



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Mar 2, 2017 – 12:13 pm GMT

PDB ID : 5A1A
EMDB ID: : EMD-2984
Title : 2.2 Å resolution cryo-EM structure of beta-galactosidase in complex with a cell-permeant inhibitor
Authors : Bartesaghi, A.; Merk, A.; Banerjee, S.; Matthies, D.; Wu, X.; Milne, J.; Subramaniam, S.
Deposited on : 2015-04-29
Resolution : 2.20 Å (reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : recalc29047

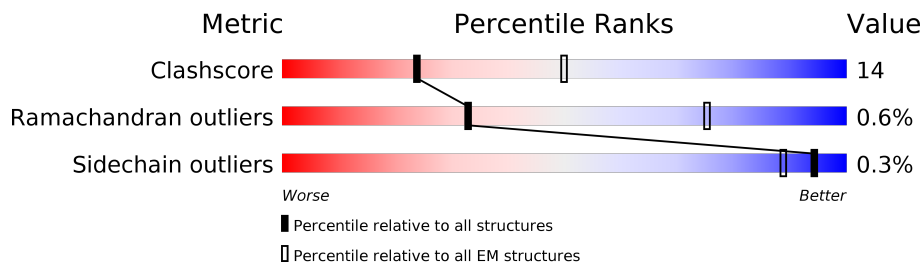
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.20 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)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	1022	72% 27% .
1	B	1022	71% 28% .
1	C	1022	72% 27% .
1	D	1022	71% 28% .

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
2	PTQ	A	2001	-	-	X	-
2	PTQ	B	2001	-	-	X	-
2	PTQ	C	2001	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PTQ	D	2001	-	-	X	-

2 Entry composition [i](#)

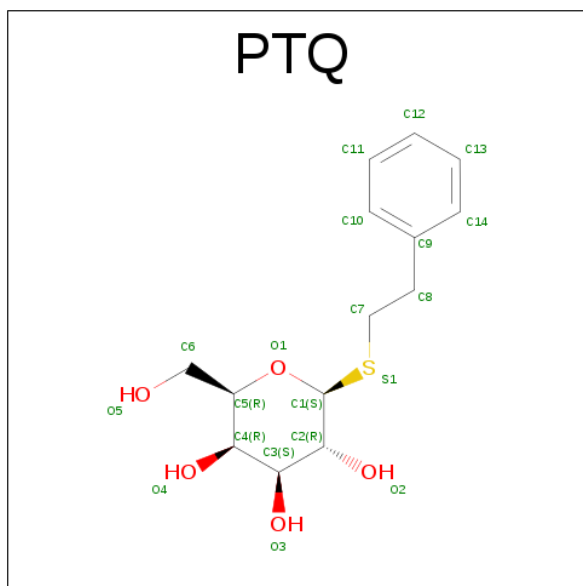
There are 5 unique types of molecules in this entry. The entry contains 33696 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 BETA-GALACTOSIDASE.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1022	Total	C	N	O	S	0	0
			8206	5190	1452	1525	39		
1	B	1022	Total	C	N	O	S	0	0
			8206	5190	1452	1525	39		
1	C	1022	Total	C	N	O	S	0	0
			8206	5190	1452	1525	39		
1	D	1022	Total	C	N	O	S	0	0
			8206	5190	1452	1525	39		

- Molecule 2 is SUGAR (2-PHENYLETHYL 1-THIO-BETA-D-GALACTOPYRANOSIDE) (three-letter code: PTQ) (formula: C₁₄H₂₀O₅S).



Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	O	S	0
			20	14	5	1	
2	B	1	Total	C	O	S	0
			20	14	5	1	

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Mol	Chain	Residues	Atoms				AltConf
2	C	1	Total	C	O	S	0
			20	14	5	1	
2	D	1	Total	C	O	S	0
			20	14	5	1	

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
3	B	2	Total	Mg	0
			2	2	
3	A	2	Total	Mg	0
			2	2	
3	D	2	Total	Mg	0
			2	2	
3	C	2	Total	Mg	0
			2	2	

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
4	B	2	Total	Na	0
			2	2	
4	A	2	Total	Na	0
			2	2	
4	D	2	Total	Na	0
			2	2	
4	C	2	Total	Na	0
			2	2	

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		AltConf
5	A	194	Total	O	0
			194	194	
5	B	194	Total	O	0
			194	194	
5	C	194	Total	O	0
			194	194	
5	D	194	Total	O	0
			194	194	

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

Chain A:

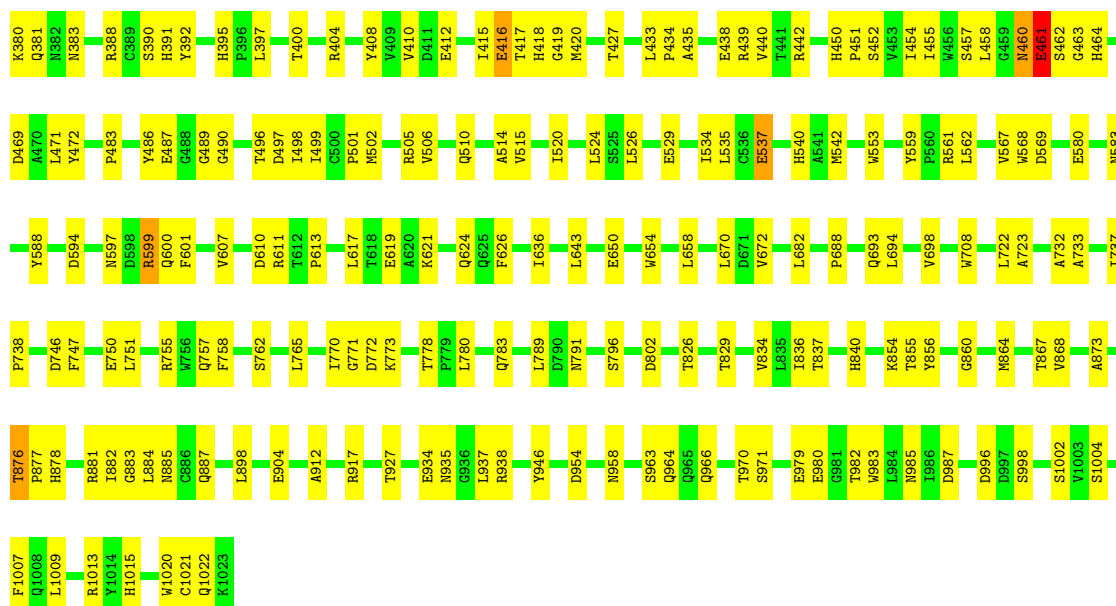
72%

27%

M1 M2 M3 M4 M5 M6 M7 M8 M9 M10 M11 M12 M13 M14 M15 M16 M17 M18 M19 M20 M21 M22 M23 M24 M25 M26 M27 M28 M29 M30 M31 M32 M33 M34 M35 M36 M37 M38 M39 M40 M41 M42 M43 M44 M45 M46 M47 M48 M49 M50 M51 M52 M53 M54 M55 M56 M57 M58 M59 M60 M61 M62 M63 M64 M65 M66 M67 M68 M69 M70 M71 M72 M73 M74 M75 M76 M77 M78 M79 M80 M81 M82 M83 M84 M85 M86 M87 M88 M89 M90 M91 M92 M93 M94 M95 M96 M97 M98 M99 M100 M101 M102 M103 M104 M105 M106 M107 M108 M109 M110 M111 M112 M113 M114 M115 M116 M117 M118 M119 M120 M121 M122 M123 M124 M125 M126 M127 M128 M129 M130 M131 M132 M133 M134 M135 M136 M137 M138 M139 M140 M141 M142 M143 M144 M145 M146 M147 M148 M149 M150 M151 M152 M153 M154 M155 M156 M157 M158 M159 M160 M161 M162 M163 M164 M165 M166 M167 M168 M169 M170 M171 M172 M173 M174 M175 M176 M177 M178 M179 M180 M181 M182 M183 M184 M185 M186 M187 M188 M189 M190 M191 M192 M193 M194 M195 M196 M197 M198 M199 M200 M201 M202 M203 M204 M205 M206 M207 M208 M209 M210 M211 M212 M213 M214 M215 M216 M217 M218 M219 M220 M221 M222 M223 M224 M225 M226 M227 M228 M229 M230 M231 M232 M233 M234 M235 M236 M237 M238 M239 M240 M241 M242 M243 M244 M245 M246 M247 M248 M249 M250 M251 M252 M253 M254 M255 M256 M257 M258 M259 M260 M261 M262 M263 M264 M265 M266 M267 M268 M269 M270 M271 M272 M273 M274 M275 M276 M277 M278 M279 M280 M281 M282 M283 M284 M285 M286 M287 M288 M289 M290 M291 M292 M293 M294 M295 M296 M297 M298 M299 M300 M301 M302 M303 M304 M305 M306 M307 M308 M309 M310 M311 M312 M313 M314 M315 M316 M317 M318 M319 M320 M321 M322 M323 M324 M325 M326 M327 M328 M329 M330 M331 M332 M333 M334 M335 M336 M337 M338 M339 M340 M341 M342 M343 M344 M345 M346 M347 M348 M349 M350 M351 M352 M353 M354 M355 M356 M357 M358 M359 M360 M361 M362 M363 M364 M365 M366 M367 M368 M369 M370 M371 M372 M373 M374 M375 M376 M377 M378 M379 M380 M381 M382 M383 M384 M385 M386 M387 M388 M389 M390 M391 M392 M393 M394 M395 M396 M397 M398 M399 M400 M401 M402 M403 M404 M405 M406 M407 M408 M409 M410 M411 M412 M413 M414 M415 M416 M417 M418 M419 M420 M421 