



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 5, 2017 – 10:56 AM EST

PDB ID : 5FFO  
Title : Integrin alpha V beta 6 in complex with pro-TGF-beta  
Authors : Dong, X.; Zhao, B.; Springer, T.A.  
Deposited on : 2015-12-18  
Resolution : 3.49 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  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20028442  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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-20028442

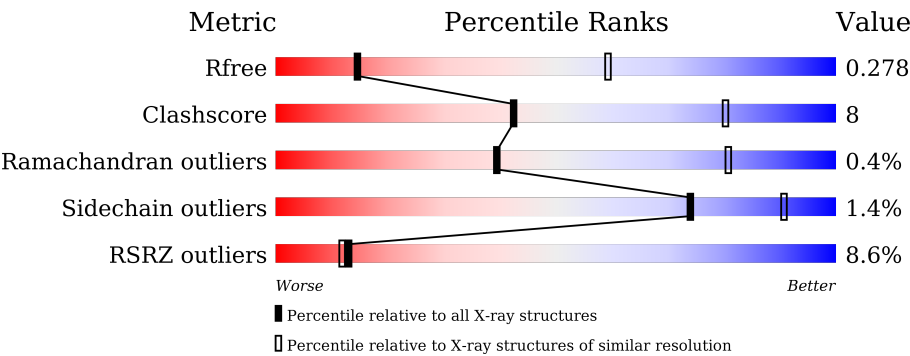
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.49 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))
$R_{free}$	91344	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

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	601	<div><div>8%</div><div><div></div><div>80%</div><div>18%</div><div>.</div></div></div>
1	E	601	<div><div>9%</div><div><div></div><div>82%</div><div>16%</div><div>.</div></div></div>
2	B	257	<div><div>%</div><div><div></div><div>68%</div><div>26%</div><div>6%</div></div></div>
2	F	257	<div><div>6%</div><div><div></div><div>72%</div><div>23%</div><div>6%</div></div></div>
3	C	363	<div><div>10%</div><div><div></div><div>62%</div><div>21%</div><div>.</div><div>16%</div></div></div>
3	D	363	<div><div>11%</div><div><div></div><div>65%</div><div>22%</div><div>.</div><div>11%</div></div></div>

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Mol	Chain	Length	Quality of chain
3	G	363	
3	H	363	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	MAN	A	2012	-	-	-	X
8	MN	B	2001	-	-	-	X
8	MN	B	2002	-	-	-	X

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 23786 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 Integrin alpha-V.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	589	Total	C	N	O	S	0	0	0
			4570	2898	776	875	21			
1	E	587	Total	C	N	O	S	0	0	0
			4547	2880	772	874	21			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	400	GLY	-	insertion	UNP P06756
A	401	CYS	MET	conflict	UNP P06756
A	597	THR	CYS	conflict	UNP P06756
A	599	GLY	-	expression tag	UNP P06756
A	600	LEU	-	expression tag	UNP P06756
A	601	GLU	-	expression tag	UNP P06756
E	400	GLY	-	insertion	UNP P06756
E	401	CYS	MET	conflict	UNP P06756
E	597	THR	CYS	conflict	UNP P06756
E	599	GLY	-	expression tag	UNP P06756
E	600	LEU	-	expression tag	UNP P06756
E	601	GLU	-	expression tag	UNP P06756

- Molecule 2 is a protein called Integrin beta-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	242	Total	C	N	O	S	0	0	0
			1891	1210	302	368	11			
2	F	242	Total	C	N	O	S	0	0	0
			1891	1210	302	368	11			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	270	CYS	ILE	conflict	UNP P18564
B	362	HIS	-	expression tag	UNP P18564
B	363	HIS	-	expression tag	UNP P18564
B	364	HIS	-	expression tag	UNP P18564
B	365	HIS	-	expression tag	UNP P18564
B	366	HIS	-	expression tag	UNP P18564
B	367	HIS	-	expression tag	UNP P18564
F	270	CYS	ILE	conflict	UNP P18564
F	362	HIS	-	expression tag	UNP P18564
F	363	HIS	-	expression tag	UNP P18564
F	364	HIS	-	expression tag	UNP P18564
F	365	HIS	-	expression tag	UNP P18564
F	366	HIS	-	expression tag	UNP P18564
F	367	HIS	-	expression tag	UNP P18564

- Molecule 3 is a protein called Transforming growth factor beta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	305	Total	C	N	O	S	0	0	0
			2445	1555	434	439	17			
3	D	322	Total	C	N	O	S	0	0	0
			2590	1650	457	466	17			
3	G	297	Total	C	N	O	S	0	0	0
			2399	1529	425	429	16			
3	H	325	Total	C	N	O	S	0	0	0
			2612	1660	465	471	16			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	GLY	-	expression tag	UNP P01137
C	0	PRO	-	expression tag	UNP P01137
C	1	LEU	-	expression tag	UNP P01137
C	2	SER	-	expression tag	UNP P01137
C	3	THR	-	expression tag	UNP P01137
C	4	SER	-	expression tag	UNP P01137
C	107	GLN	ASN	conflict	UNP P01137
C	147	GLN	ASN	conflict	UNP P01137
D	-1	GLY	-	expression tag	UNP P01137
D	0	PRO	-	expression tag	UNP P01137
D	1	LEU	-	expression tag	UNP P01137
D	2	SER	-	expression tag	UNP P01137
D	3	THR	-	expression tag	UNP P01137

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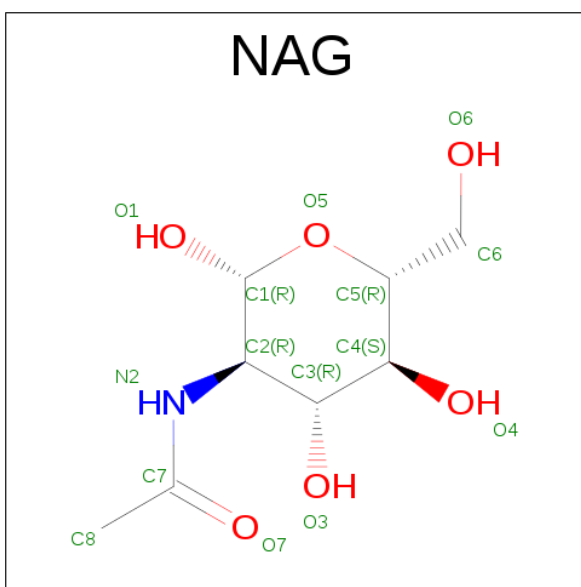
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Chain	Residue	Modelled	Actual	Comment	Reference
D	4	SER	-	expression tag	UNP P01137
D	107	GLN	ASN	conflict	UNP P01137
D	147	GLN	ASN	conflict	UNP P01137
G	-1	GLY	-	expression tag	UNP P01137
G	0	PRO	-	expression tag	UNP P01137
G	1	LEU	-	expression tag	UNP P01137
G	2	SER	-	expression tag	UNP P01137
G	3	THR	-	expression tag	UNP P01137
G	4	SER	-	expression tag	UNP P01137
G	107	GLN	ASN	conflict	UNP P01137
G	147	GLN	ASN	conflict	UNP P01137
H	-1	GLY	-	expression tag	UNP P01137
H	0	PRO	-	expression tag	UNP P01137
H	1	LEU	-	expression tag	UNP P01137
H	2	SER	-	expression tag	UNP P01137
H	3	THR	-	expression tag	UNP P01137
H	4	SER	-	expression tag	UNP P01137
H	107	GLN	ASN	conflict	UNP P01137
H	147	GLN	ASN	conflict	UNP P01137

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	4	Total Ca 4 4	0	0
4	E	4	Total Ca 4 4	0	0

- Molecule 5 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



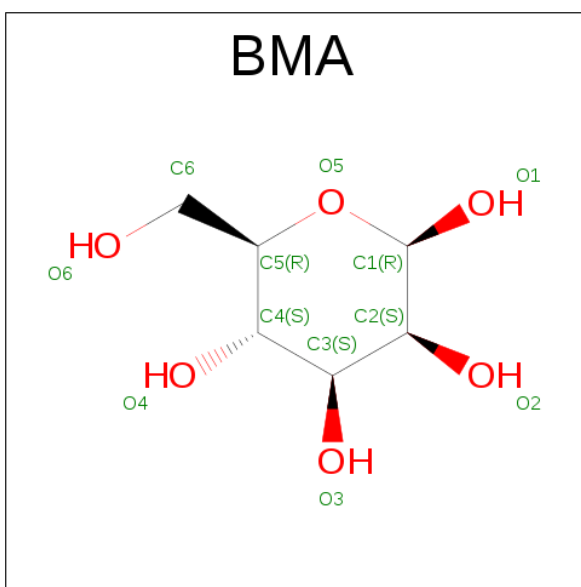
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		

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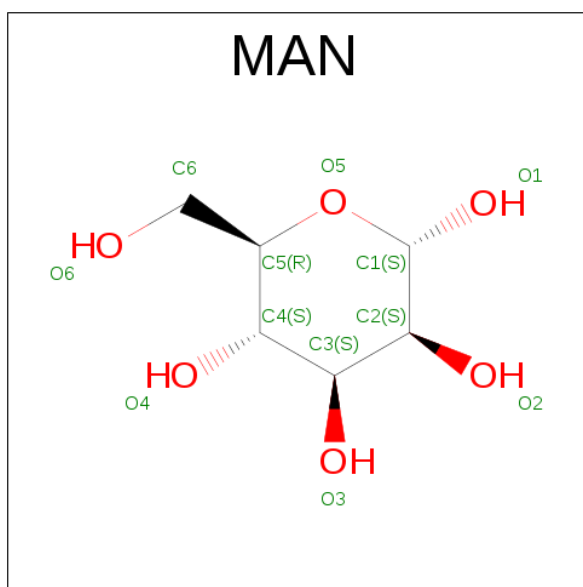
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	D	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	F	1	Total	C	N	O	0	0
			14	8	1	5		
5	G	1	Total	C	N	O	0	0
			14	8	1	5		
5	G	1	Total	C	N	O	0	0
			14	8	1	5		
5	H	1	Total	C	N	O	0	0
			14	8	1	5		
5	H	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is BETA-D-MANNOSE (three-letter code: BMA) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			11	6	5		
6	A	1	Total	C	O	0	0
			11	6	5		
6	A	1	Total	C	O	0	0
			11	6	5		
6	A	1	Total	C	O	0	0
			11	6	5		
6	C	1	Total	C	O	0	0
			11	6	5		
6	D	1	Total	C	O	0	0
			11	6	5		
6	E	1	Total	C	O	0	0
			11	6	5		
6	E	1	Total	C	O	0	0
			11	6	5		
6	E	1	Total	C	O	0	0
			11	6	5		
6	E	1	Total	C	O	0	0
			11	6	5		
6	G	1	Total	C	O	0	0
			11	6	5		
6	H	1	Total	C	O	0	0
			11	6	5		

- Molecule 7 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			11	6	5		
7	A	1	Total	C	O	0	0
			11	6	5		
7	A	1	Total	C	O	0	0
			11	6	5		
7	A	1	Total	C	O	0	0
			11	6	5		
7	A	1	Total	C	O	0	0
			11	6	5		
7	A	1	Total	C	O	0	0
			11	6	5		
7	A	1	Total	C	O	0	0
			11	6	5		
7	C	1	Total	C	O	0	0
			11	6	5		
7	D	1	Total	C	O	0	0
			11	6	5		
7	E	1	Total	C	O	0	0
			11	6	5		
7	E	1	Total	C	O	0	0
			11	6	5		
7	E	1	Total	C	O	0	0
			11	6	5		
7	E	1	Total	C	O	0	0
			11	6	5		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	E	1	Total C O 11 6 5	0	0
7	E	1	Total C O 11 6 5	0	0
7	E	1	Total C O 11 6 5	0	0
7	E	1	Total C O 11 6 5	0	0
7	G	1	Total C O 11 6 5	0	0
7	H	1	Total C O 11 6 5	0	0
7	H	1	Total C O 11 6 5	0	0
7	H	1	Total C O 11 6 5	0	0

- Molecule 8 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	3	Total Mn 3 3	0	0
8	F	3	Total Mn 3 3	0	0

