D:360:GLY:H	1:D:361:LYS:HD2	1.77	0.50
1:B:428:ILE:HD13	1:B:495:ILE:HG12	1.94	0.50
1:D:105:LYS:HD2	1:D:140:VAL:HB	1.92	0.50
1:A:140:VAL:HB	1:A:328:TYR:OH	2.12	0.50
1:A:432:ILE:HG21	1:A:494:ALA:HB2	1.94	0.50
1:A:322:SER:C	1:A:324:LEU:H	2.15	0.50
1:B:302:ARG:HH21	1:B:302:ARG:CG	2.24	0.49
1:C:215:LEU:HG	1:C:238:PHE:HE1	1.77	0.49
1:C:508:LEU:HB3	1:C:538:ILE:HG12	1.94	0.49
1:A:181:PHE:HE2	1:A:266:ILE:HD11	1.76	0.49
1:D:47:ASP:OD2	1:D:49:SER:HB3	2.12	0.49
1:D:553:TYR:HB3	1:D:560:LEU:HD11	1.95	0.49
1:A:123:LYS:HA	1:A:126:GLN:HG2	1.93	0.49
1:A:396:ILE:HD12	1:D:227:LEU:HD21	1.94	0.49
1:C:66:ILE:HD12	1:C:71:ILE:HG23	1.95	0.49
1:C:332:ARG:HB3	1:C:332:ARG:HH11	1.78	0.49
1:B:261:ILE:HG22	1:C:87:ALA:HA	1.94	0.49
1:A:405:GLN:NE2	1:A:412:GLU:OE1	2.41	0.49
1:B:442:ASN:H	1:B:442:ASN:ND2	2.10	0.49
1:B:193:LEU:O	1:B:197:ILE:HG12	2.12	0.49
1:C:20:LEU:HB3	1:C:151:LEU:HD13	1.95	0.49
1:A:513:SER:HA	1:A:542:ARG:HH12	1.78	0.48
1:C:146:MET:SD	1:C:317:LEU:HG	2.52	0.48
1:B:366:LYS:HB2	1:B:366:LYS:NZ	2.28	0.48
1:A:187:PHE:O	1:A:191:LYS:HB2	2.14	0.48
1:B:117:LEU:O	1:C:226:LYS:NZ	2.46	0.48
1:B:34:ALA:HB2	1:B:86:ARG:CD	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:373:LYS:HB2	1:C:376:GLU:HG3	1.95	0.48
1:A:243:GLU:HA	1:A:246:SER:HB3	1.94	0.48
1:B:94:PHE:CZ	1:C:260:ARG:NH1	2.81	0.48
1:D:55:LYS:HD2	1:D:55:LYS:H	1.78	0.48
1:A:108:ILE:O	1:A:112:VAL:HG23	2.13	0.48
1:B:488:GLY:O	1:B:492:ARG:HG3	2.14	0.48
1:D:391:LEU:HD12	1:D:555:LEU:HD13	1.95	0.48
1:D:529:LYS:HA	1:D:532:LYS:NZ	2.29	0.48
1:B:397:GLY:HA3	1:B:422:ARG:HG3	1.94	0.48
1:B:427:TYR:CE2	1:B:429:PRO:HB3	2.49	0.48
1:C:115:LYS:HE2	1:C:332:ARG:O	2.14	0.48
1:D:373:LYS:HB2	1:D:376:GLU:HG3	1.96	0.48
1:A:275:VAL:O	1:A:279:VAL:HG23	2.14	0.47
1:B:108:ILE:HG23	1:B:328:TYR:OH	2.13	0.47
1:D:181:PHE:CZ	1:D:266:ILE:HD11	2.49	0.47
1:D:442:ASN:O	1:D:445:PHE:N	2.30	0.47
1:B:373:LYS:HB2	1:B:376:GLU:HG3	1.96	0.47
1:B:80:ILE:HG12	1:C:269:CYS:SG	2.54	0.47
1:D:350:LYS:HB3	1:D:407:LEU:HB2	1.95	0.47
1:A:428:ILE:HG12	1:A:495:ILE:HA	1.95	0.47
1:A:378:ILE:HG22	1:A:551:LYS:HB2	1.96	0.47
1:A:133:LEU:O	1:A:137:THR:HG22	2.15	0.47
1:A:382:GLY:HA3	1:A:388:LYS:HD3	1.96	0.47
1:B:102:LYS:HB2	1:C:250:ILE:CG2	2.45	0.47
1:C:438:SER:HB2	1:C:475:GLN:HA	1.96	0.47
1:C:442:ASN:O	1:C:445:PHE:N	2.30	0.47
