



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:33 AM GMT

PDB ID : 3IU3
Title : Crystal structure of the Fab fragment of therapeutic antibody Basiliximab in complex with IL-2Ra (CD25) ectodomain
Authors : Du, J.; Yang, H.; Wang, J.; Ding, J.
Deposited on : 2009-08-29
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
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) : trunk26865

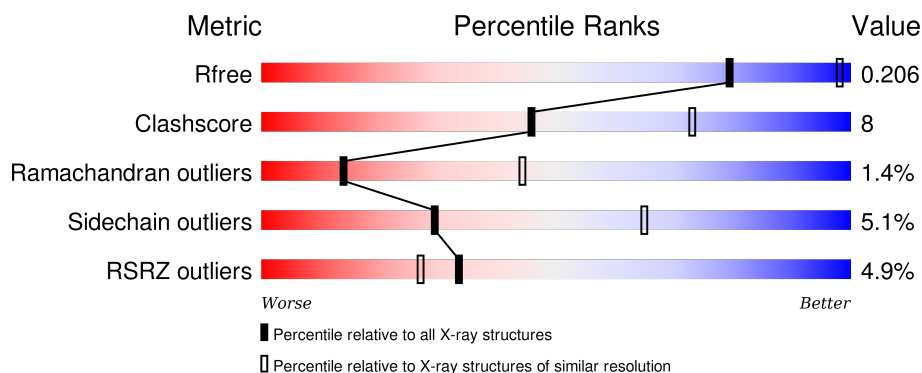
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	215	<div> <div>88%</div> <div>10%</div> <div>.</div> </div>
1	C	215	<div> <div>86%</div> <div>13%</div> <div>.</div> </div>
1	H	215	<div> <div>84%</div> <div>15%</div> <div>.</div> </div>
2	B	210	<div> <div>86%</div> <div>12%</div> <div>.</div> </div>
2	D	210	<div> <div>86%</div> <div>12%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
2	L	210	<div><div></div><div>83%</div><div>15%</div><div>••</div></div>
3	I	223	<div><div>15%</div><div>40%</div><div>10%</div><div>•</div><div>47%</div></div>
3	J	223	<div><div>10%</div><div>37%</div><div>11%</div><div>•</div><div>48%</div></div>
3	K	223	<div><div>9%</div><div>43%</div><div>5%</div><div>•</div><div>49%</div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12566 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 Heavy chain of Fab fragment of Basiliximab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	215	Total	C	N	O	S	0	0	0
			1630	1032	270	321	7			
1	C	215	Total	C	N	O	S	0	0	0
			1630	1032	270	321	7			
1	H	215	Total	C	N	O	S	0	0	0
			1630	1032	270	321	7			

- Molecule 2 is a protein called Light chain of Fab fragment of Basiliximab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	208	Total	C	N	O	S	0	0	0
			1591	989	269	325	8			
2	D	209	Total	C	N	O	S	0	0	0
			1595	991	270	326	8			
2	L	208	Total	C	N	O	S	0	0	0
			1591	989	269	325	8			

- Molecule 3 is a protein called Interleukin-2 receptor alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	119	Total	C	N	O	S	0	0	0
			954	591	174	175	14			
3	J	116	Total	C	N	O	S	0	0	0
			923	570	165	174	14			
3	K	114	Total	C	N	O	S	0	0	0
			905	560	161	170	14			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	218	HIS	-	EXPRESSION TAG	UNP P01589
I	219	HIS	-	EXPRESSION TAG	UNP P01589

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Chain	Residue	Modelled	Actual	Comment	Reference
I	220	HIS	-	EXPRESSION TAG	UNP P01589
I	221	HIS	-	EXPRESSION TAG	UNP P01589
I	222	HIS	-	EXPRESSION TAG	UNP P01589
I	223	HIS	-	EXPRESSION TAG	UNP P01589
J	218	HIS	-	EXPRESSION TAG	UNP P01589
J	219	HIS	-	EXPRESSION TAG	UNP P01589
J	220	HIS	-	EXPRESSION TAG	UNP P01589
J	221	HIS	-	EXPRESSION TAG	UNP P01589
J	222	HIS	-	EXPRESSION TAG	UNP P01589
J	223	HIS	-	EXPRESSION TAG	UNP P01589
K	218	HIS	-	EXPRESSION TAG	UNP P01589
K	219	HIS	-	EXPRESSION TAG	UNP P01589
K	220	HIS	-	EXPRESSION TAG	UNP P01589
K	221	HIS	-	EXPRESSION TAG	UNP P01589
K	222	HIS	-	EXPRESSION TAG	UNP P01589
K	223	HIS	-	EXPRESSION TAG	UNP P01589


- Molecule 4 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	I	3	Total	C	N	O	0	0
			39	22	2	15		
4	J	3	Total	C	N	O	0	0
			39	22	2	15		
4	K	3	Total	C	N	O	0	0
			39	22	2	15		

3 Residue-property plots


These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Heavy chain of Fab fragment of Basiliximab

Chain A: 




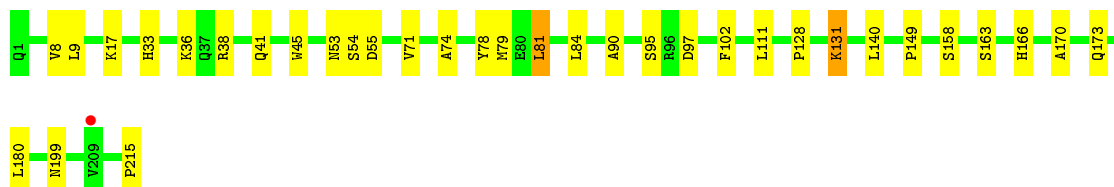
- Molecule 1: Heavy chain of Fab fragment of Basiliximab