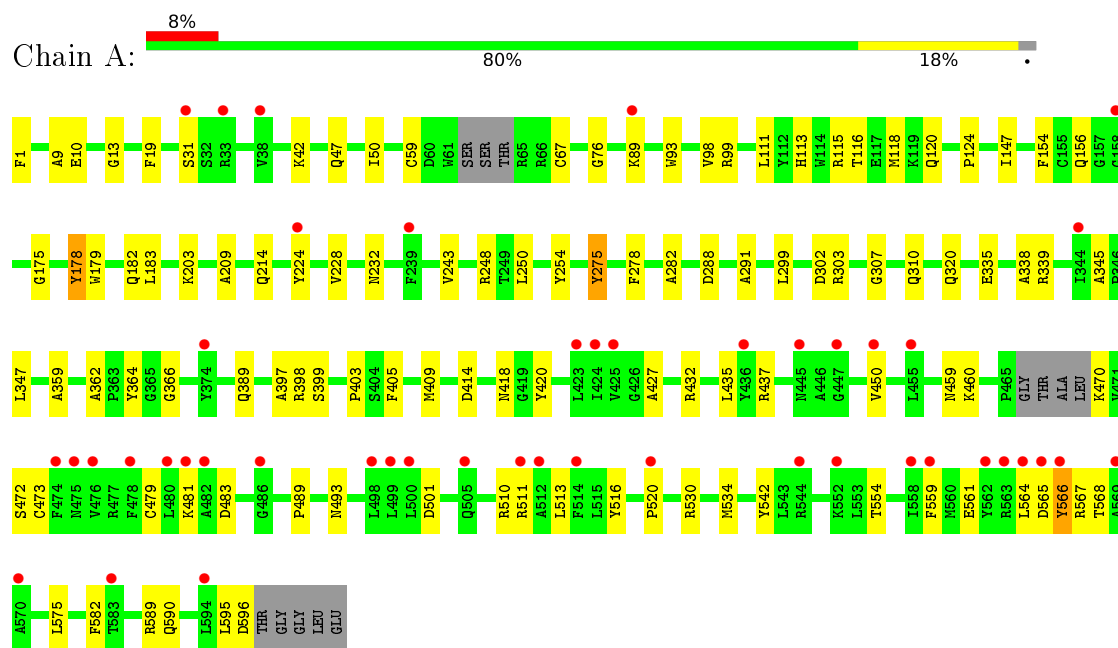
- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	3	Total O 3 3	0	0
9	F	2	Total O 2 2	0	0

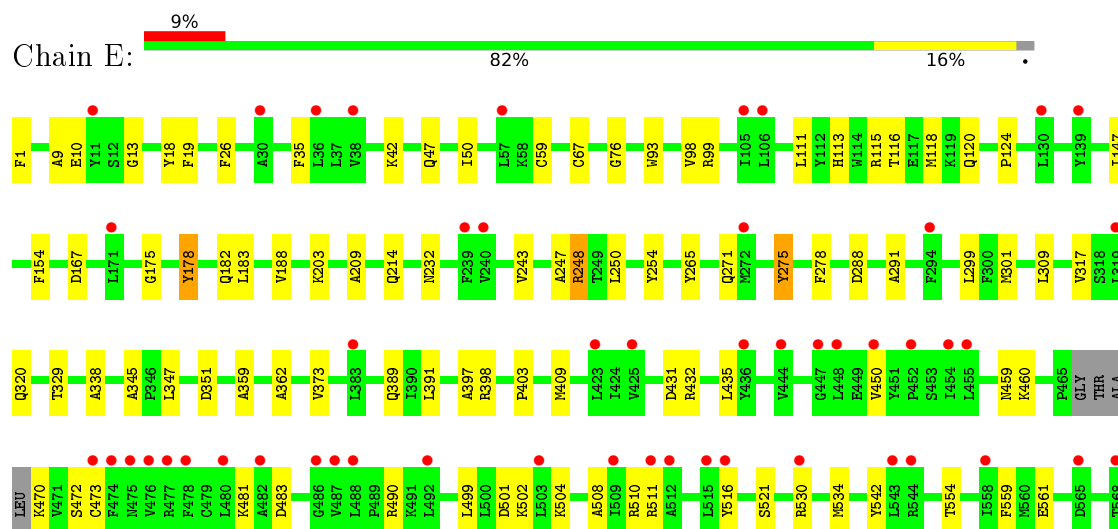
### 3 Residue-property plots [i](#)

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: Integrin alpha-V



#### • Molecule 1: Integrin alpha-V





Chain D:

11% 65% 22% 11%

GLY PRO LEU SER THR ALA GLN GLU ASP ASN LYS VAL ILE MET PHE TYR HIS ARG TRP

D217 L218 A219 T220 H222 P227 F228 W232 A233 R238 A239 Q240 H245 L246 G247 L248 S249 A250 T251 L252 S253 L254 L255 L256 L257 L258 L259 L260 L261 L262 L263 L264 L265 L266 L267 L268 L269 L270 L271 L272 L273 L274 L275 L276 L277 L278 L279 L280 W281 L282 H283 Y288 L289 L290 L291 L292 L293 L294 L295 L296 L297 L298 L299 L300 L301 L302 L303 L304 L305 L306 L307 L308 L309 L310 L311 L312 L313 L314 L315 L316 L317 L318 L319 L320 L321 L322 L323 L324 L325 L326 L327 L328 L329 L330 L331 L332 L333 L334 L335 L336 L337 L338 L339 L340 L341 L342 L343 L344 L345 L346 L347 L348 L349 L350 L351 L352 L353 L354 L355 L356 L357 L358 L359 L360 L361 L362 L363 L364 L365 L366 L367 L368 L369 L370 L371 L372 L373 L374 L375 L376 L377 L378 L379 L380 L381 L382 L383 L384 L385 L386 L387 L388 L389 L390 L391 L392 L393 L394 L395 L396 L397 L398 L399 L400 L401 L402 L403 L404 L405 L406 L407 L408 L409 L410 L411 L412 L413 L414 L415 L416 L417 L418 L419 L420 L421 L422 L423 L424 L425 L426 L427 L428 L429 L430 L431 L432 L433 L434 L435 L436 L437 L438 L439 L440 L441 L442 L443 L444 L445 L446 L447 L448 L449 L450 L451 L452 L453 L454 L455 L456 L457 L458 L459 L460 L461 L462 L463 L464 L465 L466 L467 L468 L469 L470 L471 L472 L473 L474 L475 L476 L477 L478 L479 L480 L481 L482 L483 L484 L485 L486 L487 L488 L489 L490 L491 L492 L493 L494 L495 L496 L497 L498 L499 L500 L501 L502 L503 L504 L505 L506 L507 L508 L509 L510 L511 L512 L513 L514 L515 L516 L517 L518 L519 L520 L521 L522 L523 L524 L525 L526 L527 L528 L529 L530 L531 L532 L533 L534 L535 L536 L537 L538 L539 L540 L541 L542 L543 L544 L545 L546 L547 L548 L549 L550 L551 L552 L553 L554 L555 L556 L557 L558 L559 L560 L561 L562 L563 L564 L565 L566 L567 L568 L569 L570 L571 L572 L573 L574 L575 L576 L577 L578 L579 L580 L581 L582 L583 L584 L585 L586 L587 L588 L589 L590 L591 L592 L593 L594 L595 L596 L597 L598 L599 L600 L601 L602 L603 L604 L605 L606 L607 L608 L609 L610 L611 L612 L613 L614 L615 L616 L617 L618 L619 L620 L621 L622 L623 L624 L625 L626 L627 L628 L629 L630 L631 L632 L633 L634 L635 L636 L637 L638 L639 L640 L641 L642 L643 L644 L645 L646 L647 L648 L649 L650 L651 L652 L653 L654 L655 L656 L657 L658 L659 L660 L661 L662 L663 L664 L665 L666 L667 L668 L669 L670 L671 L672 L673 L674 L675 L676 L677 L678 L679 L680 L681 L682 L683 L684 L685 L686 L687 L688 L689 L690 L691 L692 L693 L694 L695 L696 L697 L698 L699 L700 L701 L702 L703 L704 L705 L706 L707 L708 L709 L710 L711 L712 L713 L714 L715 L716 L717 L718 L719 L720 L721 L722 L723 L724 L725 L726 L727 L728 L729 L730 L731 L732 L733 L734 L735 L736 L737 L738 L739 L740 L741 L742 L743 L744 L745 L746 L747 L748 L749 L750 L751 L752 L753 L754 L755 L756 L757 L758 L759 L760 L761 L762 L763 L764 L765 L766 L767 L768 L769 L770 L771 L772 L773 L774 L775 L776 L777 L778 L779 L780 L781 L782 L783 L784 L785 L786 L787 L788 L789 L790 L791 L792 L793 L794 L795 L796 L797 L798 L799 L800 L801 L802 L803 L804 L805 L806 L807 L808 L809 L810 L811 L812 L813 L814 L815 L816 L817 L818 L819 L820 L821 L822 L823 L824 L825 L826 L827 L828 L829 L830 L831 L832 L833 L834 L835 L836 L837 L838 L839 L840 L841 L842 L843 L844 L845 L846 L847 L848 L849 L850 L851 L852 L853 L854 L855 L856 L857 L858 L859 L860 L861 L862 L863 L864 L865 L866 L867 L868 L869 L870 L871 L872 L873 L874 L875 L876 L877 L878 L879 L880 L881 L882 L883 L884 L885 L886 L887 L888 L889 L890 L891 L892 L893 L894 L895 L896 L897 L898 L899 L900 L901 L902 L903 L904 L905 L906 L907 L908 L909 L910 L911 L912 L913 L914 L915 L916 L917 L918 L919 L920 L921 L922 L923 L924 L925 L926 L927 L928 L929 L930 L931 L932 L933 L934 L935 L936 L937 L938 L939 L940 L941 L942 L943 L944 L945 L946 L947 L948 L949 L950 L951 L952 L953 L954 L955 L956 L957 L958 L959 L960 L961 L962 L963 L964 L965 L966 L967 L968 L969 L970 L971 L972 L973 L974 L975 L976 L977 L978 L979 L980 L981 L982 L983 L984 L985 L986 L987 L988 L989 L990 L991 L992 L993 L994 L995 L996 L997 L998 L999 L1000 L1001 L1002 L1003 L1004 L1005 L1006 L1007 L1008 L1009 L1010 L1011 L1012 L1013 L1014 L1015 L1016 L1017 L1018 L1019 L1020 L1021 L1022 L1023 L1024 L1025 L1026 L1027 L1028 L1029 L1030 L1031 L1032 L1033 L1034 L1035 L1036 L1037 L1038 L1039 L1040 L1041 L1042 L1043 L1044 L1045 L1046 L1047 L1048 L1049 L1050 L1051 L1052 L1053 L1054 L1055 L1056 L1057 L1058 L1059 L1060 L1061 L1062 L1063 L1064 L1065 L1066 L1067 L1068 L1069 L1070 L1071 L1072 L1073 L1074 L1075 L1076 L1077 L1078 L1079 L1080 L1081 L1082 L1083 L1084 L1085 L1086 L1087 L1088 L1089 L1090 L1091 L1092 L1093 L1094 L1095 L1096 L1097 L1098 L1099 L1100 L1101 L1102 L1103 L1104 L1105 L1106 L1107 L1108 L1109 L1110 L1111 L1112 L1113 L1114 L1115 L1116 L1117 L1118 L1119 L1120 L1121 L1122 L1123 L1124 L1125 L1126 L1127 L1128 L1129 L1130 L1131 L1132 L1133 L1134 L1135 L1136 L1137 L1138 L1139 L1140 L1141 L1142 L1143 L1144 L1145 L1146 L1147 L1148 L1149 L1150 L1151 L1152 L1153 L1

Chain G:

9%

59%

22%

18%

Chain H:

6% 69% 20% 10%

GLY PRO LEU SER THR SER K5 N9 E10 L11 R14 I17 R21 K27 L28 E38 P45 V48 S54 D57 R58 V59 A60 G61 GLU SER ALA GLU PRO GLU PRQ GLU GLU P70 E78 V79 L83 M84 E90 F95 F105 S109 E113

P116 L121 L127 L128 L129 R130 V135 F136 Q137 Y145 S146 T147 M148 R156 L157 L158 W166 L167 R176 A192 C194 S195 H193 S198 R199 D200 L202 L203 F210 T211 T212 G213 R214 R215 G216 D217 T220 I221 H222 P227 F228 M232 L236 F237 P238