1:A:226:LYS:NZ	1:D:119:ILE:O	2.40	0.47
1:B:32:THR:HG21	1:B:162:LEU:HB2	1.95	0.47
1:C:443:ILE:HA	1:C:497:ARG:HB2	1.96	0.47
1:A:349:LEU:HB2	1:A:372:ILE:HB	1.96	0.47
1:B:262:TYR:O	1:B:266:ILE:HG22	2.14	0.47
1:C:442:ASN:ND2	1:C:442:ASN:H	2.13	0.47
1:C:428:ILE:HD13	1:C:495:ILE:HG12	1.97	0.47
1:D:418:ALA:O	1:D:422:ARG:HD3	2.14	0.47
1:A:115:LYS:NZ	1:A:332:ARG:O	2.44	0.47
1:A:529:LYS:HG2	1:A:532:LYS:NZ	2.29	0.47
1:A:94:PHE:CZ	1:D:260:ARG:NH1	2.82	0.47
1:B:102:LYS:HB2	1:C:250:ILE:HG22	1.97	0.47
1:C:376:GLU:O	1:C:550:ASP:HB2	2.14	0.47
1:D:442:ASN:H	1:D:442:ASN:ND2	2.12	0.47
1:A:49:SER:OG	1:A:50:TYR:N	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:ASN:H	1:A:442:ASN:ND2	2.13	0.47
1:B:396:ILE:HD12	1:C:227:LEU:HD11	1.97	0.47
1:C:437:ASP:OD2	1:C:441:LYS:HG3	2.16	0.46
1:C:189:LEU:HD21	1:C:262:TYR:CE1	2.49	0.46
1:C:557:HIS:HA	1:C:558:GLY:HA2	1.57	0.46
1:D:389:SER:HA	1:D:539:ILE:HD13	1.97	0.46
1:A:235:LEU:HB3	1:D:110:TYR:HE1	1.80	0.46
1:A:273:PHE:HA	1:A:276:VAL:HG22	1.96	0.46
1:C:514:ALA:HB2	1:C:542:ARG:HH22	1.80	0.46
1:D:557:HIS:HA	1:D:558:GLY:HA2	1.57	0.46
1:A:328:TYR:O	1:A:332:ARG:HG2	2.16	0.46
1:C:142:ASN:HB3	1:C:320:TYR:HB3	1.97	0.46
1:B:118:ASN:HB3	1:B:336:GLU:HB3	1.97	0.46
1:B:66:ILE:HD12	1:B:71:ILE:HD13	1.96	0.46
1:B:23:PHE:CE2	1:B:96:LEU:HD12	2.51	0.46
1:C:185:ASN:O	1:C:189:LEU:HG	2.15	0.46
1:C:54:ASN:HB3	1:C:57:LEU:HB2	1.97	0.46
1:D:428:ILE:HD13	1:D:495:ILE:HG12	1.98	0.46
1:A:264:GLU:HB3	1:D:86:ARG:NH1	2.30	0.46
1:A:376:GLU:O	1:A:550:ASP:HB2	2.15	0.46
1:B:142:ASN:HB3	1:B:320:TYR:HB3	1.97	0.46
1:C:177:PHE:CD1	1:C:274:ILE:HD11	2.50	0.46
1:C:375:GLY:H	1:C:535:THR:HB	1.79	0.46
1:D:358:TYR:HB2	1:D:361:LYS:HD3	1.97	0.46
1:A:239:LYS:HA	1:D:106:HIS:HE1	1.80	0.46
1:A:421:TYR:O	1:A:424:LYS:HG2	2.16	0.46
1:C:346:ASN:HA	1:C:374:LYS:HD2	1.97	0.46
1:D:383:GLU:OE2	1:D:554:ARG:NH2	2.49	0.46
1:C:421:TYR:O	1:C:424:LYS:HG2	2.16	0.46
1:D:355:SER:HA	1:D:366:LYS:H	1.79	0.46
1:A:324:LEU:O	1:A:328:TYR:N	2.45	0.46
1:C:327:ILE:O	1:C:331:LEU:HG	2.16	0.46
1:D:49:SER:C	1:D:51:PHE:H	2.20	0.46
1:A:287:SER:O	1:A:291:SER:N	2.44	0.46
1:A:467:ILE:HG21	1:A:474:VAL:HG22	1.97	0.46
1:A:383:GLU:HG3	1:B:383:GLU:HB2	1.98	0.46
1:B:400:LYS:HD2	1:B:401:PRO:HD2	1.98	0.46
1:C:304:MET:HB2	1:C:305:PRO:HD3	1.96	0.46