Chain C: 




- Molecule 1: Heavy chain of Fab fragment of Basiliximab

Chain H: 




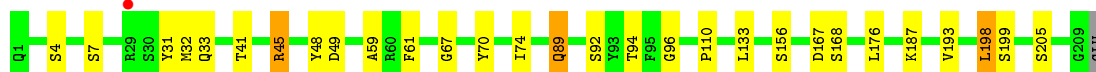
- Molecule 2: Light chain of Fab fragment of Basiliximab



Chain B: 

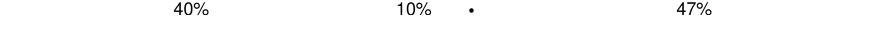


- Molecule 2: Light chain of Fab fragment of Basiliximab


Chain D: 

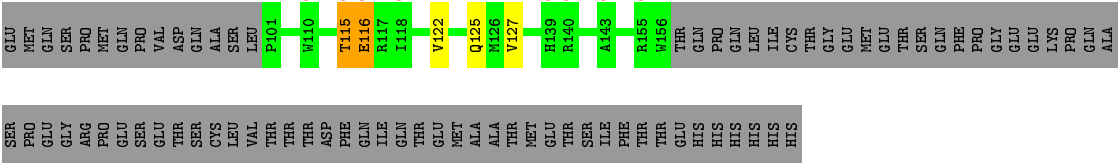


- Chain L: 
- 

- Chain I: 

- Chain J:
-
- 10% 37% 11% 48%
- E1 L2 C3 D6 E9 F15 M18 A19 H12 I10 P11 Q158 Q159 Q160 Q161 Q162 Q163 Q164 Q165 Q166 Q167 Q168 Q169 Q170 Q171 Q172 Q173 Q174 Q175 Q176 Q177 Q178 Q179 Q180 Q181 Q182 Q183 Q184 Q185 Q186 Q187 Q188 Q189 Q190 Q191 Q192 Q193 Q194 Q195 Q196 Q197 Q198 Q199 Q200 Q201 Q202 Q203 Q204 Q205 Q206 Q207 Q208 Q209 Q210 Q211 Q212 Q213 Q214 Q215 Q216 Q217 Q218 Q219 Q220 Q221 Q222 Q223 Q224 Q225 Q226 Q227 Q228 Q229 Q230 Q231 Q232 Q233 Q234 Q235 Q236 Q237 Q238 Q239 Q240 Q241 Q242 Q243 Q244 Q245 Q246 Q247 Q248 Q249 Q250 Q251 Q252 Q253 Q254 Q255 Q256 Q257 Q258 Q259 Q260 Q261 Q262 Q263 Q264 Q265 Q266 Q267 Q268 Q269 Q270 Q271 Q272 Q273 Q274 Q275 Q276 Q277 Q278 Q279 Q280 Q281 Q282 Q283 Q284 Q285 Q286 Q287 Q288 Q289 Q290 Q291 Q292 Q293 Q294 Q295 Q296 Q297 Q298 Q299 Q300 Q301 Q302 Q303 Q304 Q305 Q306 Q307 Q308 Q309 Q310 Q311 Q312 Q313 Q314 Q315 Q316 Q317 Q318 Q319 Q320 Q321 Q322 Q323 Q324 Q325 Q326 Q327 Q328 Q329 Q330 Q331 Q332 Q333 Q334 Q335 Q336 Q337 Q338 Q339 Q340 Q341 Q342 Q343 Q344 Q345 Q346 Q347 Q348 Q349 Q350 Q351 Q352 Q353 Q354 Q355 Q356 Q357 Q358 Q359 Q360 Q361 Q362 Q363 Q364 Q365 Q366 Q367 Q368 Q369 Q370 Q371 Q372 Q373 Q374 Q375 Q376 Q377 Q378 Q379 Q380 Q381 Q382 Q383 Q384 Q385 Q386 Q387 Q388 Q389 Q390 Q391 Q392 Q393 Q394 Q395 Q396 Q397 Q398 Q399 Q400 Q401 Q402 Q403 Q404 Q405 Q406 Q407 Q408 Q409 Q410 Q411 Q412 Q413 Q414 Q415 Q416 Q417 Q418 Q419 Q420 Q421 Q422 Q423 Q424 Q425 Q426 Q427 Q428 Q429 Q430 Q431 Q432 Q433 Q434 Q435 Q436 Q437 Q438 Q439 Q440 Q441 Q442 Q443 Q444 Q445 Q446 Q447 Q448 Q449 Q450 Q451 Q452 Q453 Q454 Q455 Q456 Q457 Q458 Q459 Q460 Q461 Q462 Q463 Q464 Q465 Q466 Q467 Q468 Q469 Q470 Q471 Q472 Q473 Q474 Q475 Q476 Q477 Q478 Q479 Q480 Q481 Q482 Q483 Q484 Q485 Q486 Q487 Q488 Q489 Q490 Q491 Q492 Q493 Q494 Q495 Q496 Q497 Q498 Q499 Q500 Q501 Q502 Q503 Q504 Q505 Q506 Q507 Q508 Q509 Q510 Q511 Q512 Q513 Q514 Q515 Q516 Q517 Q518 Q519 Q520 Q521 Q522 Q523 Q524 Q525 Q526 Q527 Q528 Q529 Q530 Q531 Q532 Q533 Q534 Q535 Q536 Q537 Q538 Q539 Q540 Q541 Q542 Q543 Q544 Q545 Q546 Q547 Q548 Q549 Q550 Q551 Q552 Q553 Q554 Q555 Q556 Q557 Q558 Q559 Q560 Q561 Q562 Q563 Q564 Q565 Q566 Q567 Q568 Q569 Q570 Q571 Q572 Q573 Q574 Q575 Q576 Q577 Q578 Q579 Q580 Q581 Q582 Q583 Q584 Q585 Q586 Q587 Q588 Q589 Q590 Q591 Q592 Q593 Q594 Q595 Q596 Q597 Q598 Q599 Q600 Q601 Q602 Q603 Q604 Q605 Q606 Q607 Q608 Q609 Q610 Q611 Q612 Q613 Q614 Q615 Q616 Q617 Q618 Q619 Q620 Q621 Q622 Q623 Q624 Q625 Q626 Q627 Q628 Q629 Q630 Q631 Q632 Q633 Q634 Q635 Q636 Q637 Q638 Q639 Q640 Q641 Q642 Q643 Q644 Q645 Q646 Q647 Q648 Q649 Q650 Q651 Q652 Q653 Q654 Q655 Q656 Q657 Q658 Q659 Q660 Q661 Q662 Q663 Q664 Q665 Q666 Q667 Q668 Q669 Q670 Q671 Q672 Q673 Q674 Q675 Q676 Q677 Q678 Q679 Q680 Q681 Q682 Q683 Q684 Q685 Q686 Q687 Q688 Q689 Q690 Q691 Q692 Q693 Q694 Q695 Q696 Q697 Q698 Q699 Q700 Q701 Q702 Q703 Q704 Q705 Q706 Q707 Q708 Q709 Q710 Q711 Q712 Q713 Q714 Q715 Q716 Q717 Q718 Q719 Q720 Q721 Q722 Q723 Q724 Q725 Q726 Q727 Q728 Q729 Q730 Q731 Q732 Q733 Q734 Q735 Q736 Q737 Q738 Q739 Q740 Q741 Q742 Q743 Q744 Q745 Q746 Q747 Q748 Q749 Q750 Q751 Q752 Q753 Q754 Q755 Q756 Q757 Q758 Q759 Q760 Q761 Q762 Q763 Q764 Q765 Q766 Q767 Q768 Q769 Q770 Q771 Q772 Q773 Q774 Q775 Q776 Q777 Q778 Q779 Q780 Q781 Q782 Q783 Q784 Q785 Q786 Q787 Q788 Q789 Q790 Q791 Q792 Q793 Q794 Q795 Q796 Q797 Q798 Q799 Q800 Q801 Q802 Q803 Q804 Q805 Q806 Q807 Q808 Q809 Q810 Q811 Q812 Q813 Q814 Q815 Q816 Q817 Q818 Q819 Q820 Q821 Q822 Q823 Q824 Q825 Q826 Q827 Q828 Q829 Q830 Q831 Q832 Q833 Q834 Q835 Q836 Q837 Q838 Q839 Q840 Q841 Q842 Q843 Q844 Q845 Q846 Q847 Q848 Q849 Q850 Q851 Q852 Q853 Q854 Q855 Q856 Q857 Q858 Q859 Q860 Q861 Q862 Q863 Q864 Q865 Q866 Q867 Q868 Q869 Q870 Q871 Q872 Q873 Q874 Q875 Q876 Q877 Q878 Q879 Q880 Q881 Q882 Q883 Q884 Q885 Q886 Q887 Q888 Q889 Q890 Q891 Q892 Q893 Q894 Q895 Q896 Q897 Q898 Q899 Q900 Q901 Q902 Q903 Q904 Q905 Q906 Q907 Q908 Q909 Q910 Q911 Q912 Q913 Q914 Q915 Q916 Q917 Q918 Q919 Q920 Q921 Q922 Q923 Q924 Q925 Q926 Q927 Q928 Q929 Q930 Q931 Q932 Q933 Q934 Q935 Q936 Q937 Q938 Q939 Q940 Q941 Q942 Q943 Q944 Q945 Q946 Q947 Q948 Q949 Q950 Q951 Q952 Q953 Q954 Q955 Q956 Q957 Q958 Q959 Q960 Q961 Q962 Q963 Q964 Q965 Q966 Q967 Q968 Q969 Q970 Q971 Q972 Q973 Q974 Q975 Q976 Q977 Q978 Q979 Q980 Q981 Q982 Q983 Q984 Q985 Q986 Q987 Q988 Q989 Q990 Q991 Q992 Q993 Q994 Q995 Q996 Q997 Q998 Q999 1000