M422 M423 M424 M425 M426 M427 M428 M429 M430 M431 M432 M433 M434 M435 M436 M437 M438 M439 M440 M441 M442 M443 M444 M445 M446 M447 M448 M449 M450 M451 M452 M453 M454 M455 M456 M457 M458 M459 M460 M461 M462 M463 M464 M465 M466 M467 M468 M469 M470 M471 M472 M473 M474 M475 M476 M477 M478 M479 M480 M481 M482 M483 M484 M485 M486 M487 M488 M489 M490 M491 M492 M493 M494 M495 M496 M497 M498 M499 M500 M501 M502 M503 M504 M505 M506 M507 M508 M509 M510 M511 M512 M513 M514 M515 M516 M517 M518 M519 M520 M521 M522 M523 M524 M525 M526 M527 M528 M529 M530 M531 M532 M533 M534 M535 M536 M537 M538 M539 M540 M541 M542 M543 M544 M545 M546 M547 M548 M549 M550 M551 M552 M553 M554 M555 M556 M557 M558 M559 M560 M561 M562 M563 M564 M565 M566 M567 M568 M569 M570 M571 M572 M573 M574 M575 M576 M577 M578 M579 M580 M581 M582 M583 M584 M585 M586 M587 M588 M589 M590 M591 M592 M593 M594 M595 M596 M597 M598 M599 M600 M601 M602 M603 M604 M605 M606 M607 M608 M609 M610 M611 M612 M613 M614 M615 M616 M617 M618 M619 M620 M621 M622 M623 M624 M625 M626 M627 M628 M629 M630 M631 M632 M633 M634 M635 M636 M637 M638 M639 M640 M641 M642 M643 M644 M645 M646 M647 M648 M649 M650 M651 M652 M653 M654 M655 M656 M657 M658 M659 M660 M661 M662 M663 M664 M665 M666 M667 M668 M669 M670 M671 M672 M673 M674 M675 M676 M677 M678 M679 M680 M681 M682 M683 M684 M685 M686 M687 M688 M689 M690 M691 M692 M693 M694 M695 M696 M697 M698 M699 M700 M701 M702 M703 M704 M705 M706 M707 M708 M709 M710 M711 M712 M713 M714 M715 M716 M717 M718 M719 M720 M721 M722 M723 M724 M725 M726 M727 M728 M729 M730 M731 M732 M733 M734 M735 M736 M737 M738 M739 M740 M741 M742 M743 M744 M745 M746 M747 M748 M749 M750 M751 M752 M753 M754 M755 M756 M757 M758 M759 M760 M761 M762 M763 M764 M765 M766 M767 M768 M769 M770 M771 M772 M773 M774 M775 M776 M777 M778 M779 M780 M781 M782 M783 M784 M785 M786 M787 M788 M789 M790 M791 M792 M793 M794 M795 M796 M797 M798 M799 M800 M801 M802 M803 M804 M805 M806 M807 M808 M809 M810 M811 M812 M813 M814 M815 M816 M817 M818 M819 M820 M821 M822 M823 M824 M825 M826 M827 M828 M829 M830 M831 M832 M833 M834 M835 M836 M837 M838 M839 M840 M841 M842 M843 M844 M845 M846 M847 M848 M849 M850 M851 M852 M853 M854 M855 M856 M857 M858 M859 M860 M861 M862 M863 M864 M865 M866 M867 M868 M869 M870 M871 M872 M873 M874 M875 M876 M877 M878 M879 M880 M881 M882 M883 M884 M885 M886 M887 M888 M889 M890 M891 M892 M893 M894 M895 M896 M897 M898 M899 M900 M901 M902 M903 M904 M905 M906 M907 M908 M909 M910 M911 M912 M913 M914 M915 M916 M917 M918 M919 M920 M921 M922 M923 M924 M925 M926 M927 M928 M929 M930 M931 M932 M933 M934 M935 M936 M937 M938 M939 M940 M941 M942 M943 M944 M945 M946 M947 M948 M949 M950 M951 M952 M953 M954 M955 M956 M957 M958 M959 M960 M961 M962 M963 M964 M965 M966 M967 M968 M969 M970 M971 M972 M973 M974 M975 M976 M977 M978 M979 M980 M981 M982 M983 M984 M985 M986 M987 M988 M989 M990 M991 M992 M993 M994 M995 M