1:C:365:PHE:HB3	1:C:368:LEU:HD23	1.98	0.45
1:C:481:GLY:O	1:C:490:LYS:HE2	2.15	0.45
1:D:104:ARG:HA	1:D:104:ARG:HD3	1.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:499:LEU:HD21	1:A:530:ILE:HD12	1.99	0.45
1:A:513:SER:HA	1:A:542:ARG:NH1	2.31	0.45
1:A:327:ILE:O	1:A:331:LEU:HD23	2.16	0.45
1:A:422:ARG:O	1:A:425:ILE:HG12	2.16	0.45
1:B:139:GLU:CD	1:B:324:LEU:HD12	2.37	0.45
1:C:353:ASN:O	1:C:404:GLY:HA2	2.16	0.45
1:A:7:PHE:HE2	1:A:332:ARG:HB2	1.82	0.45
1:A:350:LYS:HB3	1:A:407:LEU:HB2	1.99	0.45
1:B:101:SER:HB3	1:B:148:SER:OG	2.17	0.45
1:C:262:TYR:O	1:C:266:ILE:HG22	2.16	0.45
1:B:181:PHE:CE2	1:B:266:ILE:HD11	2.51	0.45
1:B:243:GLU:HA	1:B:246:SER:HB3	1.98	0.45
1:B:7:PHE:HE2	1:B:332:ARG:HB2	1.82	0.45
1:B:422:ARG:O	1:B:425:ILE:HG12	2.17	0.45
1:B:463:LEU:O	1:B:467:ILE:HG12	2.17	0.45
1:D:168:LEU:HA	1:D:175:THR:HG21	1.98	0.45
1:D:328:TYR:HD2	1:D:328:TYR:HA	1.68	0.45
1:A:184:LEU:O	1:A:187:PHE:HB3	2.17	0.45
1:A:350:LYS:O	1:A:407:LEU:N	2.47	0.45
1:C:274:ILE:HD13	1:C:274:ILE:HA	1.78	0.45
1:C:275:VAL:O	1:C:279:VAL:HG23	2.16	0.45
1:A:142:ASN:HB2	1:A:324:LEU:HG	1.99	0.45
1:A:391:LEU:HD12	1:A:555:LEU:HD13	2.00	0.44
1:B:228:LYS:HE2	1:B:228:LYS:HB3	1.79	0.44
1:B:8:ILE:HG12	1:B:328:TYR:HE1	1.82	0.44
1:D:181:PHE:CE2	1:D:266:ILE:HD11	2.51	0.44
1:A:235:LEU:HB3	1:D:110:TYR:CE1	2.52	0.44
1:A:437:ASP:OD2	1:A:441:LYS:HG3	2.17	0.44
1:A:87:ALA:HA	1:D:261:ILE:HG22	1.99	0.44
1:D:332:ARG:HH11	1:D:332:ARG:HB3	1.82	0.44
1:B:322:SER:C	1:B:324:LEU:H	2.20	0.44
1:C:80:ILE:O	1:C:84:VAL:HG23	2.17	0.44
1:D:155:SER:O	1:D:159:VAL:HG23	2.17	0.44
1:B:104:ARG:HD3	1:B:104:ARG:HA	1.70	0.44
1:B:418:ALA:O	1:B:422:ARG:HD3	2.17	0.44
1:C:271:LEU:HD21	1:C:293:ILE:HD11	1.99	0.44
1:A:302:ARG:O	1:A:305:PRO:HD2	2.17	0.44
1:B:152:LEU:HD22	1:B:156:GLU:HG2	1.99	0.44
1:B:255:VAL:HA	1:B:258:VAL:HG23	2.00	0.44
1:B:502:GLU:HB2	1:B:503:PRO:CD	2.44	0.44
1:A:529:LYS:HA	1:A:532:LYS:NZ	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:528:TYR:OH	1:A:545:THR:O	2.29	0.44
1:B:237:LEU:HB3	1:B:241:GLN:HE22	1.82	0.44
1:C:347:GLN:O	1:C:374:LYS:N	2.49	0.44
1:A:101:SER:HB2	1:A:148:SER:OG	2.17	0.44
1:A:279:VAL:HG12	1:D:69:PHE:CZ	2.53	0.44
1:C:463:LEU:O	1:C:467:ILE:HG12	2.18	0.44
1:D:350:LYS:O	1:D:407:LEU:N	2.50	0.44
1:D:434:LEU:HD22	1:D:442:ASN:ND2	2.33	0.44