- Chain K: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	137.05Å 137.05Å 459.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.38 – 2.90 49.84 – 2.90	Depositor EDS
% Data completeness (in resolution range)	93.0 (47.38-2.90) 97.9 (49.84-2.90)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	0.17	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.76 (at 2.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.215 , 0.262 0.214 , 0.206	Depositor DCC
R_{free} test set	2872 reflections (5.09%)	DCC
Wilson B-factor (Å ²)	74.4	Xtriage
Anisotropy	0.262	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 43.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 56725 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12566	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.05% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.35	0/1675	0.54	0/2281
1	C	0.34	0/1675	0.54	0/2281
1	H	0.33	0/1675	0.52	0/2281
2	B	0.35	0/1626	0.52	0/2203
2	D	0.36	0/1630	0.50	0/2208
2	L	0.34	0/1626	0.52	0/2203
3	I	0.38	0/981	0.52	0/1323
3	J	0.36	0/947	0.51	0/1278
3	K	0.34	0/930	0.48	0/1256
All	All	0.35	0/12765	0.52	0/17314

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	1630	0	1575	23	0
1	C	1630	0	1575	22	0
1	H	1630	0	1575	19	0
2	B	1591	0	1541	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1595	0	1544	14	0
2	L	1591	0	1541	21	0
3	I	954	0	889	25	0
3	J	923	0	856	34	0
3	K	905	0	834	22	0
4	I	39	0	34	1	0
4	J	39	0	34	2	0
4	K	39	0	34	1	0
All	All	12566	0	12032	189	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 (189) 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)
3:J:146:VAL:O	3:J:157:THR:HG23	1.56	1.04
1:C:38:ARG:HH11	1:C:38:ARG:HG2	1.23	1.00
1:C:33:HIS:HD2	1:C:45:TRP:HE1	1.09	0.96
3:I:133:GLN:HA	3:I:133:GLN:OE1	1.61	0.95
1:H:33:HIS:HD2	1:H:45:TRP:HE1	1.05	0.95
1:A:31:TRP:CH2	3:K:42:LEU:HD23	2.01	0.94
3:I:135:TYR:HB3	3:I:136:ARG:CD	2.02	0.90
1:A:38:ARG:HG2	1:A:38:ARG:HH11	1.35	0.90
1:A:131:LYS:O	1:A:132:SER:HB3	1.71	0.89
3:J:146:VAL:O	3:J:157:THR:CG2	2.23	0.86
1:A:158:SER:H	1:A:199:ASN:HD21	1.22	0.86
3:J:156:TRP:O	3:J:157:THR:HG22	1.76	0.85
3:J:145:SER:HA	3:J:157:THR:OG1	1.78	0.83
2:L:32:MET:HE2	2:L:87:CYS:HB2	1.59	0.83
3:J:156:TRP:O	3:J:157:THR:CG2	2.28	0.81
2:B:33:GLN:HE21	2:B:49:ASP:H	1.28	0.81
1:A:33:HIS:HD2	1:A:45:TRP:HE1	1.26	0.80
1:C:8:VAL:HG11	1:C:16:VAL:HG21	1.62	0.79
3:I:133:GLN:CA	3:I:133:GLN:OE1	2.30	0.79
3:J:151:HIS:ND1	3:J:151:HIS:N	2.30	0.79
1:H:33:HIS:CD2	1:H:45:TRP:HE1	1.97	0.78
3:K:17:ALA:HB2	3:K:127:VAL:HG12	1.65	0.77
3:J:156:TRP:C	3:J:157:THR:HG23	2.04	0.76
4:J:300:NAG:O3	4:J:301:NAG:O5	2.03	0.76
1:C:33:HIS:CD2	1:C:45:TRP:HE1	2.00	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:40:GLY:O	3:K:41:SER:HB3	1.87	0.75
3:J:156:TRP:C	3:J:157:THR:CG2	2.56	0.74
1:H:33:HIS:HD2	1:H:45:TRP:NE1	1.84	0.73
3:I:135:TYR:HB3	3:I:136:ARG:HD2	1.69	0.72
3:I:110:TRP:CE2	3:I:112:ASN:ND2	2.59	0.70
3:K:38:LYS:HG2	3:K:39:SER:N	2.07	0.70
1:A:31:TRP:CZ2	3:K:42:LEU:HD23	2.27	0.70
3:I:110:TRP:O	3:I:111:GLU:HB2	1.92	0.69
1:H:53:ASN:O	1:H:55:ASP:N	2.25	0.69
1:A:31:TRP:CZ3	3:K:42:LEU:CD2	2.76	0.69
3:J:51:SER:O	3:J:52:HIS:HB2	1.94	0.68
1:A:31:TRP:CH2	3:K:42:LEU:CD2	2.75	0.68
3:I:140:ARG:HG3	3:I:140:ARG:HH11	1.60	0.67
1:A:33:HIS:CD2	1:A:45:TRP:HE1	2.11	0.67
3:K:115:THR:HG22	3:K:116:GLU:H	1.60	0.66
1:H:81:LEU:HB3	1:H:84:LEU:HD21	1.78	0.66