K239 Q240 H153 L154 G155 S156 S157 A158 H159 H160 H161 H162 H163 H164 H165 H166 H167 H168 H169 H170 H171 H172 H173 H174 H175 H176 H177 H178 H179 H180 H181 H182 H183 H184 H185 H186 H187 H188 H189 H190 H191 H192 H193 H194 H195 H196 H197 H198 H199 H200 H201 H202 H203 H204 H205 H206 H207 H208 H209 H210 H211 H212 H213 H214 H215 H216 H217 H218 H219 H220 H221 H222 H223 H224 H225 H226 H227 H228 H229 H230 H231 H232 H233 H234 H235 H236 H237 H238 H239 H240 H241 H242 H243 H244 H245 H246 H247 H248 H249 H250 H251 H252 H253 H254 H255 H256 H257 H258 H259 H260 H261 H262 H263 H264 H265 H266 H267 H268 H269 H270 H271 H272 H273 H274 H275 H276 H277 H278 H279 H280 H281 H282 H283 H284 H285 H286 H287 H288 H289 H290 H291 H292 H293 H294 H295 H296 H297 H298 H299 H300 D304 T305 G306 A307 S308 T309 C310 G311 A312 S313 T314 G315 A316 S317 T318 C319 G320 A321 S322 T323 G324 A325 S326 T327 C328 G329 A330 S331 T332 G333 A334 S335 T336 C337 G338 A339 S340 T341 G342 A343 S344 T345 C346 G347 A348 S349 T350 C351 G352 A353 S354 T355 C356 G357 A358 S359 T360 C361 G362 A363 S364 T365 C366 G367 A368 S369 T370 C371 G372 A373 S374 T375 C376 G377 A378 S379 T380 C381 G382 A383 S384 T385 C386 G387 A388 S389 T390 C391 G392 A393 S394 T395 C396 G397 A398 S399 T400 C401 G402 A403 S404 T405 C406 G407 A408 S409 T410 C411 G412 A413 S414 T415 C416 G417 A418 S419 T420 C421 G422 A423 S424 T425 C426 G427 A428 S429 T430 C431 G432 A433 S434 T435 C436 G437 A438 S439 T440 C441 G442 A443 S444 T445 C446 G447 A448 S449 T450 C451 G452 A453 S454 T455 C456 G457 A458 S459 T460 C461 G462 A463 S464 T465 C466 G467 A468 S469 T470 C471 G472 A473 S474 T475 C476 G477 A478 S479 T480 C481 G482 A483 S484 T485 C486 G487 A488 S489 T490 C491 G492 A493 S494 T495 C496 G497 A498 S499 T500 C501 G502 A503 S504 T505 C506 G507 A508 S509 T510 C511 G512 A513 S514 T515 C516 G517 A518 S519 T520 C521 G522 A523 S524 T525 C526 G527 A528 S529 T530 C531 G532 A533 S534 T535 C536 G537 A538 S539 T540 C541 G542 A543 S544 T545 C546 G547 A548 S549 T550 C551 G552 A553 S554 T555 C556 G557 A558 S559 T560 C561 G562 A563 S564 T565 C566 G567 A568 S569 T570 C571 G572 A573 S574 T575 C576 G577 A578 S579 T580 C581 G582 A583 S584 T585 C586 G587 A588 S589 T590 C591 G592 A593 S594 T595 C596 G597 A598 S599 T600 C601 G602 A603 S604 T605 C606 G607 A608 S609 T610 C611 G612 A613 S614 T615 C616 G617 A618 S619 T620 C621 G622 A623 S624 T625 C626 G627 A628 S629 T630 C631 G632 A633 S634 T635 C636 G637 A638 S639 T640 C641 G642 A643 S644 T645 C646 G647 A648 S649 T650 C651 G652 A653 S654 T655 C656 G657 A658 S659 T660 C661 G662 A663 S664 T665 C666 G667 A668 S669 T670 C671 G672 A673 S674 T675 C676 G677 A678 S679 T680 C681 G682 A683 S684 T685 C686 G687 A688 S689 T690 C691 G692 A693 S694 T695 C696 G697 A698 S699 T700 C701 G702 A703 S704 T705 C706 G707 A708 S709 T710 C711 G712 A713 S714 T715 C716 G717 A718 S719 T720 C721 G722 A723 S724 T725 C726 G727 A728 S729 T730 C731 G732 A733 S734 T735 C736 G737 A738 S739 T740 C741 G742 A743 S744 T745 C746 G747 A748 S749 T750 C751 G752 A753 S754 T755 C756 G757 A758 S759 T760 C761 G762 A763 S764 T765 C766 G767 A768 S769 T770 C771 G772 A773 S774 T775 C776 G777 A778 S779 T780 C781 G782 A783 S784 T785 C786 G787 A788 S789 T790 C791 G792 A793 S794 T795 C796 G797 A798 S799 T800 C801 G802 A803 S804 T805 C806 G807 A808 S809 T810 C811 G812 A813 S814 T815 C816 G817 A818 S819 T820 C821 G822 A823 S824 T825 C826 G827 A828 S829 T830 C831 G832 A833 S834 T835 C836 G837 A838 S839 T840 C841 G842 A843 S844 T845 C846 G847 A848 S849 T850 C851 G852 A853 S854 T855 C856 G857 A858 S859 T860 C861 G862 A863 S864 T865 C866 G867 A868 S869 T870 C871 G872 A873 S874 T875 C876 G877 A878 S879 T880 C881 G882 A883 S884 T885 C886 G887 A888 S889 T890 C891 G892 A893 S894 T895 C896 G897 A898 S899 T900 C901 G902 A903 S904 T905 C906 G907 A908 S909 T910 C911 G912 A913 S914 T915 C916 G917 A918 S919 T920 C921 G922 A923 S924 T925 C926 G927 A928 S929 T930 C931 G932 A933 S934 T935 C936 G937 A938 S939 T940 C941 G942 A943 S944 T945 C946 G947 A948 S949 T950 C951 G952 A953 S954 T955 C956 G957 A958 S959 T960 C961 G962 A963 S964 T965 C966 G967 A968 S969 T970 C971 G972 A973 S974 T975 C976 G977 A978 S979 T980 C981 G982 A983 S984 T985 C986 G987 A988 S989 T990 C991 G992 A993 S994 T995 C996 G997 A998 S999 T1000 C1001 G1002 A1003 S1004 T1005 C1006 G1007 A1008 S1009 T1010 C1011 G1012 A1013 S1014 T1015 C1016 G1017 A1018 S1019 T1020 C1021 G1022 A1023 S1024 T1025 C1026 G1027 A1028 S1029 T1030 C1031 G1032 A1033 S1034 T1035 C1036 G1037 A1038 S1039 T1040 C1041 G1042 A1043 S1044 T1045 C1046 G1047 A1048 S1049 T1050 C1051 G1052 A1053 S1054 T1055 C1056 G1057 A1058 S1059 T1060 C10

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.44Å 91.44Å 131.03Å 89.98° 86.25° 89.85°	Depositor
Resolution (Å)	45.72 – 3.49 45.72 – 3.49	Depositor EDS
% Data completeness (in resolution range)	94.4 (45.72-3.49) 94.0 (45.72-3.49)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.05 (at 3.48Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, $R_{free}$	0.224 , 0.277 0.224 , 0.278	Depositor DCC
$R_{free}$ test set	1059 reflections (2.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	124.4	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 159.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.286 for -h,k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	23786	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	217.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.95% 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 ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, CA, BMA, NAG, MN

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	0/4672	0.49	1/6321 (0.0%)
1	E	0.28	0/4649	0.48	0/6291
2	B	0.35	0/1930	0.50	0/2618
2	F	0.32	1/1930 (0.1%)	0.44	0/2618
3	C	0.35	2/2501 (0.1%)	0.47	1/3381 (0.0%)
3	D	0.45	5/2650 (0.2%)	0.51	0/3585
3	G	0.37	2/2454 (0.1%)	0.45	0/3317
3	H	0.45	4/2672 (0.1%)	0.52	0/3616
All	All	0.35	14/23458 (0.1%)	0.48	2/31747 (0.0%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	38	GLU	CG-CD	8.88	1.65	1.51
3	D	38	GLU	CG-CD	8.35	1.64	1.51
3	C	38	GLU	CG-CD	8.05	1.64	1.51
3	H	148	ASN	CB-CG	7.88	1.69	1.51
3	H	38	GLU	CB-CG	7.88	1.67	1.52
3	G	38	GLU	CG-CD	7.64	1.63	1.51
3	D	38	GLU	CB-CG	6.93	1.65	1.52
3	H	261	GLU	CD-OE1	6.15	1.32	1.25
3	D	38	GLU	CD-OE1	6.11	1.32	1.25
3	D	148	ASN	CB-CG	5.76	1.64	1.51
3	G	38	GLU	CB-CG	5.50	1.62	1.52
2	F	342	ASN	CB-CG	5.41	1.63	1.51
3	D	112	ARG	CG-CD	5.19	1.65	1.51
3	C	38	GLU	CB-CG	5.17	1.61	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	595	LEU	CA-CB-CG	7.55	132.66	115.30
3	C	319	PRO	N-CA-CB	5.96	110.45	103.30

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	4570	0	4414	73	0
1	E	4547	0	4388	60	0
2	B	1891	0	1866	48	0
2	F	1891	0	1866	33	0
3	C	2445	0	2435	51	0
3	D	2590	0	2580	55	0
3	G	2399	0	2394	52	0
3	H	2612	0	2608	45	0
4	A	4	0	0	0	0
4	E	4	0	0	0	0
5	A	154	0	134	3	0
5	B	14	0	13	0	0
5	C	28	0	24	1	0
5	D	28	0	24	0	0
5	E	154	0	134	6	0
5	F	14	0	13	0	0
5	G	28	0	24	0	0
5	H	28	0	24	0	0
6	A	44	0	35	2	0
6	C	11	0	9	0	0
6	D	11	0	9	0	0
6	E	44	0	35	2	0
6	G	11	0	9	0	0
6	H	11	0	8	0	0
7	A	88	0	77	1	0
7	C	11	0	10	0	0
7	D	11	0	10	0	0
7	E	88	0	77	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	G	11	0	10	0	0
7	H	33	0	29	0	0
8	B	3	0	0	0	0
8	F	3	0	0	0	0
9	B	3	0	0	0	0
9	F	2	0	0	0	0
All	All	23786	0	23259	390	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 8.