1:B:368:LEU:HD22	1:B:368:LEU:HA	1.89	0.43
1:B:80:ILE:HG13	1:C:272:VAL:HB	2.00	0.43
1:C:46:SER:HA	1:C:47:ASP:HA	1.84	0.43
1:C:488:GLY:O	1:C:492:ARG:HG3	2.18	0.43
1:A:365:PHE:HB3	1:A:368:LEU:HD23	2.00	0.43
1:C:432:ILE:HG21	1:C:494:ALA:HB2	2.00	0.43
1:D:322:SER:C	1:D:324:LEU:H	2.22	0.43
1:B:400:LYS:HZ2	1:D:516:ASP:HB2	1.83	0.43
1:B:178:LEU:O	1:B:182:MET:HB2	2.18	0.43
1:B:121:TYR:HA	1:C:222:PHE:HE2	1.83	0.43
1:A:434:LEU:HD22	1:A:442:ASN:ND2	2.34	0.43
1:C:504:GLU:O	1:C:534:LYS:HB3	2.17	0.43
1:A:332:ARG:HG2	1:A:332:ARG:H	1.61	0.43
1:A:438:SER:HB2	1:A:475:GLN:HA	2.00	0.43
1:A:90:ASN:HB3	1:D:261:ILE:HD13	2.00	0.43
1:B:122:GLU:HA	1:B:125:THR:HG22	2.00	0.43
1:C:478:VAL:O	1:C:483:SER:OG	2.37	0.43
1:C:499:LEU:HD21	1:C:530:ILE:HD12	1.99	0.43
1:D:112:VAL:HG22	1:D:332:ARG:NH2	2.29	0.43
1:D:247:LYS:O	1:D:250:ILE:HG12	2.18	0.43
1:D:383:GLU:O	1:D:384:SER:OG	2.36	0.43
1:D:177:PHE:CE1	1:D:274:ILE:HD11	2.53	0.43
1:D:397:GLY:HA3	1:D:422:ARG:HG3	2.00	0.43
1:D:482:GLY:HA2	1:D:485:LEU:H	1.83	0.43
1:D:523:ILE:O	1:D:527:ILE:HG13	2.19	0.43
1:A:260:ARG:HG3	1:A:261:ILE:N	2.33	0.43
1:A:365:PHE:HE1	1:A:394:LEU:HD12	1.84	0.43
1:B:119:ILE:HA	1:B:336:GLU:HA	2.01	0.43
1:B:119:ILE:HG13	1:B:335:GLU:O	2.18	0.43
1:D:143:LEU:O	1:D:147:ILE:HG13	2.19	0.43
1:D:463:LEU:O	1:D:467:ILE:HG12	2.18	0.43
1:C:502:GLU:HB2	1:C:503:PRO:CD	2.44	0.43
1:B:235:LEU:HD22	1:C:110:TYR:CE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:501:LEU:CD1	1:D:228:LYS:HZ1	2.28	0.43
1:D:203:ARG:HE	1:D:203:ARG:HA	1.84	0.42
1:D:343:LEU:HD22	1:D:417:ASN:ND2	2.34	0.42
1:B:223:LYS:HE3	1:C:427:TYR:OH	2.19	0.42
1:C:365:PHE:HE1	1:C:394:LEU:HD12	1.83	0.42
1:C:428:ILE:HG12	1:C:495:ILE:HA	2.01	0.42
1:A:492:ARG:NH1	1:A:523:ILE:HG12	2.34	0.42
1:B:249:ASN:O	1:B:253:GLU:HB2	2.18	0.42
1:D:432:ILE:HG21	1:D:494:ALA:HB2	2.02	0.42
1:A:457:VAL:HG21	1:A:500:TYR:HA	2.00	0.42
1:B:146:MET:HG2	1:B:321:HIS:ND1	2.34	0.42
1:B:419:LYS:HG2	1:C:229:THR:HG21	2.01	0.42
1:C:427:TYR:H	1:C:498:ALA:HB1	1.84	0.42
1:A:106:HIS:HB2	1:D:246:SER:OG	2.19	0.42
1:A:252:ASN:HA	1:A:255:VAL:HG12	2.01	0.42
1:A:323:SER:O	1:A:324:LEU:HD13	2.19	0.42
1:A:557:HIS:HA	1:A:558:GLY:HA2	1.74	0.42
1:B:32:THR:HG21	1:B:162:LEU:CB	2.50	0.42
1:C:203:ARG:NH1	1:C:207:ALA:N	2.67	0.42
1:D:154:MET:O	1:D:157:ILE:HG13	2.20	0.42