1:C:33:HIS:HD2	1:C:45:TRP:NE1	1.89	0.65
3:K:40:GLY:O	3:K:41:SER:CB	2.44	0.65
3:K:38:LYS:HG2	3:K:39:SER:H	1.61	0.65
3:J:149:MET:O	3:J:150:THR:C	2.36	0.64
3:J:145:SER:HA	3:J:157:THR:HG1	1.62	0.64
1:C:158:SER:H	1:C:199:ASN:HD21	1.46	0.63
3:I:135:TYR:HB3	3:I:136:ARG:HD3	1.80	0.62
2:B:89:GLN:HE21	2:B:91:SER:HB2	1.65	0.62
3:K:38:LYS:O	3:K:39:SER:C	2.38	0.62
1:A:38:ARG:HG2	1:A:38:ARG:NH1	2.12	0.62
3:K:38:LYS:O	3:K:40:GLY:N	2.33	0.62
1:C:38:ARG:HG2	1:C:38:ARG:NH1	2.01	0.61
2:B:60:ARG:NH1	2:B:81:ASP:OD1	2.33	0.61
1:C:28:THR:HA	1:C:51:PRO:HB2	1.82	0.61
3:I:135:TYR:CD1	3:I:136:ARG:NH1	2.68	0.61
3:J:150:THR:OG1	3:J:151:HIS:N	2.34	0.61
2:D:89:GLN:HE22	2:D:92:SER:H	1.49	0.61
2:B:89:GLN:HG2	2:B:91:SER:H	1.69	0.58
2:B:33:GLN:NE2	2:B:49:ASP:H	1.99	0.58
1:A:53:ASN:HD21	1:A:55:ASP:HB2	1.69	0.58
1:H:166:HIS:CE1	2:L:135:ASN:HD21	2.22	0.58
3:J:150:THR:HG1	3:J:151:HIS:H	1.50	0.57
2:B:89:GLN:NE2	2:B:92:SER:H	2.02	0.57
1:A:158:SER:N	1:A:199:ASN:HD21	1.98	0.56
3:K:38:LYS:CG	3:K:39:SER:N	2.66	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:29:ARG:HD3	2:B:89:GLN:HG3	1.86	0.56
2:D:33:GLN:HE21	2:D:49:ASP:H	1.53	0.56
2:B:33:GLN:HE21	2:B:49:ASP:N	2.02	0.56
3:I:135:TYR:CB	3:I:136:ARG:HD2	2.35	0.56
3:J:150:THR:HB	3:J:151:HIS:CE1	2.41	0.56
2:L:32:MET:CE	2:L:87:CYS:HB2	2.35	0.55
1:A:99:GLY:HA2	3:K:43:TYR:OH	2.06	0.55
3:J:157:THR:O	3:J:158:GLN:C	2.44	0.55
3:J:149:MET:O	3:J:149:MET:HG3	2.06	0.55
3:I:110:TRP:CZ2	3:I:112:ASN:ND2	2.74	0.55
3:I:140:ARG:HG3	3:I:140:ARG:NH1	2.22	0.55
2:D:59:ALA:HB1	2:L:202:VAL:HG11	1.87	0.55
1:H:166:HIS:HE1	2:L:135:ASN:HD21	1.55	0.54
3:I:115:THR:C	3:I:117:ARG:H	2.11	0.54
2:L:2:ILE:HD12	2:L:2:ILE:H	1.73	0.54
3:J:146:VAL:HB	3:J:157:THR:HG21	1.91	0.53
1:A:183:VAL:HG11	2:B:132:LEU:CD2	2.38	0.53
1:C:8:VAL:HG11	1:C:16:VAL:CG2	2.37	0.53
2:B:187:LYS:HE3	2:B:207:ASN:HD22	1.74	0.53
3:I:135:TYR:C	3:I:136:ARG:HD2	2.30	0.53
1:A:38:ARG:CG	1:A:38:ARG:HH11	2.17	0.52
2:B:33:GLN:HG3	2:B:48:TYR:HA	1.91	0.52
3:J:146:VAL:N	3:J:157:THR:OG1	2.36	0.52
3:J:3:CYS:HA	3:J:154:THR:HG21	1.90	0.52
3:I:126:MET:HG2	3:I:146:VAL:HG22	1.91	0.51
3:J:150:THR:HB	3:J:151:HIS:ND1	2.25	0.51
3:K:37:ILE:HD11	3:K:41:SER:HB3	1.91	0.51
1:H:38:ARG:HG2	1:H:90:ALA:HB2	1.93	0.51
1:C:33:HIS:CE1	1:C:97:ASP:OD2	2.63	0.51
3:K:25:MET:HE2	3:K:43:TYR:CD2	2.46	0.51
1:A:183:VAL:HG11	2:B:132:LEU:HD22	1.93	0.51
3:I:115:THR:O	3:I:117:ARG:N	2.44	0.51
3:I:110:TRP:CD2	3:I:112:ASN:ND2	2.80	0.50
1:C:158:SER:N	1:C:199:ASN:HD21	2.09	0.50
2:L:105:ARG:NH2	2:L:106:THR:HG22	2.26	0.50
2:L:65:GLY:HA3	2:L:70:TYR:HA	1.93	0.50
1:C:33:HIS:HE1	1:C:97:ASP:OD2	1.95	0.50
2:B:142:LYS:HB3	2:B:194:THR:HB	1.94	0.50
2:L:49:ASP:HB2	2:L:52:LYS:HD2	1.94	0.49
2:L:33:GLN:NE2	2:L:49:ASP:H	2.10	0.49
2:L:105:ARG:HG2	2:L:106:THR:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:25:ALA:O	2:L:68:THR:HG23	2.13	0.49
1:H:158:SER:H	1:H:199:ASN:HD21	1.60	0.49
3:J:149:MET:O	3:J:150:THR:O	2.30	0.49
3:K:25:MET:CE	3:K:43:TYR:CE2	2.96	0.49
2:D:31:TYR:HB3	2:D:49:ASP:HA	1.94	0.49
3:I:115:THR:C	3:I:117:ARG:N	2.66	0.49
3:K:2:LEU:HD23	3:K:122:VAL:HG12	1.95	0.48
2:L:105:ARG:HG2	2:L:106:THR:H	1.78	0.48
3:I:42:LEU:HD12	3:I:43:TYR:CD2	2.48	0.48
1:C:38:ARG:CG	1:C:38:ARG:NH1	2.73	0.47
2:B:6:GLN:HG3	2:B:87:CYS:SG	2.54	0.47
3:K:28:CYS:HB2	3:K:42:LEU:O	2.15	0.47
1:H:36:LYS:HE2	1:H:38:ARG:HG3	1.97	0.47
1:C:121:PRO:HB3	1:C:147:TYR:HB3	1.95	0.47