All (390) 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:A:248:ARG:HE	2:B:320:LEU:HD12	1.35	0.92
1:A:460:LYS:HB3	1:A:470:LYS:HB3	1.63	0.80
1:E:502:LYS:HE2	5:E:2026:NAG:H81	1.65	0.79
3:C:100:HIS:HA	3:C:210:PHE:HB2	1.68	0.75
3:C:261:GLU:HG3	3:C:263:ASN:H	1.51	0.74
1:E:397:ALA:HB2	1:E:403:PRO:HD3	1.66	0.74
1:E:460:LYS:HB3	1:E:470:LYS:HB3	1.68	0.73
2:B:218:ASN:ND2	3:D:217:ASP:OD2	2.21	0.72
3:G:261:GLU:HG3	3:G:263:ASN:H	1.55	0.72
3:C:194:CYS:HB2	3:D:194:CYS:HB2	1.73	0.71
3:G:194:CYS:HB2	3:H:194:CYS:HB2	1.73	0.70
3:D:54:SER:O	3:D:127:ARG:NH1	2.24	0.70
3:G:79:VAL:HG22	3:G:232:MET:HG2	1.75	0.67
3:G:220:THR:HG23	3:G:227:PRO:HD3	1.75	0.67
3:C:84:MET:O	3:C:226:ARG:NH2	2.28	0.67
3:C:79:VAL:HG22	3:C:232:MET:HG2	1.76	0.67
3:G:156:ARG:NH1	3:G:168:SER:O	2.27	0.67
3:H:59:VAL:HG11	3:H:167:LEU:HA	1.76	0.67
1:A:116:THR:HG22	1:A:118:MET:H	1.59	0.66
1:A:10:GLU:OE2	1:A:432:ARG:NH1	2.28	0.66
1:E:116:THR:HG22	1:E:118:MET:H	1.60	0.66
3:C:156:ARG:NH1	3:C:168:SER:O	2.29	0.66
1:E:214:GLN:NE2	6:E:2016:BMA:O2	2.29	0.66
2:F:218:ASN:ND2	3:H:217:ASP:OD2	2.28	0.66
3:H:84:MET:HE2	3:H:227:PRO:HD2	1.77	0.65
1:A:115:ARG:HE	1:A:120:GLN:HG2	1.63	0.64
3:D:8:ASP:O	3:D:9:MET:HB3	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:44:LEU:HB2	3:G:45:PRO:HD2	1.79	0.64
3:C:86:GLU:HA	3:C:226:ARG:HH12	1.61	0.64
2:B:118:LEU:HD21	2:B:250:VAL:HG23	1.80	0.64
3:D:79:VAL:HG22	3:D:232:MET:HG2	1.79	0.64
3:G:135:VAL:HG12	3:G:136:GLU:H	1.61	0.64
1:A:214:GLN:NE2	6:A:2016:BMA:O2	2.30	0.64
3:H:79:VAL:HG22	3:H:232:MET:HG2	1.81	0.62
1:E:115:ARG:HE	1:E:120:GLN:HG2	1.64	0.62
1:A:414:ASP:OD1	1:A:418:ASN:OD1	2.18	0.62
3:C:135:VAL:HG12	3:C:136:GLU:H	1.66	0.61
2:B:311:PHE:O	2:B:334:GLY:N	2.33	0.61
3:D:156:ARG:HH11	3:D:167:LEU:HD12	1.66	0.61
3:D:166:TRP:HZ2	3:D:228:PHE:HE1	1.50	0.60
2:F:115:PRO:HA	2:F:152:ASN:HB2	1.84	0.60
2:B:115:PRO:HG3	2:B:152:ASN:HD22	1.66	0.59
1:A:338:ALA:HB1	1:A:362:ALA:HB1	1.84	0.59
3:D:9:MET:SD	3:D:10:GLU:N	2.75	0.59
3:D:84:MET:HE2	3:D:227:PRO:HD2	1.85	0.59
3:D:102:ILE:HG21	3:D:207:ILE:HD11	1.83	0.59
3:D:28:LEU:O	3:D:238:ARG:NH1	2.36	0.59
1:A:397:ALA:HB2	1:A:403:PRO:HD3	1.85	0.59
2:F:194:LYS:HG2	2:F:283:GLU:HG2	1.83	0.59
2:B:127:SER:HA	3:D:220:THR:OG1	2.02	0.59
3:D:272:ASP:HB3	3:D:275:LYS:HB3	1.85	0.58
3:G:329:PRO:HA	3:G:358:CYS:HA	1.85	0.58
3:C:276:ASP:HB3	3:D:17:ILE:HD13	1.86	0.58
3:G:100:HIS:HA	3:G:210:PHE:HB2	1.86	0.58
3:H:166:TRP:HZ2	3:H:228:PHE:HE1	1.50	0.57
1:A:483:ASP:HA	1:A:530:ARG:HB2	1.86	0.57
3:C:348:GLU:HG2	3:D:78:GLU:HA	1.87	0.57
1:A:564:LEU:HG	1:A:566:TYR:H	1.70	0.57
1:E:1:PHE:HA	1:E:389:GLN:HB2	1.85	0.57
3:G:351:SER:O	3:H:27:LYS:NZ	2.34	0.57
3:H:14:ARG:HD2	3:H:17:ILE:HD12	1.86	0.57
1:A:398:ARG:HG3	1:A:399:SER:H	1.69	0.57
1:A:275:TYR:HD2	1:A:278:PHE:HB2	1.69	0.57
5:E:2009:NAG:H62	6:E:2010:BMA:H2	1.85	0.57
3:G:78:GLU:HA	3:H:348:GLU:HG2	1.87	0.56
3:H:137:GLN:HB3	3:H:158:LEU:HD22	1.87	0.56
3:G:13:LYS:HD3	3:H:269:LEU:HD13	1.86	0.56
2:B:122:MET:HG3	2:B:135:ILE:HG21	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:261:GLU:OE1	3:D:262:LYS:NZ	2.39	0.56
1:E:347:LEU:HD11	1:E:359:ALA:HB2	1.86	0.56
2:F:118:LEU:HD21	2:F:250:VAL:HG23	1.87	0.56
2:B:121:LEU:HD11	2:B:228:ALA:HB1	1.86	0.56
2:B:152:ASN:OD1	2:B:242:ARG:NH2	2.39	0.56
1:E:42:LYS:HE3	1:E:93:TRP:CZ2	2.40	0.56
1:A:481:LYS:HB2	1:A:534:MET:HG3	1.87	0.56
3:G:83:LEU:HD23	3:G:228:PHE:HB3	1.88	0.56
3:G:265:CYS:HB3	3:G:267:ARG:CZ	2.36	0.56
3:C:78:GLU:HA	3:D:348:GLU:HG2	1.87	0.55
3:C:86:GLU:CA	3:C:226:ARG:HH12	2.18	0.55
3:H:11:LEU:HD12	3:H:14:ARG:HB2	1.87	0.55
1:A:345:ALA:HB2	1:A:409:MET:HG3	1.88	0.55
1:A:501:ASP:O	1:A:510:ARG:NH1	2.35	0.55
1:E:450:VAL:H	1:E:589:ARG:NH1	2.05	0.55
3:H:28:LEU:O	3:H:238:ARG:NH1	2.40	0.55
1:A:291:ALA:O	1:A:320:GLN:NE2	2.36	0.55
3:D:341:VAL:O	3:D:343:ARG:N	2.40	0.55
1:A:178:TYR:HB2	3:D:215:ARG:HH21	1.70	0.55
2:F:187:CYS:HB2	2:F:215:ILE:O	2.07	0.55
1:A:232:ASN:HB2	5:A:2009:NAG:H81	1.89	0.54
1:A:47:GLN:HB3	1:A:50:ILE:HD12	1.89	0.54
1:E:338:ALA:HB1	1:E:362:ALA:HB1	1.89	0.54
3:D:214:ARG:HG3	3:D:222:HIS:CD2	2.43	0.54
3:H:272:ASP:HB3	3:H:275:LYS:HB3	1.88	0.54
3:C:83:LEU:HD23	3:C:228:PHE:HB3	1.90	0.54
3:G:152:TYR:OH	3:G:155:ASN:HB2	2.08	0.54
2:F:322:GLU:HA	2:F:333:VAL:HG11	1.90	0.54
1:E:481:LYS:HB2	1:E:534:MET:HG3	1.90	0.53
3:G:348:GLU:HG2	3:H:78:GLU:HA	1.90	0.53
3:H:210:PHE:C	3:H:212:THR:H	2.12	0.53
5:A:2009:NAG:H62	6:A:2010:BMA:H2	1.90	0.53
1:E:483:ASP:HA	1:E:530:ARG:HB2	1.90	0.53
3:H:83:LEU:HD23	3:H:228:PHE:HB3	1.90	0.53
1:E:47:GLN:HB3	1:E:50:ILE:HD12	1.90	0.53
2:F:311:PHE:O	2:F:334:GLY:N	2.41	0.53
1:A:450:VAL:H	1:A:589:ARG:NH1	2.06	0.53
2:F:136:LYS:HG2	2:F:210:VAL:HG12	1.90	0.53
1:A:182:GLN:HE21	1:A:209:ALA:HB1	1.74	0.53
3:C:96:LYS:HA	3:C:215:ARG:NH2	2.24	0.52
3:G:266:VAL:HB	3:G:358:CYS:SG	2.49	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:152:TYR:OH	3:C:155:ASN:HB2	2.09	0.52
2:F:118:LEU:HD23	2:F:248:LEU:HB2	1.91	0.52
3:G:334:PRO:O	3:H:58:ARG:NH2	2.41	0.52
1:A:93:TRP:CD1	1:A:111:LEU:HD12	2.45	0.52
3:C:272:ASP:HB3	3:C:275:LYS:HB3	1.92	0.52
1:E:345:ALA:HB2	1:E:409:MET:HG3	1.92	0.52
3:C:351:SER:O	3:D:27:LYS:NZ	2.38	0.52
3:D:61:GLY:HA2	3:D:156:ARG:NH1	2.25	0.52
5:E:2021:NAG:H61	5:E:2022:NAG:N2	2.24	0.52
1:E:559:PHE:CE2	1:E:561:GLU:HB2	2.44	0.52
1:A:1:PHE:HA	1:A:389:GLN:HB2	1.91	0.52
1:A:414:ASP:OD1	1:A:420:TYR:O	2.28	0.52
5:E:2021:NAG:H61	5:E:2022:NAG:HN2	1.75	0.52
2:B:136:LYS:HG2	2:B:210:VAL:HG12	1.91	0.52
2:F:256:ASP:OD1	2:F:257:SER:N	2.38	0.52
2:B:157:PHE:HE2	2:B:196:ILE:HD12	1.74	0.51
3:G:46:GLU:HA	3:G:49:LEU:HB2	1.93	0.51
3:H:304:ASP:HA	3:H:310:VAL:HA	1.92	0.51
1:A:154:PHE:O	1:A:175:GLY:HA3	2.10	0.51
3:C:46:GLU:HA	3:C:49:LEU:HB2	1.92	0.51
3:H:214:ARG:HG3	3:H:222:HIS:CD2	2.45	0.51
3:G:279:TRP:CZ2	3:H:21:ARG:HG3	2.45	0.51
3:H:326:CYS:O	3:H:360:CYS:HA	2.11	0.51
1:A:98:VAL:O	1:A:99:ARG:NE	2.44	0.51
2:B:187:CYS:HB2	2:B:215:ILE:O	2.11	0.51
2:B:238:LYS:HD3	2:B:278:LEU:HB2	1.92	0.51
3:C:210:PHE:CE2	3:C:218:LEU:HD23	2.45	0.51
3:C:122:SER:OG	3:C:232:MET:O	2.18	0.51
1:A:589:ARG:HG2	1:A:590:GLN:H	1.76	0.51
3:C:54:SER:O	3:C:127:ARG:NH1	2.44	0.51
1:E:98:VAL:O	1:E:99:ARG:NE	2.44	0.51
1:E:9:ALA:HB3	1:E:435:LEU:HB3	1.92	0.50
1:A:113:HIS:HA	1:A:124:PRO:HA	1.93	0.50
5:A:2008:NAG:H61	5:A:2009:NAG:HN2	1.75	0.50
1:E:183:LEU:O	1:E:209:ALA:HA	2.11	0.50
1:E:182:GLN:HE21	1:E:209:ALA:HB1	1.75	0.50
2:B:194:LYS:HG2	2:B:283:GLU:HG2	1.94	0.50
3:D:329:PRO:HB3	3:D:355:VAL:HG13	1.94	0.50
2:F:121:LEU:HD11	2:F:228:ALA:HB1	1.92	0.50
1:A:511:ARG:NH1	1:A:554:THR:O	2.42	0.50
2:B:226:PHE:HB3	2:B:293:PRO:HG2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:86:GLU:HA	3:C:226:ARG:NH1	2.27	0.50
1:E:178:TYR:HB2	3:H:215:ARG:HH21	1.76	0.50
3:G:54:SER:O	3:G:127:ARG:NH1	2.45	0.50
3:C:59:VAL:HB	3:C:166:TRP:O	2.11	0.49
2:B:235:CYS:HB2	2:B:239:ILE:HD13	1.93	0.49
3:D:210:PHE:C	3:D:212:THR:H	2.15	0.49
3:G:272:ASP:HB3	3:G:275:LYS:HB3	1.93	0.49
2:B:259:PHE:O	2:B:292:TYR:HB2	2.12	0.49
3:H:211:THR:OG1	3:H:214:ARG:HG2	2.12	0.49
2:B:278:LEU:HA	2:B:283:GLU:O	2.13	0.49
1:E:271:GLN:NE2	1:E:301:MET:O	2.34	0.49
1:E:42:LYS:HE3	1:E:93:TRP:HZ2	1.77	0.49
1:A:405:PHE:HA	1:A:427:ALA:HB2	1.95	0.49
3:C:321:ALA:HB2	3:D:355:VAL:HG21	1.92	0.49
1:A:565:ASP:O	1:A:567:ARG:N	2.40	0.49
1:E:291:ALA:O	1:E:320:GLN:NE2	2.43	0.49
2:F:302:LEU:HD22	2:F:307:VAL:HB	1.94	0.49
3:G:333:GLU:HB3	3:H:58:ARG:HH12	1.77	0.49
3:G:96:LYS:HA	3:G:215:ARG:NH2	2.28	0.49
3:C:144:LYS:HE2	3:C:147:GLN:HG2	1.95	0.49
3:C:329:PRO:HA	3:C:358:CYS:HA	1.94	0.49
2:B:325:ALA:HB1	2:B:331:ALA:O	2.12	0.49
3:D:83:LEU:HD23	3:D:228:PHE:HB3	1.93	0.49
3:C:266:VAL:HB	3:C:358:CYS:SG	2.52	0.48
2:F:154:ARG:NH2	2:F:242:ARG:HG3	2.28	0.48
3:H:299:TYR:CD2	3:H:300:ILE:HG12	2.48	0.48
1:E:232:ASN:HB2	5:E:2009:NAG:H81	1.94	0.48
3:C:56:ARG:NH2	5:C:401:NAG:O6	2.46	0.48
3:C:29:ARG:HE	3:C:238:ARG:HB3	1.77	0.48
3:G:269:LEU:HB3	3:G:291:ASN:HA	1.95	0.48
3:C:130:ARG:HD3	3:C:165:GLU:HB3	1.94	0.48
2:F:314:THR:O	2:F:318:VAL:HG23	2.14	0.48
3:G:124:ALA:HB3	3:G:172:THR:HA	1.94	0.48
1:A:459:ASN:O	1:A:472:SER:HA	2.14	0.48
2:B:217:ALA:HB1	3:D:218:LEU:HD13	1.96	0.48
3:C:108:THR:HB	3:C:184:GLU:HA	1.95	0.48
1:E:459:ASN:O	1:E:472:SER:HA	2.13	0.48
3:G:108:THR:HB	3:G:184:GLU:HA	1.96	0.48
2:B:236:LYS:HA	2:B:241:TRP:HD1	1.78	0.48
1:E:113:HIS:HA	1:E:124:PRO:HA	1.96	0.48
2:F:235:CYS:HB2	2:F:239:ILE:HD13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:88:HIS:O	3:G:91:ILE:HG12	2.14	0.48
1:A:42:LYS:HE3	1:A:93:TRP:CZ2	2.49	0.48
2:F:238:LYS:HD3	2:F:278:LEU:HB2	1.95	0.48
1:E:116:THR:HG23	1:E:147:ILE:HG21	1.96	0.47
1:E:243:VAL:HG21	1:E:254:TYR:CD2	2.49	0.47
3:D:206:ASP:OD1	3:D:206:ASP:N	2.46	0.47
2:F:122:MET:HG3	2:F:135:ILE:HG21	1.95	0.47
2:B:118:LEU:HD23	2:B:248:LEU:HB2	1.97	0.47
3:D:326:CYS:O	3:D:360:CYS:HA	2.14	0.47