1:D:156:GLU:HG3	1:D:309:ARG:HD2	2.02	0.42
1:A:6:PHE:HD1	1:A:14:LYS:HG2	1.84	0.42
1:A:450:ASP:O	1:A:452:GLU:N	2.51	0.42
1:B:139:GLU:HB3	1:B:324:LEU:HB3	2.01	0.42
1:B:438:SER:HB2	1:B:475:GLN:HA	2.00	0.42
1:D:391:LEU:O	1:D:395:ILE:HG13	2.20	0.42
1:D:436:ASN:ND2	1:D:479:GLY:O	2.52	0.42
1:B:374:LYS:NZ	1:B:504:GLU:OE1	2.52	0.42
1:B:557:HIS:HA	1:B:558:GLY:HA2	1.54	0.42
1:C:116:PHE:O	1:C:119:ILE:HG22	2.19	0.42
1:C:12:GLU:OE1	1:C:12:GLU:N	2.41	0.42
1:A:181:PHE:HZ	1:A:266:ILE:HG13	1.85	0.42
1:C:382:GLY:HA3	1:C:388:LYS:HD3	2.01	0.42
1:C:34:ALA:HA	1:C:82:PHE:HE2	1.84	0.42
1:A:69:PHE:HE1	1:D:280:LEU:HD13	1.85	0.42
1:A:527:ILE:HA	1:A:530:ILE:HG12	2.01	0.42
1:B:181:PHE:HE2	1:B:266:ILE:HD11	1.84	0.42
1:C:122:GLU:HA	1:C:125:THR:HG22	2.02	0.42
1:D:226:LYS:HD3	1:D:226:LYS:HA	1.89	0.42
1:D:346:ASN:HA	1:D:374:LYS:HD2	2.02	0.42
1:D:372:ILE:HD11	1:D:395:ILE:HD13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:39:MET:HB3	1:D:40:PRO:HD3	2.01	0.42
1:B:262:TYR:HD1	1:B:263:LEU:HD22	1.85	0.42
1:C:221:ASN:O	1:C:225:ILE:HG13	2.20	0.42
1:B:177:PHE:CE1	1:B:274:ILE:HD11	2.55	0.41
1:B:383:GLU:O	1:B:384:SER:OG	2.36	0.41
1:D:7:PHE:HE2	1:D:332:ARG:HG3	1.85	0.41
1:B:185:ASN:OD1	1:B:262:TYR:OH	2.27	0.41
1:B:247:LYS:O	1:B:250:ILE:HG12	2.19	0.41
1:B:108:ILE:HG23	1:B:328:TYR:CZ	2.55	0.41
1:B:438:SER:HA	1:B:476:THR:O	2.19	0.41
1:D:32:THR:HG21	1:D:162:LEU:HB3	2.02	0.41
1:B:405:GLN:NE2	1:B:412:GLU:OE1	2.53	0.41
1:A:108:ILE:HG22	1:A:328:TYR:OH	2.21	0.41
1:A:234:VAL:O	1:A:237:LEU:HG	2.21	0.41
1:B:112:VAL:HA	1:B:332:ARG:NH2	2.36	0.41
1:D:231:GLU:HG3	1:D:231:GLU:H	1.67	0.41
1:D:343:LEU:HD23	1:D:408:ILE:HD12	2.02	0.41
1:D:354:LEU:HD22	1:D:394:LEU:HD13	2.02	0.41
1:A:397:GLY:HA3	1:A:422:ARG:HG3	2.03	0.41
1:B:146:MET:SD	1:B:317:LEU:HG	2.61	0.41
1:D:116:PHE:O	1:D:119:ILE:HG22	2.21	0.41
1:A:188:ILE:HA	1:A:192:ILE:HD12	2.02	0.41
1:B:176:LEU:HA	1:B:176:LEU:HD13	1.97	0.41
1:C:171:ASN:O	1:C:175:THR:HG22	2.20	0.41
1:A:116:PHE:O	1:A:119:ILE:HG22	2.21	0.41
1:A:190:VAL:HA	1:A:194:SER:HB3	2.03	0.41
1:B:441:LYS:HA	1:B:442:ASN:O	2.20	0.41
1:C:372:ILE:HG12	1:C:378:ILE:HD13	2.03	0.41
1:B:225:ILE:HG12	1:C:445:PHE:HE2	1.86	0.41
1:C:262:TYR:HD1	1:C:263:LEU:HD22	1.84	0.41
1:C:39:MET:HE3	1:C:42:ILE:HG21	2.03	0.41
1:B:106:HIS:HB2	1:C:246:SER:HB2	2.03	0.41