3:I:52:HIS:CE1	4:I:300:NAG:H4	2.50	0.46
3:J:150:THR:CB	3:J:151:HIS:ND1	2.79	0.46
3:J:110:TRP:CE2	3:J:113:GLU:HG2	2.50	0.46
3:J:37:ILE:HG13	3:J:38:LYS:H	1.81	0.46
3:J:62:THR:HG22	3:J:63:SER:H	1.79	0.46
3:K:25:MET:HE3	3:K:43:TYR:CE2	2.50	0.46
1:A:53:ASN:ND2	1:A:55:ASP:HB2	2.31	0.45
2:L:31:TYR:HB3	2:L:49:ASP:HA	1.99	0.45
2:L:89:GLN:NE2	2:L:91:SER:H	2.14	0.45
3:I:24:THR:HG22	3:I:121:PHE:HA	1.99	0.45
3:I:2:LEU:HD12	3:I:122:VAL:HG12	1.99	0.45
2:L:133:LEU:HD21	2:L:193:VAL:HG13	1.97	0.45
4:J:300:NAG:O3	4:J:300:NAG:O7	2.34	0.45
2:D:167:ASP:O	2:D:168:SER:HB2	2.16	0.45
1:A:28:THR:HG23	1:A:52:GLY:HA2	1.99	0.44
2:D:4:SER:HB2	2:D:96:GLY:HA2	1.99	0.44
4:K:300:NAG:C3	4:K:301:NAG:O5	2.66	0.44
2:B:110:PRO:HD2	2:B:198:LEU:HD13	2.00	0.44
1:A:33:HIS:HD2	1:A:45:TRP:NE1	2.03	0.44
1:H:128:PRO:HD2	1:H:215:PRO:HA	2.00	0.44
2:L:194:THR:HG23	2:L:200:SER:HB3	2.01	0.43
1:H:95:SER:OG	1:H:102:PHE:HB3	2.18	0.43
1:C:9:LEU:HD21	1:C:149:PRO:HG3	2.00	0.43
2:L:2:ILE:O	2:L:94:THR:HG21	2.18	0.43
2:D:61:PHE:CE1	2:D:74:ILE:HG12	2.54	0.43
2:L:157:GLN:HB3	2:L:157:GLN:HE21	1.58	0.43
1:A:16:VAL:HG12	1:A:84:LEU:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:LYS:HB2	1:C:46:ILE:HD11	1.99	0.43
1:C:36:LYS:HB3	1:C:44:GLU:HB3	1.99	0.43
3:J:61:CYS:HB2	3:J:112:ASN:HB2	2.00	0.43
1:C:131:LYS:HE2	2:D:205:SER:O	2.19	0.43
2:B:183:TYR:HA	2:B:189:TYR:OH	2.18	0.43
3:J:150:THR:HG1	3:J:151:HIS:CE1	2.36	0.43
2:D:133:LEU:HD21	2:D:193:VAL:HG13	2.01	0.43
1:H:173:GLN:HE21	1:H:173:GLN:HB2	1.67	0.43
1:C:203:LYS:HB2	1:C:204:PRO:HD3	2.00	0.43
1:C:128:PRO:HG3	1:C:140:LEU:HB3	2.00	0.43
1:A:38:ARG:CG	1:A:38:ARG:NH1	2.80	0.43
3:J:145:SER:CA	3:J:157:THR:OG1	2.57	0.42
1:C:65:LYS:HG2	1:C:81:LEU:HD12	2.00	0.42
2:D:32:MET:HE3	2:D:70:TYR:CD1	2.54	0.42
2:D:33:GLN:HG3	2:D:48:TYR:HA	2.00	0.42
2:L:23:CYS:SG	2:L:32:MET:HE1	2.60	0.42
1:H:33:HIS:HE1	1:H:97:ASP:OD2	2.02	0.42
3:J:107:PRO:HA	3:J:108:PRO:HD3	1.93	0.42
3:J:146:VAL:H	3:J:157:THR:CG2	2.33	0.42
2:L:29:ARG:NE	2:L:30:SER:H	2.17	0.42
2:B:60:ARG:HH11	2:B:81:ASP:CG	2.22	0.42
1:A:8:VAL:HG11	1:A:16:VAL:HG21	2.01	0.42
1:H:9:LEU:HD21	1:H:149:PRO:HG3	2.02	0.42
2:D:45:ARG:HG3	2:D:45:ARG:H	1.59	0.42
1:H:17:LYS:HE2	1:H:78:TYR:CD2	2.55	0.41
2:B:60:ARG:HD2	2:B:76:SER:O	2.20	0.41
2:D:156:SER:HB3	2:D:176:LEU:HD23	2.02	0.41
1:H:128:PRO:HG3	1:H:140:LEU:HB3	2.02	0.41
3:I:106:GLU:HA	3:I:107:PRO:HD3	1.90	0.41
3:K:25:MET:HE2	3:K:43:TYR:CE2	2.56	0.41
1:H:170:ALA:HA	1:H:180:LEU:HB3	2.02	0.41
3:J:115:THR:O	3:J:116:GLU:CB	2.68	0.41
1:C:127:ALA:HA	1:C:128:PRO:HD3	1.99	0.41
1:H:71:VAL:HG12	1:H:74:ALA:H	1.86	0.41
3:I:15:PHE:HA	3:I:128:TYR:O	2.21	0.41
3:J:32:ARG:HD2	3:J:32:ARG:H	1.84	0.41
2:D:110:PRO:HD2	2:D:198:LEU:HD13	2.03	0.41
1:A:31:TRP:CE3	3:K:42:LEU:HD22	2.57	0.40
3:J:15:PHE:HB2	3:J:127:VAL:CG1	2.51	0.40
3:I:135:TYR:CB	3:I:136:ARG:CD	2.87	0.40
3:J:121:PHE:CD2	3:J:125:GLN:HG2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	213/215 (99%)	201 (94%)	11 (5%)	1 (0%)	34	71
1	C	213/215 (99%)	206 (97%)	7 (3%)	0	100	100
1	H	213/215 (99%)	198 (93%)	13 (6%)	2 (1%)	21	57
2	B	206/210 (98%)	201 (98%)	5 (2%)	0	100	100
2	D	207/210 (99%)	198 (96%)	8 (4%)	1 (0%)	34	71
2	L	206/210 (98%)	198 (96%)	6 (3%)	2 (1%)	19	54
3	I	115/223 (52%)	100 (87%)	11 (10%)	4 (4%)	4	18
3	J	110/223 (49%)	88 (80%)	14 (13%)	8 (7%)	1	3
3	K	108/223 (48%)	93 (86%)	11 (10%)	4 (4%)	4	17
All	All	1591/1944 (82%)	1483 (93%)	86 (5%)	22 (1%)	14	44