3:G:121:LEU:HD11	3:G:124:ALA:HB2	1.95	0.47
1:A:50:ILE:HD11	1:A:76:GLY:HA2	1.96	0.47
3:H:109:SER:O	3:H:113:GLU:HB2	2.15	0.47
2:B:162:GLU:OE2	2:B:223:GLU:HA	2.14	0.47
3:H:195:SER:HB3	3:H:200:ASP:HB2	1.97	0.47
3:H:329:PRO:HB3	3:H:355:VAL:HG13	1.97	0.47
1:A:275:TYR:HD1	2:B:259:PHE:HE2	1.63	0.47
1:E:265:TYR:HH	7:E:2012:MAN:HO4	1.63	0.47
1:A:565:ASP:HB3	1:A:568:THR:HG22	1.97	0.47
2:B:256:ASP:OD1	2:B:257:SER:N	2.44	0.47
3:C:273:PHE:O	3:C:278:GLY:N	2.47	0.47
2:F:157:PHE:HE2	2:F:196:ILE:HD12	1.80	0.47
3:G:329:PRO:HB2	3:G:332:LEU:HD11	1.97	0.47
3:C:27:LYS:NZ	3:C:74:TYR:O	2.33	0.47
3:D:271:ILE:HD12	3:D:290:ALA:HB3	1.97	0.47
1:E:154:PHE:O	1:E:175:GLY:HA3	2.15	0.47
1:E:589:ARG:HG2	1:E:590:GLN:H	1.80	0.47
2:F:260:GLY:HA3	2:F:294:THR:HG22	1.97	0.47
2:F:234:VAL:HG11	2:F:275:LEU:HA	1.96	0.46
2:B:222:PRO:HB3	2:B:256:ASP:HB3	1.96	0.46
3:C:333:GLU:HB2	3:C:354:ILE:HB	1.97	0.46
1:E:511:ARG:NH1	1:E:554:THR:O	2.44	0.46
1:A:183:LEU:O	1:A:209:ALA:HA	2.16	0.46
2:F:236:LYS:HA	2:F:241:TRP:HD1	1.79	0.46
3:G:117:GLU:HB3	3:G:120:LEU:HG	1.96	0.46
3:C:84:MET:HE2	3:C:226:ARG:HB2	1.98	0.46
1:A:116:THR:HG23	1:A:147:ILE:HG21	1.96	0.46
3:C:261:GLU:HG3	3:C:263:ASN:N	2.27	0.46
3:D:262:LYS:HB2	3:D:267:ARG:NH2	2.30	0.46
3:G:276:ASP:HB3	3:H:17:ILE:HD13	1.97	0.46
1:A:31:SER:HB3	3:G:262:LYS:HD3	1.98	0.46
3:D:263:ASN:O	3:D:265:CYS:N	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:144:LYS:HE2	3:G:147:GLN:HG2	1.98	0.46
2:B:118:LEU:HD12	2:B:142:LEU:HD21	1.97	0.46
5:E:2008:NAG:H61	5:E:2009:NAG:HN2	1.81	0.46
2:F:127:SER:HA	3:H:220:THR:OG1	2.16	0.46
2:B:311:PHE:HB2	2:B:333:VAL:HG12	1.97	0.45
3:G:143:GLN:HB2	3:G:153:LEU:HD11	1.97	0.45
1:E:373:VAL:HB	1:E:391:LEU:HB2	1.97	0.45
2:B:234:VAL:HG11	2:B:275:LEU:HA	1.97	0.45
2:B:259:PHE:C	2:B:292:TYR:HB2	2.36	0.45
3:D:211:THR:OG1	3:D:214:ARG:HG2	2.16	0.45
2:B:314:THR:O	2:B:318:VAL:HG23	2.16	0.45
3:C:143:GLN:HB2	3:C:153:LEU:HD11	1.97	0.45
3:H:271:ILE:HD12	3:H:290:ALA:HB3	1.99	0.45
1:E:13:GLY:HA3	1:E:19:PHE:CD1	2.52	0.45
1:E:501:ASP:O	1:E:510:ARG:NH1	2.46	0.45
2:B:157:PHE:CE2	2:B:196:ILE:HD12	2.52	0.45
1:E:450:VAL:H	1:E:589:ARG:HH11	1.64	0.45
1:A:559:PHE:CE2	1:A:561:GLU:HB2	2.52	0.45
1:A:243:VAL:HG21	1:A:254:TYR:CD2	2.52	0.45
1:A:489:PRO:O	1:A:530:ARG:NH1	2.50	0.45
3:H:130:ARG:CZ	3:H:158:LEU:HG	2.47	0.45
1:A:182:GLN:NE2	1:A:209:ALA:HB1	2.32	0.45
1:A:299:LEU:HD22	2:B:294:THR:HG21	1.98	0.45
2:B:336:LEU:HD13	2:B:336:LEU:HA	1.82	0.44
3:C:265:CYS:HB3	3:C:267:ARG:CZ	2.47	0.44
3:C:33:PRO:HB3	3:D:281:TRP:CE2	2.52	0.44
1:E:275:TYR:HD2	1:E:278:PHE:HB2	1.82	0.44
3:G:128:LEU:HD22	3:G:227:PRO:HB3	1.98	0.44
3:H:84:MET:HB2	3:H:105:PHE:O	2.16	0.44
3:D:9:MET:HG3	3:D:11:LEU:H	1.82	0.44
1:A:13:GLY:HA3	1:A:19:PHE:CD1	2.53	0.44
1:A:59:CYS:HA	1:A:67:CYS:HA	1.99	0.44
2:B:170:LYS:N	2:B:219:ILE:HD11	2.33	0.44
3:D:14:ARG:HD2	3:D:17:ILE:HD12	1.99	0.44
1:E:301:MET:HE2	1:E:309:LEU:HB3	1.99	0.44
3:H:192:ALA:HB2	3:H:203:LEU:HD13	1.98	0.44
3:H:45:PRO:HG2	3:H:48:VAL:HG22	2.00	0.44
3:D:205:VAL:HG12	3:D:207:ILE:HG23	1.99	0.44
3:D:87:THR:HG22	3:D:91:ILE:HB	2.00	0.44
1:E:499:LEU:HD23	1:E:521:SER:HB3	1.98	0.44
1:A:250:LEU:HA	1:A:250:LEU:HD12	1.87	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:302:LEU:HD22	2:B:307:VAL:HB	2.00	0.44
2:F:126:ALA:HB2	2:F:217:ALA:HA	1.99	0.44
3:H:130:ARG:NH2	3:H:158:LEU:HG	2.33	0.44
3:H:156:ARG:HH11	3:H:167:LEU:HD12	1.83	0.44
1:A:303:ARG:NH1	1:A:307:GLY:O	2.51	0.43
1:A:493:ASN:HB2	1:A:568:THR:HG21	2.00	0.43
3:D:84:MET:HB2	3:D:105:PHE:O	2.18	0.43
2:B:207:ASN:HB3	2:B:211:LYS:HE3	2.00	0.43
3:C:100:HIS:CD2	3:C:207:ILE:HD12	2.53	0.43
3:C:121:LEU:HD11	3:C:124:ALA:HB2	1.99	0.43
3:D:121:LEU:O	3:D:176:ARG:NH2	2.51	0.43
7:E:2018:MAN:H61	7:E:2019:MAN:H2	1.82	0.43
1:E:50:ILE:HD11	1:E:76:GLY:HA2	2.00	0.43
1:A:473:CYS:HA	1:A:542:TYR:HA	2.01	0.43
3:G:264:CYS:HA	3:G:295:GLY:HA3	2.01	0.43
3:D:288:TYR:CZ	3:D:290:ALA:HB2	2.54	0.43
1:E:398:ARG:H	1:E:398:ARG:HG3	1.63	0.43
3:G:115:VAL:HG21	3:G:121:LEU:HD23	2.01	0.43
3:G:122:SER:OG	3:G:232:MET:O	2.26	0.43
3:C:116:PRO:HG2	3:C:236:LEU:HD11	1.99	0.43
2:B:322:GLU:O	2:B:326:LYS:HG3	2.18	0.43
2:F:154:ARG:HH21	2:F:242:ARG:HG3	1.83	0.43
1:A:156:GLN:OE1	2:B:167:PRO:HG3	2.18	0.42
3:D:288:TYR:CE2	3:D:290:ALA:HB2	2.54	0.42
1:A:339:ARG:HD2	1:A:364:TYR:CE2	2.54	0.42
3:C:135:VAL:HG12	3:C:136:GLU:N	2.32	0.42
3:H:54:SER:O	3:H:127:ARG:NH1	2.52	0.42
3:C:264:CYS:HA	3:C:295:GLY:HA3	2.01	0.42
2:F:226:PHE:HB3	2:F:293:PRO:HG2	2.02	0.42
3:D:129:LEU:HD13	3:D:166:TRP:CE3	2.54	0.42
2:F:163:LYS:NZ	2:F:287:SER:O	2.41	0.42
1:A:347:LEU:HD11	1:A:359:ALA:HB2	2.02	0.42
1:E:167:ASP:HB3	1:E:188:VAL:HG22	2.00	0.42
1:A:335:GLU:CD	1:A:366:GLY:H	2.23	0.42
3:C:88:HIS:O	3:C:91:ILE:HG12	2.19	0.42
3:H:121:LEU:O	3:H:176:ARG:NH2	2.53	0.42
1:A:224:TYR:OH	2:B:264:LYS:HD3	2.18	0.42
1:A:437:ARG:CZ	1:A:575:LEU:HD13	2.49	0.42
1:E:351:ASP:OD1	1:E:351:ASP:N	2.49	0.42
3:H:116:PRO:HG2	3:H:236:LEU:HD11	2.02	0.42
2:B:130:ASP:OD1	2:B:130:ASP:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:131:ASP:O	2:F:135:ILE:HG12	2.20	0.42
3:G:95:PHE:O	3:G:96:LYS:HB3	2.18	0.42
1:A:111:LEU:HD23	1:A:111:LEU:HA	1.90	0.42
1:E:182:GLN:NE2	1:E:209:ALA:HB1	2.34	0.42
1:E:26:PHE:HB3	1:E:35:PHE:HB2	2.01	0.42
1:E:59:CYS:HA	1:E:67:CYS:HA	2.02	0.42
1:A:50:ILE:HD13	1:A:89:LYS:HB2	2.01	0.41
1:A:275:TYR:CD1	2:B:259:PHE:HE2	2.38	0.41
1:E:10:GLU:OE2	1:E:432:ARG:NH1	2.53	0.41
3:G:138:HIS:ND1	3:G:157:LEU:HG	2.35	0.41
1:A:288:ASP:OD1	1:A:288:ASP:N	2.54	0.41
1:A:302:ASP:OD1	1:A:310:GLN:HG3	2.20	0.41
2:B:235:CYS:O	2:B:239:ILE:HB	2.20	0.41
1:E:203:LYS:HA	1:E:203:LYS:HD2	1.82	0.41
2:F:153:PHE:HZ	2:F:155:LEU:HD13	1.85	0.41
3:G:329:PRO:HB3	3:G:355:VAL:HG13	2.01	0.41
3:D:78:GLU:N	3:D:233:ALA:O	2.53	0.41
3:G:102:ILE:HG12	3:G:215:ARG:HG2	2.01	0.41
3:G:340:TYR:HA	3:G:345:PRO:HA	2.02	0.41
1:A:203:LYS:HD2	1:A:203:LYS:HA	1.81	0.41
3:D:192:ALA:HB2	3:D:203:LEU:HD13	2.02	0.41
1:E:93:TRP:CD1	1:E:111:LEU:HD12	2.56	0.41
1:E:317:VAL:HB	1:E:329:THR:HG23	2.02	0.41
2:F:170:LYS:N	2:F:219:ILE:HD11	2.34	0.41
3:G:333:GLU:HB2	3:G:354:ILE:HB	2.02	0.41
3:H:129:LEU:HD13	3:H:166:TRP:CE3	2.56	0.41
1:A:224:TYR:HE2	1:A:278:PHE:CD1	2.39	0.41
3:C:252:ASP:O	3:C:256:CYS:HB2	2.21	0.41
3:D:115:VAL:HG21	3:D:121:LEU:HD23	2.02	0.41
1:E:167:ASP:HB3	1:E:188:VAL:CG2	2.50	0.41
2:F:222:PRO:HG2	2:F:258:HIS:NE2	2.35	0.41
3:D:133:LEU:HD11	3:D:204:GLN:O	2.21	0.41
3:G:116:PRO:HG2	3:G:236:LEU:HD11	2.02	0.41
1:A:513:LEU:HA	1:A:520:PRO:HA	2.01	0.41
3:C:269:LEU:HB3	3:C:291:ASN:HA	2.02	0.41
3:D:118:PRO:HG3	3:D:179:LEU:HB3	2.02	0.41
3:D:53:ASN:O	3:D:57:ASP:HB2	2.20	0.41
2:F:157:PHE:CE2	2:F:196:ILE:HD12	2.55	0.41
3:G:60:ALA:HA	3:G:167:LEU:HA	2.03	0.41
1:A:175:GLY:HA2	1:A:179:TRP:CD1	2.56	0.41
1:A:479:CYS:HB3	1:A:534:MET:SD	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:153:PHE:HZ	2:B:155:LEU:HD13	1.86	0.41
3:C:13:LYS:HD3	3:D:269:LEU:HD13	2.03	0.41
1:A:9:ALA:HB3	1:A:435:LEU:HB3	2.02	0.41
3:D:58:ARG:HD3	3:D:127:ARG:NH2	2.36	0.41
1:E:288:ASP:OD1	1:E:288:ASP:N	2.54	0.41
3:G:210:PHE:CD2	3:G:218:LEU:HD23	2.56	0.41
3:G:340:TYR:CE2	3:G:345:PRO:HB3	2.56	0.41
3:G:279:TRP:HZ2	3:H:21:ARG:HG3	1.86	0.41
3:G:333:GLU:HB3	3:H:58:ARG:NH1	2.36	0.41
3:C:128:LEU:HD22	3:C:227:PRO:HB3	2.03	0.41
3:D:172:THR:HG22	3:D:176:ARG:HH12	1.86	0.41
1:E:473:CYS:HA	1:E:542:TYR:HA	2.03	0.41
1:A:450:VAL:H	1:A:589:ARG:HH11	1.70	0.40
2:B:263:SER:HB2	2:B:268:ILE:HB	2.03	0.40
3:C:214:ARG:C	3:C:216:GLY:H	2.24	0.40
3:D:137:GLN:HG2	3:D:205:VAL:HG23	2.03	0.40
1:A:154:PHE:HZ	2:B:170:LYS:HG2	1.86	0.40
2:B:223:GLU:H	2:B:257:SER:HA	1.86	0.40
1:E:247:ALA:O	1:E:250:LEU:HB2	2.22	0.40
1:E:575:LEU:HA	1:E:575:LEU:HD12	1.88	0.40
2:F:212:ASN:OD1	2:F:212:ASN:N	2.54	0.40
3:G:273:PHE:O	3:G:278:GLY:N	2.55	0.40
7:A:2011:MAN:H61	7:A:2012:MAN:H2	1.47	0.40
1:A:228:VAL:O	1:A:282:ALA:HB3	2.22	0.40
3:D:130:ARG:NH2	3:D:158:LEU:HG	2.36	0.40
1:E:248:ARG:HD3	1:E:248:ARG:N	2.37	0.40
1:E:18:TYR:N	1:E:431:ASP:OD1	2.54	0.40
1:A:42:LYS:HE3	1:A:93:TRP:HZ2	1.86	0.40
1:A:575:LEU:HA	1:A:575:LEU:HD12	1.85	0.40
2:B:172:THR:O	2:B:176:ILE:HG13	2.21	0.40
3:C:340:TYR:CE2	3:C:345:PRO:HB3	2.56	0.40
3:D:133:LEU:HA	3:D:133:LEU:HD12	1.87	0.40
1:E:299:LEU:HD22	2:F:294:THR:HG21	2.03	0.40
1:E:504:LYS:HB3	1:E:508:ALA:HB3	2.03	0.40
3:H:57:ASP:O	3:H:127:ARG:NH1	2.52	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	583/601 (97%)	548 (94%)	34 (6%)	1 (0%)	52	88
1	E	583/601 (97%)	552 (95%)	31 (5%)	0	100	100
2	B	240/257 (93%)	217 (90%)	23 (10%)	0	100	100
2	F	240/257 (93%)	218 (91%)	22 (9%)	0	100	100
3	C	295/363 (81%)	263 (89%)	30 (10%)	2 (1%)	26	72
3	D	310/363 (85%)	272 (88%)	35 (11%)	3 (1%)	19	66
3	G	285/363 (78%)	254 (89%)	28 (10%)	3 (1%)	17	63
3	H	315/363 (87%)	273 (87%)	39 (12%)	3 (1%)	19	66
All	All	2851/3168 (90%)	2597 (91%)	242 (8%)	12 (0%)	39	81