1:C:112:VAL:HG21	1:C:328:TYR:HE1	1.86	0.41
1:C:152:LEU:HD11	1:C:309:ARG:HB3	2.03	0.41
1:C:166:LEU:HA	1:C:166:LEU:HD23	1.91	0.41
1:C:39:MET:HA	1:C:42:ILE:HG22	2.03	0.41
1:B:166:LEU:HD22	1:B:170:ILE:HD11	2.03	0.41
1:D:16:PHE:O	1:D:20:LEU:HD23	2.20	0.41
1:D:260:ARG:HG3	1:D:261:ILE:N	2.36	0.41
1:D:304:MET:HB2	1:D:305:PRO:HD3	2.03	0.41
1:D:380:PHE:CE1	1:D:391:LEU:HD13	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:467:ILE:CG2	1:D:474:VAL:HG22	2.50	0.41
1:D:49:SER:OG	1:D:50:TYR:N	2.53	0.41
1:A:289:ILE:HG21	1:D:46:SER:HB2	2.03	0.41
1:A:396:ILE:HB	1:A:425:ILE:HD12	2.03	0.41
1:B:318:LEU:HD23	1:B:318:LEU:HA	1.93	0.41
1:B:337:ASN:HD22	1:B:338:LEU:H	1.69	0.41
1:B:454:LEU:O	1:B:458:ILE:HG13	2.20	0.41
1:D:176:LEU:HA	1:D:176:LEU:HD13	1.90	0.41
1:A:110:TYR:HA	1:D:238:PHE:CE2	2.56	0.40
1:A:271:LEU:HD21	1:A:293:ILE:HD11	2.03	0.40
1:B:100:PHE:HA	1:B:104:ARG:HH21	1.85	0.40
1:B:189:LEU:HD21	1:B:262:TYR:CE1	2.56	0.40
1:B:156:GLU:HG3	1:B:309:ARG:HD2	2.03	0.40
1:B:518:GLN:HG3	1:B:518:GLN:H	1.72	0.40
1:C:32:THR:HG22	1:C:163:LEU:HG	2.02	0.40
1:A:401:PRO:O	1:C:515:LEU:HD21	2.21	0.40
1:D:96:LEU:HA	1:D:96:LEU:HD23	1.89	0.40
1:C:9:LEU:HB3	1:C:13:ASP:HB2	2.03	0.40
1:C:6:PHE:CD1	1:C:14:LYS:HG2	2.54	0.40
1:C:154:MET:O	1:C:157:ILE:HG13	2.21	0.40
1:A:427:TYR:CZ	1:D:223:LYS:HG2	2.56	0.40
1:D:400:LYS:HA	1:D:401:PRO:HD2	1.96	0.40
1:B:35:ILE:HG23	1:B:298:LEU:HB3	2.03	0.40
1:A:380:PHE:HA	1:A:553:TYR:O	2.21	0.40
1:C:133:LEU:O	1:C:137:THR:HG22	2.21	0.40
1:C:462:ASN:ND2	1:C:492:ARG:HD3	2.36	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	562/564 (100%)	478 (85%)	68 (12%)	16 (3%)	6	42
1	B	562/564 (100%)	478 (85%)	65 (12%)	19 (3%)	4	39
1	C	562/564 (100%)	478 (85%)	69 (12%)	15 (3%)	6	43
1	D	562/564 (100%)	477 (85%)	68 (12%)	17 (3%)	5	41
All	All	2248/2256 (100%)	1911 (85%)	270 (12%)	67 (3%)	5	41

All (67) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	321	HIS
1	A	436	ASN
1	A	439	ILE
1	A	442	ASN
1	A	443	ILE
1	A	502	GLU
1	B	443	ILE
1	B	487	GLY
1	B	502	GLU
1	C	443	ILE
1	C	502	GLU
1	D	443	ILE
1	D	487	GLY
1	D	502	GLU
1	A	67	PRO
1	A	399	LEU
1	A	487	GLY
1	B	67	PRO
1	B	436	ASN
1	B	439	ILE
1	B	442	ASN
1	C	67	PRO
1	C	399	LEU
1	C	436	ASN
1	C	439	ILE
1	C	480	ASP
1	C	487	GLY
1	D	54	ASN
1	D	67	PRO
1	D	436	ASN
1	D	439	ILE