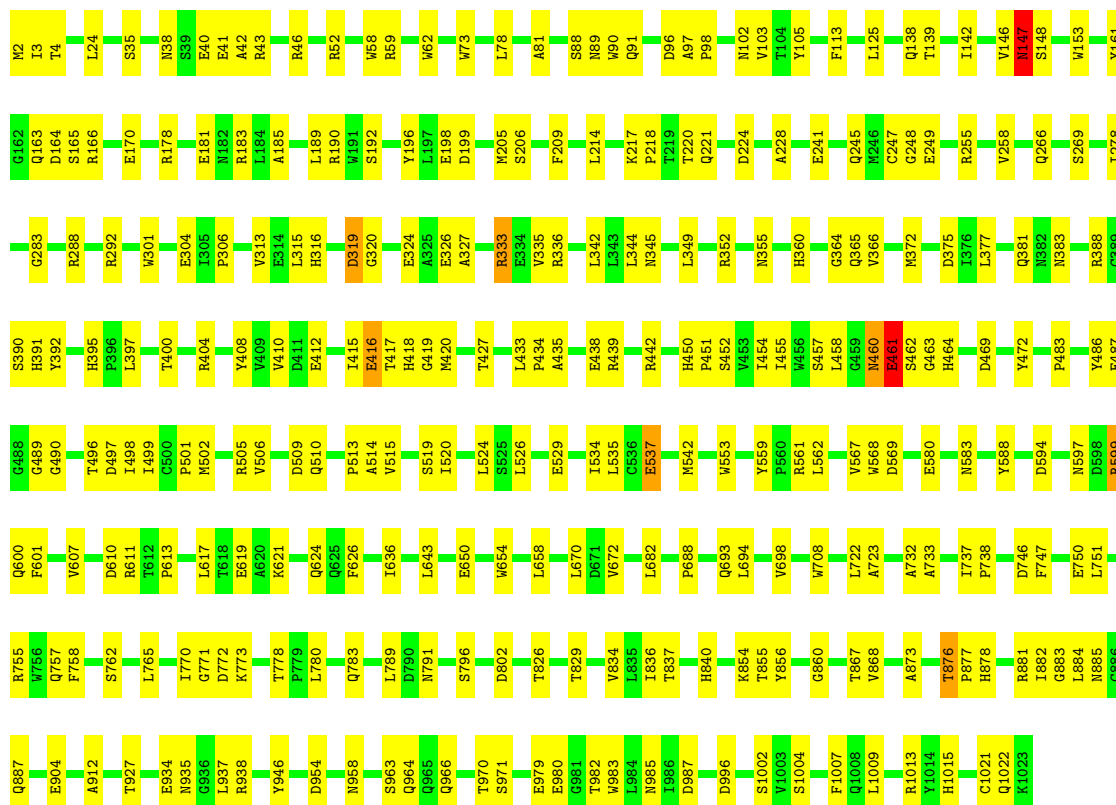
Chain B:

Category	Value
M2	71%
T4	71%
L24	71%
H30	71%
P31	71%
S35	71%
M38	71%
S39	71%
E40	71%
E41	71%
A42	71%
R43	71%
R46	71%
R52	71%
W58	71%
R59	71%
W62	71%
W73	71%
L78	71%
A81	71%
S88	71%
R90	71%
Q91	71%
D96	71%
A97	71%
P98	71%
M102	71%
V103	71%
T104	71%
Y105	71%
F113	71%
S124	71%
L125	71%
Q138	71%
T139	71%
I142	71%
V146	71%
R147	71%
W153	28%
Y161	28%
G162	28%
D164	28%
S165	28%
A166	28%
E170	28%
R178	28%
E181	28%
G182	28%
L183	28%
L184	28%
A185	28%
L189	28%
R190	28%
Y191	28%
S192	28%
D193	28%
Y196	28%
L197	28%
E198	28%
D199	28%
M205	28%
S206	28%
F209	28%
L214	28%
K217	28%
P218	28%
T219	28%
T220	28%
Q221	28%
D224	28%
A228	28%
E241	28%
Q245	28%
M246	28%
C247	28%
G248	28%
E249	28%
R255	28%
V258	28%
C266	28%



• Molecule 1: BETA-GALACTOSIDASE

Chain C:  72% 27%



• Molecule 1: BETA-GALACTOSIDASE

Chain D:  71% 28%




4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	EACH PARTICLE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	215000	Depositor
Image detector	GATAN K2 (4K X 4K)	Depositor

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: NA, MG, PTQ

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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	0.40	6/8448 (0.1%)	0.52	14/11526 (0.1%)
1	B	0.40	6/8448 (0.1%)	0.52	14/11526 (0.1%)
1	C	0.40	6/8448 (0.1%)	0.52	14/11526 (0.1%)
1	D	0.40	6/8448 (0.1%)	0.52	14/11526 (0.1%)
All	All	0.40	24/33792 (0.1%)	0.52	56/46104 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	3
1	C	0	3
1	D	0	3
All	All	0	12

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	146	VAL	C-N	-18.42	0.91	1.34
1	B	146	VAL	C-N	-18.42	0.91	1.34
1	C	146	VAL	C-N	-18.42	0.91	1.34
1	D	146	VAL	C-N	-18.42	0.91	1.34
1	A	461	GLU	C-N	-15.25	0.98	1.34

The worst 5 of 56 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	461	GLU	O-C-N	19.17	153.38	122.70
1	B	461	GLU	O-C-N	19.17	153.38	122.70
1	C	461	GLU	O-C-N	19.17	153.38	122.70
1	D	461	GLU	O-C-N	19.17	153.38	122.70
1	A	147	ASN	O-C-N	-14.44	99.59	122.70