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	135	VAL
3	G	135	VAL
1	A	566	TYR
3	H	135	VAL
3	H	202	THR
3	D	135	VAL
3	H	90	GLU
3	G	222	HIS
3	D	58	ARG
3	D	264	CYS
3	G	39	VAL
3	C	59	VAL

### 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	483/491 (98%)	478 (99%)	5 (1%)	82	93
1	E	481/491 (98%)	475 (99%)	6 (1%)	78	92
2	B	215/230 (94%)	213 (99%)	2 (1%)	84	94
2	F	215/230 (94%)	213 (99%)	2 (1%)	84	94
3	C	268/323 (83%)	265 (99%)	3 (1%)	80	92
3	D	286/323 (88%)	278 (97%)	8 (3%)	51	82
3	G	265/323 (82%)	262 (99%)	3 (1%)	80	92
3	H	288/323 (89%)	281 (98%)	7 (2%)	57	85
All	All	2501/2734 (92%)	2465 (99%)	36 (1%)	74	91

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	178	TYR
1	A	275	TYR
1	A	516	TYR
1	A	582	PHE
1	A	596	ASP
2	B	131	ASP
2	B	336	LEU
3	C	44	LEU
3	C	207	ILE
3	C	256	CYS
3	D	95	PHE
3	D	206	ASP
3	D	220	THR
3	D	222	HIS
3	D	256	CYS
3	D	262	LYS
3	D	299	TYR
3	D	311	LEU
1	E	178	TYR
1	E	248	ARG
1	E	275	TYR
1	E	490	ARG
1	E	516	TYR

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Mol	Chain	Res	Type
1	E	583	THR
2	F	284	TYR
2	F	336	LEU
3	G	38	GLU
3	G	207	ILE
3	G	256	CYS
3	H	95	PHE
3	H	146	SER
3	H	147	GLN
3	H	198	SER
3	H	222	HIS
3	H	299	TYR
3	H	314	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	342	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 80 ligands modelled in this entry, 14 are monoatomic - leaving 66 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	$\# Z  > 2$
5	NAG	A	2005	1,5	14,14,15	0.45	0	15,19,21	0.37	0
5	NAG	A	2006	5,6	14,14,15	0.28	0	15,19,21	0.40	0
6	BMA	A	2007	5	11,11,12	0.52	0	15,15,17	0.92	0
5	NAG	A	2008	1,5	14,14,15	0.28	0	15,19,21	0.30	0
5	NAG	A	2009	5,6	14,14,15	0.43	0	15,19,21	0.38	0
6	BMA	A	2010	5,7	11,11,12	1.00	1 (9%)	15,15,17	1.17	2 (13%)
7	MAN	A	2011	7,6	11,11,12	0.77	0	15,15,17	1.36	4 (26%)
7	MAN	A	2012	7	11,11,12	0.84	1 (9%)	15,15,17	1.19	2 (13%)
7	MAN	A	2013	6	11,11,12	1.01	1 (9%)	15,15,17	1.13	1 (6%)
5	NAG	A	2014	1,5	14,14,15	0.58	1 (7%)	15,19,21	0.43	0
5	NAG	A	2015	5,6	14,14,15	0.34	0	15,19,21	0.35	0
6	BMA	A	2016	5,7	11,11,12	0.75	0	15,15,17	1.14	1 (6%)
7	MAN	A	2017	6	11,11,12	0.65	0	15,15,17	1.04	2 (13%)
7	MAN	A	2018	7,6	11,11,12	1.19	2 (18%)	15,15,17	2.14	4 (26%)
7	MAN	A	2019	7	11,11,12	0.77	0	15,15,17	1.07	2 (13%)
7	MAN	A	2020	7	11,11,12	0.77	0	15,15,17	0.85	1 (6%)
5	NAG	A	2021	1,5	14,14,15	0.20	0	15,19,21	0.27	0
5	NAG	A	2022	5,6	14,14,15	0.28	0	15,19,21	0.35	0
6	BMA	A	2023	5,7	11,11,12	0.71	0	15,15,17	1.29	4 (26%)
7	MAN	A	2024	6	11,11,12	0.69	0	15,15,17	1.28	2 (13%)
5	NAG	A	2025	1	14,14,15	0.57	0	15,19,21	0.27	0
5	NAG	A	2026	1,5	14,14,15	0.43	0	15,19,21	0.35	0
5	NAG	A	2027	5	14,14,15	0.36	0	15,19,21	0.36	0
5	NAG	B	2004	2	14,14,15	0.32	0	15,19,21	0.26	0
5	NAG	C	401	3,5	14,14,15	0.40	0	15,19,21	0.32	0
5	NAG	C	402	5,6	14,14,15	0.35	0	15,19,21	0.53	0
6	BMA	C	403	5,7	11,11,12	0.58	0	15,15,17	0.86	0
7	MAN	C	404	6	11,11,12	0.85	0	15,15,17	1.12	1 (6%)
5	NAG	D	401	3,5	14,14,15	0.38	0	15,19,21	0.49	0
5	NAG	D	402	5,6	14,14,15	0.35	0	15,19,21	0.22	0
6	BMA	D	403	5,7	11,11,12	0.53	0	15,15,17	0.86	0
7	MAN	D	404	6	11,11,12	0.57	0	15,15,17	1.10	2 (13%)
5	NAG	E	2005	1,5	14,14,15	0.34	0	15,19,21	0.36	0
5	NAG	E	2006	5,6	14,14,15	0.51	0	15,19,21	0.52	0
6	BMA	E	2007	5	11,11,12	0.62	0	15,15,17	1.04	2 (13%)
5	NAG	E	2008	1,5	14,14,15	0.32	0	15,19,21	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	E	2009	5,6	14,14,15	0.44	0	15,19,21	0.40	0
6	BMA	E	2010	5,7	11,11,12	1.01	1 (9%)	15,15,17	1.15	2 (13%)
7	MAN	E	2011	7,6	11,11,12	0.80	0	15,15,17	1.32	2 (13%)
7	MAN	E	2012	7	11,11,12	0.76	0	15,15,17	1.15	1 (6%)
7	MAN	E	2013	6	11,11,12	1.04	1 (9%)	15,15,17	1.13	1 (6%)
5	NAG	E	2014	1,5	14,14,15	0.64	1 (7%)	15,19,21	0.47	0
5	NAG	E	2015	5,6	14,14,15	0.30	0	15,19,21	0.30	0
6	BMA	E	2016	5,7	11,11,12	0.67	0	15,15,17	1.12	1 (6%)
7	MAN	E	2017	6	11,11,12	0.65	0	15,15,17	1.03	1 (6%)
7	MAN	E	2018	7,6	11,11,12	1.25	2 (18%)	15,15,17	2.16	4 (26%)
7	MAN	E	2019	7	11,11,12	0.90	0	15,15,17	1.12	2 (13%)
7	MAN	E	2020	7	11,11,12	0.84	1 (9%)	15,15,17	0.86	1 (6%)
5	NAG	E	2021	1,5	14,14,15	0.23	0	15,19,21	0.26	0
5	NAG	E	2022	5,6	14,14,15	0.22	0	15,19,21	0.35	0
6	BMA	E	2023	5,7	11,11,12	0.83	0	15,15,17	1.38	3 (20%)
7	MAN	E	2024	6	11,11,12	0.71	0	15,15,17	1.41	3 (20%)
5	NAG	E	2025	1	14,14,15	0.65	1 (7%)	15,19,21	0.26	0
5	NAG	E	2026	1,5	14,14,15	0.57	0	15,19,21	0.23	0
5	NAG	E	2027	5	14,14,15	0.32	0	15,19,21	0.33	0
5	NAG	F	2004	2	14,14,15	0.20	0	15,19,21	0.21	0
5	NAG	G	401	3,5	14,14,15	0.48	0	15,19,21	0.57	0
5	NAG	G	402	5,6	14,14,15	0.33	0	15,19,21	0.58	0
6	BMA	G	403	5,7	11,11,12	1.19	1 (9%)	15,15,17	1.23	1 (6%)
7	MAN	G	404	6	11,11,12	1.11	1 (9%)	15,15,17	1.72	4 (26%)
5	NAG	H	401	3,5	14,14,15	0.33	0	15,19,21	0.59	0
5	NAG	H	402	5,6	14,14,15	0.39	0	15,19,21	0.32	0
6	BMA	H	403	5,7	11,11,12	1.33	1 (9%)	15,15,17	1.33	2 (13%)
7	MAN	H	404	7,6	11,11,12	1.64	2 (18%)	15,15,17	1.53	2 (13%)
7	MAN	H	405	6	11,11,12	0.88	1 (9%)	15,15,17	1.23	2 (13%)
7	MAN	H	406	7	11,11,12	0.69	0	15,15,17	0.99	2 (13%)