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	54	SER
1	H	131	LYS
3	I	111	GLU
3	J	52	HIS
3	J	150	THR
3	K	39	SER
3	I	134	GLY
3	J	38	LYS
3	J	133	GLN
3	K	41	SER
1	A	132	SER
2	L	67	GLY
3	I	116	GLU

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Mol	Chain	Res	Type
3	J	11	PRO
3	J	49	ASN
3	J	111	GLU
3	K	37	ILE
3	K	38	LYS
2	L	82	ALA
2	D	67	GLY
3	I	11	PRO
3	J	107	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	181/181 (100%)	171 (94%)	10 (6%)	27	61
1	C	181/181 (100%)	173 (96%)	8 (4%)	35	70
1	H	181/181 (100%)	174 (96%)	7 (4%)	39	75
2	B	181/182 (100%)	174 (96%)	7 (4%)	39	75
2	D	181/182 (100%)	173 (96%)	8 (4%)	35	70
2	L	181/182 (100%)	172 (95%)	9 (5%)	30	65
3	I	104/200 (52%)	95 (91%)	9 (9%)	13	36
3	J	102/200 (51%)	96 (94%)	6 (6%)	24	58
3	K	100/200 (50%)	93 (93%)	7 (7%)	19	47
All	All	1392/1689 (82%)	1321 (95%)	71 (5%)	29	65