1	D	442	ASN
1	D	480	ASP

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Mol	Chain	Res	Type
1	A	54	ASN
1	A	355	SER
1	A	480	ASP
1	B	54	ASN
1	B	355	SER
1	B	360	GLY
1	B	399	LEU
1	B	471	PRO
1	B	480	ASP
1	C	54	ASN
1	C	321	HIS
1	C	471	PRO
1	D	399	LEU
1	C	355	SER
1	C	442	ASN
1	D	321	HIS
1	D	355	SER
1	D	360	GLY
1	A	360	GLY
1	A	384	SER
1	A	471	PRO
1	B	321	HIS
1	B	354	LEU
1	B	406	ILE
1	B	451	GLU
1	C	360	GLY
1	C	406	ILE
1	D	323	SER
1	D	406	ILE
1	D	471	PRO
1	B	515	LEU
1	A	406	ILE
1	D	286	ILE
1	B	286	ILE

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	505/505 (100%)	475 (94%)	30 (6%)	23	59
1	B	505/505 (100%)	472 (94%)	33 (6%)	20	56
1	C	505/505 (100%)	474 (94%)	31 (6%)	22	58
1	D	505/505 (100%)	476 (94%)	29 (6%)	24	61
All	All	2020/2020 (100%)	1897 (94%)	123 (6%)	22	58

All (123) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	4	LYS
1	A	12	GLU
1	A	16	PHE
1	A	23	PHE
1	A	47	ASP
1	A	48	PHE
1	A	56	TYR
1	A	58	ILE
1	A	104	ARG
1	A	139	GLU
1	A	172	TYR
1	A	203	ARG
1	A	215	LEU
1	A	249	ASN
1	A	264	GLU
1	A	266	ILE
1	A	281	LYS
1	A	289	ILE
1	A	301	TYR
1	A	328	TYR
1	A	332	ARG
1	A	335	GLU
1	A	368	LEU
1	A	383	GLU
1	A	442	ASN
1	A	451	GLU
1	A	483	SER
1	A	543	LEU
1	A	555	LEU
1	B	3	LYS
1	B	5	LEU
1	B	16	PHE

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Mol	Chain	Res	Type
1	B	23	PHE
1	B	48	PHE
1	B	58	ILE
1	B	104	ARG
1	B	139	GLU
1	B	152	LEU
1	B	172	TYR
1	B	203	ARG
1	B	215	LEU
1	B	238	PHE
1	B	266	ILE
1	B	278	LEU
1	B	281	LYS
1	B	301	TYR
1	B	302	ARG
1	B	317	LEU
1	B	319	TYR
1	B	332	ARG
1	B	337	ASN
1	B	366	LYS
1	B	368	LEU
1	B	386	CYS
1	B	437	ASP
1	B	442	ASN
1	B	451	GLU
1	B	483	SER
1	B	525	ASP
1	B	542	ARG
1	B	543	LEU
1	B	557	HIS
1	C	3	LYS
1	C	23	PHE
1	C	39	MET
1	C	104	ARG
1	C	137	THR
1	C	139	GLU
1	C	140	VAL
1	C	146	MET
1	C	203	ARG
1	C	215	LEU
1	C	231	GLU
1	C	249	ASN

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Mol	Chain	Res	Type
1	C	255	VAL
1	C	266	ILE
1	C	281	LYS
1	C	289	ILE
1	C	290	LEU
1	C	317	LEU
1	C	319	TYR
1	C	324	LEU
1	C	332	ARG
1	C	368	LEU
1	C	370	LEU
1	C	437	ASP
1	C	442	ASN
1	C	451	GLU
1	C	483	SER
1	C	515	LEU
1	C	535	THR
1	C	542	ARG
1	C	555	LEU
1	D	3	LYS
1	D	23	PHE
1	D	104	ARG
1	D	108	ILE
1	D	140	VAL
1	D	172	TYR
1	D	203	ARG
1	D	213	GLU
1	D	214	ILE
1	D	215	LEU
1	D	231	GLU
1	D	246	SER