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
5	NAG	A	2005	1,5	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	2006	5,6	-	0/6/23/26	0/1/1/1
6	BMA	A	2007	5	-	0/2/19/22	0/1/1/1
5	NAG	A	2008	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	2009	5,6	-	0/6/23/26	0/1/1/1
6	BMA	A	2010	5,7	-	0/2/19/22	0/1/1/1
7	MAN	A	2011	7,6	-	0/2/19/22	0/1/1/1
7	MAN	A	2012	7	-	0/2/19/22	0/1/1/1
7	MAN	A	2013	6	-	0/2/19/22	0/1/1/1
5	NAG	A	2014	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	2015	5,6	-	0/6/23/26	0/1/1/1
6	BMA	A	2016	5,7	-	0/2/19/22	0/1/1/1
7	MAN	A	2017	6	-	0/2/19/22	0/1/1/1
7	MAN	A	2018	7,6	-	0/2/19/22	0/1/1/1
7	MAN	A	2019	7	-	0/2/19/22	0/1/1/1
7	MAN	A	2020	7	-	0/2/19/22	0/1/1/1
5	NAG	A	2021	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	2022	5,6	-	0/6/23/26	0/1/1/1
6	BMA	A	2023	5,7	-	0/2/19/22	0/1/1/1
7	MAN	A	2024	6	-	0/2/19/22	1/1/1/1
5	NAG	A	2025	1	-	0/6/23/26	0/1/1/1
5	NAG	A	2026	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	2027	5	-	0/6/23/26	0/1/1/1
5	NAG	B	2004	2	-	0/6/23/26	0/1/1/1
5	NAG	C	401	3,5	-	0/6/23/26	0/1/1/1
5	NAG	C	402	5,6	-	0/6/23/26	0/1/1/1
6	BMA	C	403	5,7	-	0/2/19/22	0/1/1/1
7	MAN	C	404	6	-	0/2/19/22	0/1/1/1
5	NAG	D	401	3,5	-	0/6/23/26	0/1/1/1
5	NAG	D	402	5,6	-	0/6/23/26	0/1/1/1
6	BMA	D	403	5,7	-	0/2/19/22	0/1/1/1
7	MAN	D	404	6	-	0/2/19/22	0/1/1/1
5	NAG	E	2005	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	2006	5,6	-	0/6/23/26	0/1/1/1
6	BMA	E	2007	5	-	0/2/19/22	0/1/1/1
5	NAG	E	2008	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	2009	5,6	-	0/6/23/26	0/1/1/1
6	BMA	E	2010	5,7	-	0/2/19/22	0/1/1/1
7	MAN	E	2011	7,6	-	0/2/19/22	0/1/1/1
7	MAN	E	2012	7	-	0/2/19/22	0/1/1/1
7	MAN	E	2013	6	-	0/2/19/22	0/1/1/1
5	NAG	E	2014	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	2015	5,6	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	BMA	E	2016	5,7	-	0/2/19/22	0/1/1/1
7	MAN	E	2017	6	-	0/2/19/22	0/1/1/1
7	MAN	E	2018	7,6	-	0/2/19/22	0/1/1/1
7	MAN	E	2019	7	-	0/2/19/22	0/1/1/1
7	MAN	E	2020	7	-	0/2/19/22	0/1/1/1
5	NAG	E	2021	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	2022	5,6	-	0/6/23/26	0/1/1/1
6	BMA	E	2023	5,7	-	0/2/19/22	0/1/1/1
7	MAN	E	2024	6	-	0/2/19/22	0/1/1/1
5	NAG	E	2025	1	-	0/6/23/26	0/1/1/1
5	NAG	E	2026	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	2027	5	-	0/6/23/26	0/1/1/1
5	NAG	F	2004	2	-	0/6/23/26	0/1/1/1
5	NAG	G	401	3,5	-	0/6/23/26	0/1/1/1
5	NAG	G	402	5,6	-	0/6/23/26	0/1/1/1
6	BMA	G	403	5,7	-	0/2/19/22	0/1/1/1
7	MAN	G	404	6	-	0/2/19/22	0/1/1/1
5	NAG	H	401	3,5	-	0/6/23/26	0/1/1/1
5	NAG	H	402	5,6	-	0/6/23/26	0/1/1/1
6	BMA	H	403	5,7	-	0/2/19/22	0/1/1/1
7	MAN	H	404	7,6	-	0/2/19/22	0/1/1/1
7	MAN	H	405	6	-	0/2/19/22	0/1/1/1
7	MAN	H	406	7	-	0/2/19/22	0/1/1/1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	E	2020	MAN	O5-C1	-2.29	1.40	1.43
5	E	2014	NAG	O5-C1	-2.18	1.40	1.43
5	A	2014	NAG	O5-C1	-2.02	1.40	1.43
5	E	2025	NAG	O5-C1	-2.01	1.40	1.43
6	A	2010	BMA	O3-C3	2.01	1.47	1.43
6	E	2010	BMA	O3-C3	2.04	1.47	1.43
7	H	404	MAN	C1-C2	2.09	1.57	1.52
7	H	405	MAN	C1-C2	2.12	1.57	1.52
6	G	403	BMA	O3-C3	2.17	1.48	1.43
7	A	2012	MAN	C1-C2	2.22	1.57	1.52
7	E	2018	MAN	C1-C2	2.34	1.57	1.52
7	E	2013	MAN	C1-C2	2.38	1.58	1.52
7	A	2018	MAN	C1-C2	2.45	1.58	1.52
7	A	2013	MAN	C1-C2	2.48	1.58	1.52
6	H	403	BMA	C4-C5	2.49	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	2018	MAN	C2-C3	2.59	1.56	1.52
7	E	2018	MAN	C2-C3	2.90	1.56	1.52
7	G	404	MAN	C1-C2	3.55	1.60	1.52
7	H	404	MAN	C2-C3	4.04	1.58	1.52

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	H	405	MAN	O2-C2-C3	-2.82	104.50	110.19
7	E	2019	MAN	O2-C2-C3	-2.67	104.80	110.19
7	G	404	MAN	O2-C2-C3	-2.55	105.06	110.19
7	A	2024	MAN	O2-C2-C3	-2.44	105.26	110.19
7	A	2011	MAN	O2-C2-C3	-2.43	105.28	110.19
7	A	2019	MAN	O2-C2-C3	-2.42	105.30	110.19
7	A	2013	MAN	O2-C2-C3	-2.39	105.37	110.19
7	E	2017	MAN	O2-C2-C3	-2.37	105.42	110.19
7	C	404	MAN	O2-C2-C3	-2.33	105.48	110.19
7	A	2012	MAN	O2-C2-C3	-2.32	105.51	110.19
6	E	2023	BMA	O5-C5-C4	-2.25	106.41	110.13
7	D	404	MAN	O2-C2-C3	-2.25	105.66	110.19
7	E	2011	MAN	O2-C2-C3	-2.24	105.67	110.19
7	E	2024	MAN	O2-C2-C3	-2.23	105.69	110.19
7	E	2013	MAN	O2-C2-C3	-2.20	105.74	110.19
7	H	406	MAN	O2-C2-C3	-2.17	105.80	110.19
7	E	2020	MAN	O2-C2-C3	-2.17	105.81	110.19
6	A	2023	BMA	O5-C5-C4	-2.08	106.69	110.13
7	E	2018	MAN	O2-C2-C3	-2.06	106.04	110.19
7	A	2020	MAN	O2-C2-C3	-2.02	106.11	110.19
7	A	2017	MAN	O2-C2-C3	-2.02	106.12	110.19
7	A	2018	MAN	O2-C2-C3	-2.01	106.13	110.19
6	E	2007	BMA	C1-C2-C3	2.01	111.98	109.55
7	E	2019	MAN	C1-O5-C5	2.02	115.11	112.14
7	A	2019	MAN	C1-O5-C5	2.03	115.13	112.14
7	A	2012	MAN	C1-O5-C5	2.04	115.13	112.14
7	E	2012	MAN	C1-O5-C5	2.04	115.14	112.14
6	E	2007	BMA	C1-O5-C5	2.07	115.18	112.14
7	A	2011	MAN	C1-C2-C3	2.07	112.06	109.55
6	A	2023	BMA	C1-C2-C3	2.12	112.11	109.55
7	A	2011	MAN	O5-C1-C2	2.14	114.32	110.89
7	H	405	MAN	C1-O5-C5	2.20	115.37	112.14
7	A	2017	MAN	C1-O5-C5	2.20	115.38	112.14
7	H	406	MAN	C1-O5-C5	2.23	115.42	112.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	2010	BMA	O3-C3-C2	2.26	114.16	110.01
7	E	2024	MAN	O5-C1-C2	2.27	114.53	110.89
6	A	2010	BMA	O3-C3-C2	2.27	114.17	110.01
6	A	2023	BMA	C1-O5-C5	2.33	115.57	112.14
6	E	2023	BMA	O5-C1-C2	2.43	114.78	110.89
6	A	2023	BMA	O5-C1-C2	2.44	114.80	110.89
6	H	403	BMA	O5-C1-C2	2.50	114.90	110.89
6	E	2016	BMA	C1-O5-C5	2.52	115.84	112.14
7	G	404	MAN	O5-C1-C2	2.54	114.95	110.89
7	D	404	MAN	C1-O5-C5	2.54	115.87	112.14
7	G	404	MAN	C1-O5-C5	2.56	115.91	112.14
6	A	2016	BMA	C1-O5-C5	2.61	115.97	112.14
6	G	403	BMA	O3-C3-C2	2.69	114.94	110.01
7	A	2011	MAN	C1-O5-C5	2.71	116.12	112.14
6	E	2010	BMA	C1-O5-C5	2.76	116.20	112.14
6	E	2023	BMA	C1-C2-C3	2.80	112.95	109.55
6	H	403	BMA	O3-C3-C2	2.86	115.25	110.01
6	A	2010	BMA	C1-O5-C5	2.88	116.38	112.14
7	H	404	MAN	O2-C2-C1	2.88	115.01	109.23
7	E	2011	MAN	C1-O5-C5	2.89	116.39	112.14
7	A	2024	MAN	C1-O5-C5	3.42	117.17	112.14
7	H	404	MAN	C1-C2-C3	3.52	113.82	109.55
7	E	2024	MAN	C1-O5-C5	3.74	117.64	112.14
7	A	2018	MAN	C1-O5-C5	4.07	118.13	112.14
7	G	404	MAN	C1-C2-C3	4.12	114.54	109.55
7	E	2018	MAN	O5-C1-C2	4.12	117.48	110.89
7	A	2018	MAN	O5-C1-C2	4.15	117.53	110.89
7	E	2018	MAN	C1-O5-C5	4.29	118.45	112.14
7	A	2018	MAN	C1-C2-C3	4.61	115.14	109.55
7	E	2018	MAN	C1-C2-C3	4.67	115.21	109.55

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	2024	MAN	C1-C2-C3-C4-C5-O5

17 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2008	NAG	1	0
5	A	2009	NAG	3	0
6	A	2010	BMA	1	0
7	A	2011	MAN	1	0
7	A	2012	MAN	1	0
6	A	2016	BMA	1	0
5	C	401	NAG	1	0
5	E	2008	NAG	1	0
5	E	2009	NAG	3	0
6	E	2010	BMA	1	0
7	E	2012	MAN	1	0
6	E	2016	BMA	1	0
7	E	2018	MAN	1	0
7	E	2019	MAN	1	0
5	E	2021	NAG	2	0
5	E	2022	NAG	2	0
5	E	2026	NAG	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	589/601 (98%)	0.37	46 (7%) 16 13	133, 206, 281, 311	0
1	E	587/601 (97%)	0.44	53 (9%) 12 10	139, 222, 286, 333	0
2	B	242/257 (94%)	0.17	3 (1%) 81 72	63, 146, 259, 309	0
2	F	242/257 (94%)	0.38	16 (6%) 22 16	171, 224, 261, 287	0
3	C	305/363 (84%)	0.59	38 (12%) 5 6	159, 243, 294, 338	0
3	D	322/363 (88%)	0.50	40 (12%) 5 6	158, 225, 274, 300	0
3	G	297/363 (81%)	0.46	32 (10%) 8 7	127, 227, 284, 315	0
3	H	325/363 (89%)	0.35	22 (6%) 20 16	133, 202, 256, 273	0
All	All	2909/3168 (91%)	0.41	250 (8%) 13 12	63, 219, 280, 338	0

All (250) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	455	LEU	11.9
1	A	482	ALA	10.4
3	G	35	SER	9.0
1	E	487	VAL	8.9
1	A	455	LEU	8.6
1	E	486	GLY	8.3
3	C	41	PRO	6.1
3	C	126	LEU	6.0
1	A	512	ALA	6.0
1	A	552	LYS	5.9
1	E	476	VAL	5.9
1	A	480	LEU	5.9
3	G	188	PHE	5.9
3	C	106	PHE	5.8
3	H	213	GLY	5.7
1	E	583	THR	5.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	E	482	ALA	5.6
3	G	127	ARG	5.5
1	A	475	ASN	5.5
1	A	447	GLY	5.4
3	G	227	PRO	5.4
3	C	211	THR	5.3
3	H	291	ASN	5.3
3	C	167	LEU	5.3
3	D	270	TYR	5.2
1	E	475	ASN	5.1
1	E	477	ARG	5.1
3	G	106	PHE	5.0
1	A	425	VAL	5.0
1	A	481	LYS	5.0
3	D	279	TRP	4.9
1	E	480	LEU	4.8
3	C	105	PHE	4.8
1	E	444	VAL	4.8
3	D	339	TYR	4.7
3	C	361	SER	4.7
3	C	230	LEU	4.7
2	F	261	MET	4.6
3	D	337	ILE	4.6
3	H	275	LYS	4.6
1	E	516	TYR	4.5
1	A	476	VAL	4.5
3	D	338	VAL	4.5
1	E	488	LEU	4.5
1	E	591	ALA	4.5
1	E	450	VAL	4.4
1	E	448	LEU	4.4
2	F	259	PHE	4.4
1	E	544	ARG	4.4
3	H	290	ALA	4.3
1	E	474	PHE	4.3
3	H	282	ILE	4.3
3	C	127	ARG	4.2
3	G	167	LEU	4.2
3	G	222	HIS	4.2
1	E	452	PRO	4.2
2	F	262	ASP	4.1
3	C	187	GLY	4.1