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	VAL
1	A	38	ARG
1	A	41	GLN
1	A	107	GLN
1	A	111	LEU

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Mol	Chain	Res	Type
1	A	152	VAL
1	A	195	THR
1	A	201	ASN
1	A	208	LYS
1	A	209	VAL
2	B	20	THR
2	B	45	ARG
2	B	89	GLN
2	B	105	ARG
2	B	126	THR
2	B	139	ARG
2	B	176	LEU
1	C	11	ARG
1	C	38	ARG
1	C	41	GLN
1	C	111	LEU
1	C	131	LYS
1	C	140	LEU
1	C	195	THR
1	C	209	VAL
2	D	7	SER
2	D	41	THR
2	D	45	ARG
2	D	89	GLN
2	D	94	THR
2	D	187	LYS
2	D	198	LEU
2	D	199	SER
1	H	8	VAL
1	H	41	GLN
1	H	79	MET
1	H	81	LEU
1	H	111	LEU
1	H	131	LYS
1	H	163	SER
2	L	19	VAL
2	L	45	ARG
2	L	89	GLN
2	L	106	THR
2	L	132	LEU
2	L	157	GLN
2	L	174	SER

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Mol	Chain	Res	Type
2	L	176	LEU
2	L	198	LEU
3	I	6	ASP
3	I	36	ARG
3	I	42	LEU
3	I	45	LEU
3	I	113	GLU
3	I	133	GLN
3	I	135	TYR
3	I	136	ARG
3	I	140	ARG
3	J	3	CYS
3	J	6	ASP
3	J	32	ARG
3	J	62	THR
3	J	116	GLU
3	J	151	HIS
3	K	3	CYS
3	K	6	ASP
3	K	30	CYS
3	K	42	LEU
3	K	115	THR
3	K	116	GLU
3	K	125	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	HIS
1	A	41	GLN
1	A	199	ASN
1	A	201	ASN
2	B	33	GLN
2	B	89	GLN
2	B	196	GLN
2	B	207	ASN
1	C	33	HIS
1	C	199	ASN
2	D	33	GLN
2	D	89	GLN
2	D	144	GLN
1	H	33	HIS

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Mol	Chain	Res	Type
1	H	41	GLN
1	H	166	HIS
1	H	173	GLN
1	H	199	ASN
1	H	201	ASN
2	L	33	GLN
2	L	157	GLN
3	I	125	GLN
3	K	57	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 ⓘ

9 carbohydrates are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	I	300	3,4	14,14,15	0.69	0	15,19,21	1.79	4 (26%)
4	NAG	I	301	4	14,14,15	0.49	0	15,19,21	1.35	1 (6%)
4	BMA	I	302	4	11,11,12	0.89	1 (9%)	14,15,17	1.64	3 (21%)
4	NAG	J	300	3,4	14,14,15	0.54	0	15,19,21	0.59	0
4	NAG	J	301	4	14,14,15	0.62	0	15,19,21	0.89	0
4	BMA	J	302	4	11,11,12	0.71	0	14,15,17	0.72	0
4	NAG	K	300	3,4	14,14,15	0.76	1 (7%)	15,19,21	2.32	5 (33%)
4	NAG	K	301	4	14,14,15	0.50	0	15,19,21	1.84	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	BMA	K	302	4	11,11,12	0.77	0	14,15,17	1.38	2 (14%)

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
4	NAG	I	300	3,4	-	0/6/23/26	0/1/1/1
4	NAG	I	301	4	-	0/6/23/26	0/1/1/1
4	BMA	I	302	4	-	0/2/19/22	0/1/1/1
4	NAG	J	300	3,4	-	0/6/23/26	0/1/1/1
4	NAG	J	301	4	-	0/6/23/26	0/1/1/1
4	BMA	J	302	4	-	0/2/19/22	0/1/1/1
4	NAG	K	300	3,4	-	0/6/23/26	0/1/1/1
4	NAG	K	301	4	-	0/6/23/26	0/1/1/1
4	BMA	K	302	4	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	K	300	NAG	C1-C2	2.15	1.55	1.52
4	I	302	BMA	C2-C3	2.18	1.55	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	300	NAG	C3-C4-C5	-2.21	106.35	110.20
4	K	301	NAG	C6-C5-C4	-2.16	107.69	113.02
4	I	300	NAG	O4-C4-C5	-2.00	103.94	109.24
4	I	300	NAG	O5-C5-C6	2.02	111.72	107.35
4	K	302	BMA	C1-O5-C5	2.39	115.28	112.25
4	I	302	BMA	O5-C5-C6	2.49	112.74	107.35
4	I	300	NAG	C2-N2-C7	2.71	126.52	123.04
4	K	300	NAG	C6-C5-C4	2.77	119.84	113.02
4	K	300	NAG	C1-O5-C5	2.79	115.78	112.25
4	K	301	NAG	C1-O5-C5	2.79	115.78	112.25
4	I	302	BMA	C2-C3-C4	3.03	116.19	111.04
4	K	300	NAG	O4-C4-C3	3.36	117.90	110.34
4	I	301	NAG	C4-C3-C2	3.37	116.47	111.23
4	K	301	NAG	C3-C4-C5	3.86	116.93	110.20
4	K	302	BMA	C1-C2-C3	3.88	114.14	109.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	301	NAG	C4-C3-C2	4.03	117.50	111.23
4	I	302	BMA	C1-C2-C3	4.16	114.46	109.54
4	I	300	NAG	C4-C3-C2	4.71	118.54	111.23
4	K	300	NAG	C2-N2-C7	5.45	130.04	123.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	300	NAG	1	0
4	J	300	NAG	2	0
4	J	301	NAG	1	0
4	K	300	NAG	1	0
4	K	301	NAG	1	0