1	D	249	ASN
1	D	266	ILE
1	D	281	LYS
1	D	289	ILE
1	D	301	TYR
1	D	317	LEU
1	D	319	TYR
1	D	328	TYR
1	D	332	ARG
1	D	368	LEU
1	D	373	LYS

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Mol	Chain	Res	Type
1	D	437	ASP
1	D	442	ASN
1	D	451	GLU
1	D	483	SER
1	D	535	THR
1	D	542	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	218	ASN
1	B	241	GLN
1	D	329	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	564/564 (100%)	-0.21	13 (2%) 61 51	122, 177, 272, 322	0
1	B	564/564 (100%)	-0.22	20 (3%) 44 35	156, 204, 285, 320	0
1	C	564/564 (100%)	-0.07	22 (3%) 40 31	139, 215, 288, 326	0
1	D	564/564 (100%)	-0.04	29 (5%) 29 23	127, 218, 286, 328	0
All	All	2256/2256 (100%)	-0.14	84 (3%) 42 33	122, 202, 284, 328	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	52	ASP	8.3
1	B	564	LYS	7.5
1	C	541	HIS	7.5
1	B	287	SER	7.2
1	A	282	ASN	6.6
1	B	46	SER	6.5
1	B	282	ASN	6.3
1	D	52	ASP	5.4
1	D	362	LYS	5.4
1	D	518	GLN	5.3
1	D	357	GLY	5.2
1	B	285	ASP	5.1
1	C	366	LYS	5.1
1	D	361	LYS	5.0
1	C	287	SER	4.4
1	C	62	GLU	4.3
1	B	47	ASP	4.3
1	C	284	SER	4.2
1	D	516	ASP	4.2
1	D	285	ASP	4.2
1	C	355	SER	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	282	ASN	3.9
1	D	562	GLU	3.9
1	B	281	LYS	3.9
1	B	514	ALA	3.8
1	C	403	GLU	3.7
1	B	410	LYS	3.7
1	D	515	LEU	3.6
1	A	51	PHE	3.6
1	D	360	GLY	3.5
1	B	277	PHE	3.5
1	B	286	ILE	3.5
1	D	287	SER	3.4
1	D	448	ALA	3.4
1	C	52	ASP	3.4
1	C	276	VAL	3.4
1	D	359	GLU	3.3
1	C	286	ILE	3.3
1	B	460	GLN	3.2
1	A	469	ASN	3.2
1	C	546	ILE	3.1
1	A	564	LYS	3.0
1	D	561	LYS	3.0
1	D	126	GLN	3.0
1	B	515	LEU	3.0
1	C	285	ASP	2.9
1	A	62	GLU	2.9
1	A	277	PHE	2.9
1	B	465	HIS	2.8
1	B	62	GLU	2.8
1	B	278	LEU	2.8
1	D	557	HIS	2.8
1	C	363	TYR	2.7
1	D	323	SER	2.7
1	C	55	LYS	2.6
1	C	277	PHE	2.6
1	B	464	GLU	2.5
1	B	321	HIS	2.5
1	A	191	LYS	2.5
1	A	323	SER	2.4
1	D	340	GLU	2.4
1	B	517	THR	2.4
1	D	358	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	283	GLU	2.4
1	A	561	LYS	2.3
1	C	402	LYS	2.3
1	D	447	ASP	2.3
1	A	549	CYS	2.3
1	D	55	LYS	2.3
1	B	6	PHE	2.3
1	D	128	ASN	2.3
1	C	511	ALA	2.2
1	C	512	THR	2.2
1	A	198	LYS	2.2
1	A	281	LYS	2.2
1	D	54	ASN	2.2
1	D	363	TYR	2.1
1	C	417	ASN	2.1
1	D	414	ASN	2.1
1	D	129	GLN	2.1
1	D	564	LYS	2.0
1	D	342	LYS	2.0
1	D	51	PHE	2.0
1	C	63	TYR	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.