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Mol	Chain	Res	Type	RSRZ
3	G	57	ASP	4.0
1	A	498	LEU	4.0
1	E	272	MET	3.9
3	C	104	MET	3.9
3	G	104	MET	3.9
3	G	231	LEU	3.9
1	E	512	ALA	3.9
3	G	126	LEU	3.8
3	H	339	TYR	3.8
1	A	474	PHE	3.8
1	E	423	LEU	3.7
1	A	570	ALA	3.7
1	E	57	LEU	3.7
1	E	454	ILE	3.7
3	C	229	LEU	3.7
3	D	221	ILE	3.7
3	H	337	ILE	3.6
3	C	222	HIS	3.6
3	C	166	TRP	3.6
3	H	286	LYS	3.6
3	D	274	ARG	3.6
1	A	499	LEU	3.6
1	E	565	ASP	3.6
2	F	260	GLY	3.6
1	E	239	PHE	3.5
3	C	234	THR	3.5
3	C	299	TYR	3.5
2	F	119	TYR	3.4
1	E	30	ALA	3.4
3	G	361	SER	3.4
3	H	221	ILE	3.4
1	A	436	TYR	3.4
1	A	564	LEU	3.3
3	D	197	ASP	3.3
1	E	568	THR	3.3
3	G	44	LEU	3.3
1	A	511	ARG	3.3
2	F	118	LEU	3.3
3	D	288	TYR	3.3
2	F	226	PHE	3.3
3	G	228	PHE	3.3
3	C	13	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
3	D	341	VAL	3.3
3	C	322	SER	3.2
3	C	42	GLY	3.2
3	C	147	GLN	3.2
3	D	7	ILE	3.2
3	D	347	VAL	3.2
3	D	283	HIS	3.2
1	E	436	TYR	3.2
3	G	353	MET	3.1
2	F	161	VAL	3.1
3	G	41	PRO	3.1
3	G	229	LEU	3.1
1	A	239	PHE	3.1
1	E	171	LEU	3.0
1	A	478	PHE	3.0
1	E	240	VAL	3.0
3	D	167	LEU	3.0
1	A	31	SER	3.0
3	C	231	LEU	3.0
3	D	276	ASP	2.9
1	E	294	PHE	2.9
1	E	558	ILE	2.9
3	G	168	SER	2.9
1	A	569	ALA	2.9
3	G	190	LEU	2.9
3	C	188	PHE	2.9
3	D	257	PHE	2.8
1	A	566	TYR	2.8
3	H	147	GLN	2.8
1	A	544	ARG	2.8
3	C	240	GLN	2.8
1	A	158	GLY	2.8
1	A	423	LEU	2.8
3	D	335	LEU	2.8
3	G	115	VAL	2.8
1	E	383	LEU	2.8
1	E	515	LEU	2.8
1	A	559	PHE	2.8
3	C	321	ALA	2.8
3	D	212	THR	2.8
3	D	275	LYS	2.8
3	D	188	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
2	F	249	LEU	2.7
3	D	361	SER	2.7
1	A	500	LEU	2.7
1	E	425	VAL	2.7
3	D	336	PRO	2.7
3	D	345	PRO	2.7
1	E	543	LEU	2.7
3	G	186	GLU	2.7
1	E	36	LEU	2.7
3	C	140	GLU	2.7
1	E	569	ALA	2.6
1	E	503	LEU	2.6
2	F	298	LEU	2.6
3	G	128	LEU	2.6
1	E	492	LEU	2.6
3	H	288	TYR	2.6
3	G	166	TRP	2.6
1	E	447	GLY	2.6
3	C	319	PRO	2.6
3	H	146	SER	2.6
3	D	106	PHE	2.6
3	D	189	ARG	2.6
2	B	146	MET	2.6
1	E	511	ARG	2.5
1	A	520	PRO	2.5
3	D	273	PHE	2.5
1	A	563	ARG	2.5
1	E	38	VAL	2.5
3	C	118	PRO	2.5
3	D	271	ILE	2.5
1	E	478	PHE	2.5
3	G	79	VAL	2.5
3	G	103	TYR	2.5
1	A	224	TYR	2.5
3	D	130	ARG	2.5
3	C	346	LYS	2.4
1	A	558	ILE	2.4
1	A	450	VAL	2.4
3	H	317	HIS	2.4
3	H	145	TYR	2.4
1	E	473	CYS	2.4
3	C	207	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
2	F	160	PHE	2.4
3	C	169	PHE	2.4
3	G	43	PRO	2.4
3	D	269	LEU	2.4
3	H	130	ARG	2.4
1	A	374	TYR	2.4
3	G	97	GLN	2.3
1	E	319	LEU	2.3
3	C	81	ARG	2.3
2	F	232	ALA	2.3
1	A	505	GLN	2.3
1	A	565	ASP	2.3
3	C	269	LEU	2.3
2	F	271	PRO	2.3
3	D	165	GLU	2.3
1	A	594	LEU	2.3
1	A	89	LYS	2.3
1	A	424	ILE	2.2
3	D	135	VAL	2.2
3	H	346	LYS	2.2
3	C	102	ILE	2.2
1	E	130	LEU	2.2
1	A	33	ARG	2.2
3	D	289	HIS	2.2
1	E	509	ILE	2.2
2	B	343	ILE	2.2
1	E	530	ARG	2.2
3	G	226	ARG	2.2
3	D	318	ASN	2.2
3	C	111	LEU	2.1
1	A	562	TYR	2.1
1	A	344	ILE	2.1
1	A	486	GLY	2.1
1	E	139	TYR	2.1
2	B	153	PHE	2.1
2	F	310	ILE	2.1
3	D	282	ILE	2.1
3	D	323	ALA	2.1
3	C	228	PHE	2.1
1	A	583	THR	2.1
3	G	187	GLY	2.1
3	D	210	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	445	ASN	2.1
3	C	179	LEU	2.1
3	H	9	MET	2.1
3	C	227	PRO	2.1
1	E	105	ILE	2.1
2	F	343	ILE	2.1
3	G	105	PHE	2.0
1	E	11	TYR	2.0
3	C	186	GLU	2.0
3	H	314	TYR	2.0
3	G	118	PRO	2.0
3	G	83	LEU	2.0
3	H	269	LEU	2.0
3	H	280	LYS	2.0
3	H	276	ASP	2.0
1	A	38	VAL	2.0
1	E	106	LEU	2.0
3	D	332	LEU	2.0
2	F	186	PHE	2.0
3	D	166	TRP	2.0
3	H	361	SER	2.0
3	D	160	PRO	2.0
1	A	514	PHE	2.0
3	D	218	LEU	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
8	MN	B	2002	1/1	0.99	0.26	2.48	110,110,110,110	0
8	MN	B	2001	1/1	0.99	0.25	2.35	181,181,181,181	0
7	MAN	A	2012	11/12	0.74	0.40	1.81	210,237,246,247	0
5	NAG	E	2008	14/15	0.90	0.24	1.40	210,229,277,283	0
8	MN	F	2001	1/1	0.98	0.26	0.96	217,217,217,217	0
4	CA	A	2004	1/1	0.99	0.27	0.92	155,155,155,155	0
8	MN	F	2002	1/1	0.95	0.20	0.78	233,233,233,233	0
5	NAG	A	2005	14/15	0.88	0.25	0.72	155,202,243,244	0
5	NAG	D	401	14/15	0.90	0.23	0.12	193,229,252,259	0
7	MAN	E	2012	11/12	0.81	0.21	0.05	170,229,254,263	0
5	NAG	E	2014	14/15	0.94	0.26	-0.03	157,187,255,258	0
5	NAG	A	2008	14/15	0.86	0.21	-0.03	188,238,257,265	0
5	NAG	A	2021	14/15	0.78	0.37	-0.21	239,291,308,308	0
4	CA	E	2004	1/1	0.98	0.14	-0.36	225,225,225,225	0
8	MN	F	2003	1/1	0.99	0.16	-0.38	213,213,213,213	0
5	NAG	E	2015	14/15	0.97	0.21	-0.40	156,199,262,266	0
5	NAG	E	2005	14/15	0.93	0.19	-0.50	157,203,222,230	0
5	NAG	A	2014	14/15	0.93	0.21	-0.72	157,208,243,252	0
8	MN	B	2003	1/1	0.99	0.18	-0.81	144,144,144,144	0
5	NAG	A	2015	14/15	0.96	0.19	-0.83	165,185,197,203	0
5	NAG	H	401	14/15	0.94	0.16	-0.83	178,216,248,264	0
4	CA	A	2001	1/1	0.99	0.15	-0.84	189,189,189,189	0
4	CA	E	2001	1/1	0.95	0.14	-0.91	218,218,218,218	0
4	CA	A	2002	1/1	0.94	0.10	-0.95	222,222,222,222	0
4	CA	E	2002	1/1	0.96	0.12	-1.03	256,256,256,256	0
4	CA	A	2003	1/1	0.99	0.16	-1.07	199,199,199,199	0
4	CA	E	2003	1/1	0.91	0.10	-1.10	219,219,219,219	0
5	NAG	E	2021	14/15	0.84	0.19	-1.52	255,303,326,328	0
6	BMA	D	403	11/12	0.90	0.16	-	193,230,238,242	0
7	MAN	A	2013	11/12	0.79	0.21	-	144,256,279,288	0
5	NAG	C	401	14/15	0.79	0.19	-	181,240,272,278	0
6	BMA	C	403	11/12	0.88	0.14	-	246,266,287,288	0
7	MAN	H	404	11/12	0.91	0.20	-	241,259,269,273	0
7	MAN	A	2019	11/12	0.87	0.20	-	210,220,237,246	0
7	MAN	G	404	11/12	0.65	0.26	-	210,251,267,270	0
5	NAG	E	2022	14/15	0.87	0.14	-	251,293,309,313	0
5	NAG	C	402	14/15	0.84	0.30	-	257,291,310,311	0
6	BMA	G	403	11/12	0.90	0.12	-	207,247,255,268	0
7	MAN	H	405	11/12	0.91	0.24	-	227,249,268,271	0
7	MAN	E	2017	11/12	0.95	0.13	-	208,229,241,241	0
7	MAN	E	2018	11/12	0.86	0.12	-	205,229,252,264	0
5	NAG	E	2025	14/15	0.80	0.32	-	223,252,285,293	0
5	NAG	A	2026	14/15	0.78	0.22	-	170,256,290,295	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	BMA	E	2023	11/12	0.70	0.21	-	268,283,319,345	0
5	NAG	A	2006	14/15	0.87	0.22	-	194,225,238,255	0
6	BMA	A	2023	11/12	0.77	0.17	-	279,294,313,321	0
7	MAN	E	2020	11/12	0.81	0.32	-	216,259,290,308	0
6	BMA	H	403	11/12	0.82	0.15	-	204,259,281,282	0
7	MAN	A	2020	11/12	0.85	0.32	-	257,283,289,293	0
5	NAG	E	2027	14/15	0.56	0.44	-	251,324,342,342	0
6	BMA	E	2016	11/12	0.94	0.13	-	190,205,228,232	0
5	NAG	E	2026	14/15	0.81	0.22	-	256,296,331,332	0
5	NAG	A	2009	14/15	0.73	0.26	-	251,285,298,299	0
6	BMA	E	2010	11/12	0.86	0.08	-	260,279,289,294	0
5	NAG	B	2004	14/15	0.91	0.19	-	234,258,269,269	0
7	MAN	H	406	11/12	0.78	0.21	-	182,265,283,288	0
5	NAG	H	402	14/15	0.85	0.16	-	215,238,266,275	0
5	NAG	A	2025	14/15	0.76	0.60	-	280,323,340,345	0
7	MAN	A	2018	11/12	0.89	0.17	-	187,214,265,277	0
5	NAG	G	402	14/15	0.85	0.19	-	202,251,281,284	0
7	MAN	E	2024	11/12	0.76	0.31	-	260,296,321,322	0
5	NAG	E	2006	14/15	0.92	0.17	-	181,186,204,214	0
6	BMA	A	2016	11/12	0.91	0.15	-	117,192,216,216	0
7	MAN	E	2019	11/12	0.90	0.20	-	236,241,265,267	0
5	NAG	A	2027	14/15	0.72	0.27	-	189,242,281,286	0
5	NAG	D	402	14/15	0.83	0.18	-	188,213,241,242	0
7	MAN	A	2011	11/12	0.61	0.18	-	238,258,280,291	0
5	NAG	G	401	14/15	0.90	0.17	-	231,270,278,279	0
5	NAG	E	2009	14/15	0.84	0.20	-	223,250,271,275	0
7	MAN	E	2013	11/12	0.85	0.17	-	228,253,286,286	0
7	MAN	C	404	11/12	0.82	0.20	-	206,239,263,266	0
7	MAN	D	404	11/12	0.91	0.18	-	156,208,226,234	0
6	BMA	A	2010	11/12	0.77	0.12	-	242,283,305,308	0
6	BMA	A	2007	11/12	0.73	0.34	-	181,242,253,260	0
6	BMA	E	2007	11/12	0.89	0.19	-	195,223,230,231	0
7	MAN	A	2017	11/12	0.94	0.20	-	167,197,224,249	0
5	NAG	F	2004	14/15	0.85	0.21	-	258,270,279,284	0
7	MAN	E	2011	11/12	0.87	0.15	-	224,281,298,305	0
7	MAN	A	2024	11/12	0.82	0.30	-	223,243,287,291	0
5	NAG	A	2022	14/15	0.86	0.14	-	253,281,301,303	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.