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	215/215 (100%)	0.00	0 100 100	49, 71, 101, 122	0
1	C	215/215 (100%)	0.01	1 (0%) 91 90	46, 74, 104, 136	0
1	H	215/215 (100%)	0.02	1 (0%) 91 90	53, 78, 113, 154	0
2	B	208/210 (99%)	-0.10	1 (0%) 91 90	43, 64, 102, 121	0
2	D	209/210 (99%)	-0.05	1 (0%) 91 90	42, 65, 111, 126	0
2	L	208/210 (99%)	-0.13	0 100 100	52, 71, 111, 136	0
3	I	119/223 (53%)	1.32	34 (28%) 1 0	79, 130, 186, 224	0
3	J	116/223 (52%)	1.08	23 (19%) 1 1	65, 132, 175, 191	0
3	K	114/223 (51%)	0.99	19 (16%) 2 1	71, 131, 179, 202	0
All	All	1619/1944 (83%)	0.21	80 (4%) 33 27	42, 77, 159, 224	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	I	115	THR	7.0
3	I	116	GLU	6.6
3	K	18	MET	6.1
3	I	114	ALA	6.0
3	J	116	GLU	5.5
3	I	35	ARG	5.3
3	J	130	GLN	5.1
3	I	138	LEU	4.4
3	K	19	ALA	4.1
3	I	34	PHE	4.0
3	K	139	HIS	4.0
3	K	116	GLU	3.9
3	K	60	GLN	3.9
3	J	19	ALA	3.9
3	K	143	ALA	3.8

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Mol	Chain	Res	Type	RSRZ
3	I	143	ALA	3.6
3	I	118	ILE	3.6
3	I	20	TYR	3.6
3	I	29	GLU	3.5
3	K	140	ARG	3.5
3	K	42	LEU	3.4
3	I	19	ALA	3.4
3	I	12	HIS	3.4
3	I	104	CYS	3.3
3	I	39	SER	3.3
3	K	59	CYS	3.2
3	I	132	VAL	3.2
3	I	9	GLU	3.2
3	I	33	GLY	3.2
3	I	13	ALA	3.1
3	K	62	THR	3.1
3	K	43	TYR	3.1
3	J	144	GLU	3.1
3	J	140	ARG	3.0
3	K	29	GLU	3.0
3	K	115	THR	2.9
3	J	18	MET	2.9
3	I	61	CYS	2.9
3	J	60	GLN	2.9
3	J	133	GLN	2.9
3	J	111	GLU	2.9
3	I	14	THR	2.9
3	J	138	LEU	2.8
3	K	155	ARG	2.8
3	J	9	GLU	2.7
3	I	130	GLN	2.7
3	I	119	TYR	2.6
3	I	60	GLN	2.6
3	K	58	GLN	2.6
3	I	128	TYR	2.6
3	J	106	GLU	2.5
3	K	61	CYS	2.5
3	I	45	LEU	2.5
3	I	18	MET	2.5
3	J	12	HIS	2.5
3	J	135	TYR	2.5
3	J	119	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
3	K	110	TRP	2.4
3	I	139	HIS	2.4
3	J	105	ARG	2.4
1	C	1	GLN	2.4
3	I	112	ASN	2.3
2	D	29	ARG	2.3
3	I	30	CYS	2.3
3	J	63	SER	2.3
3	I	41	SER	2.3
1	H	209	VAL	2.2
3	J	62	THR	2.2
2	B	29	ARG	2.2
3	I	31	LYS	2.2
3	J	118	ILE	2.2
3	K	118	ILE	2.1
3	I	46	CYS	2.1
3	I	58	GLN	2.1
3	I	55	TRP	2.1
3	J	134	GLY	2.1
3	J	121	PHE	2.1
3	J	117	ARG	2.1
3	J	26	LEU	2.0
3	K	45	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	NAG	I	301	14/15	0.89	0.12	-	101,129,148,153	0
4	NAG	K	301	14/15	0.79	0.18	-	125,138,154,157	0
4	NAG	K	300	14/15	0.73	0.21	-	71,101,135,138	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	BMA	K	302	11/12	0.83	0.14	-	126,148,157,160	0
4	NAG	I	300	14/15	0.76	0.15	-	66,115,130,135	0
4	BMA	I	302	11/12	0.79	0.18	-	141,157,168,168	0
4	BMA	J	302	11/12	0.70	0.18	-	137,155,169,172	0
4	NAG	J	300	14/15	0.66	0.22	-	66,113,133,134	0
4	NAG	J	301	14/15	0.72	0.21	-	125,141,168,169	0

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.