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	147	ASN	Mainchain
1	A	460	ASN	Mainchain
1	A	882	ILE	Peptide
1	B	147	ASN	Mainchain
1	B	460	ASN	Mainchain

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	8206	0	7802	218	0
1	B	8206	0	7802	221	0
1	C	8206	0	7802	218	0
1	D	8206	0	7802	218	0
2	A	20	0	18	20	0
2	B	20	0	18	20	0
2	C	20	0	18	20	0
2	D	20	0	18	19	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
5	A	194	0	0	19	0
5	B	194	0	0	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	194	0	0	19	0
5	D	194	0	0	19	0
All	All	33696	0	31280	878	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 14.

The worst 5 of 878 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:C:601:PHE:CG	2:C:2001:PTQ:H11	1.82	1.15
1:A:601:PHE:CG	2:A:2001:PTQ:H11	1.82	1.15
1:D:601:PHE:CG	2:D:2001:PTQ:H11	1.82	1.14
1:B:601:PHE:CG	2:B:2001:PTQ:H11	1.82	1.14
1:B:601:PHE:CD1	2:B:2001:PTQ:H11	1.97	1.00

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 PDB entries followed by that with respect to all EM entries.

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	1020/1022 (100%)	974 (96%)	40 (4%)	6 (1%)	28	29
1	B	1020/1022 (100%)	974 (96%)	40 (4%)	6 (1%)	28	29
1	C	1020/1022 (100%)	974 (96%)	40 (4%)	6 (1%)	28	29
1	D	1020/1022 (100%)	974 (96%)	40 (4%)	6 (1%)	28	29
All	All	4080/4088 (100%)	3896 (96%)	160 (4%)	24 (1%)	33	29

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	ILE
1	A	461	GLU
1	B	3	ILE
1	B	461	GLU
1	C	3	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	874/874 (100%)	871 (100%)	3 (0%)	94	97
1	B	874/874 (100%)	871 (100%)	3 (0%)	94	97
1	C	874/874 (100%)	871 (100%)	3 (0%)	94	97
1	D	874/874 (100%)	871 (100%)	3 (0%)	94	97
All	All	3496/3496 (100%)	3484 (100%)	12 (0%)	94	97

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	537	GLU
1	C	333	ARG
1	D	333	ARG
1	B	416	GLU
1	C	537	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 76 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	775	GLN
1	C	163	GLN
1	D	653	HIS
1	B	935	ASN
1	C	25	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 20 ligands modelled in this entry, 16 are monoatomic - leaving 4 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$
2	PTQ	A	2001	4	21,21,21	2.59	4 (19%)	26,28,28	1.51	2 (7%)
2	PTQ	B	2001	4	21,21,21	2.59	4 (19%)	26,28,28	1.51	2 (7%)
2	PTQ	C	2001	4	21,21,21	2.59	4 (19%)	26,28,28	1.51	2 (7%)
2	PTQ	D	2001	4	21,21,21	2.59	4 (19%)	26,28,28	1.51	2 (7%)

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
2	PTQ	A	2001	4	-	0/8/28/28	0/2/2/2
2	PTQ	B	2001	4	-	0/8/28/28	0/2/2/2
2	PTQ	C	2001	4	-	0/8/28/28	0/2/2/2
2	PTQ	D	2001	4	-	0/8/28/28	0/2/2/2

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2001	PTQ	C7-S1	-2.83	1.77	1.81
2	C	2001	PTQ	C7-S1	-2.83	1.77	1.81
2	B	2001	PTQ	C7-S1	-2.83	1.77	1.81
2	D	2001	PTQ	C7-S1	-2.83	1.77	1.81
2	A	2001	PTQ	C12-C11	5.66	1.51	1.38

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2001	PTQ	C7-C8-C9	-3.27	108.41	114.05
2	C	2001	PTQ	C7-C8-C9	-3.27	108.41	114.05
2	B	2001	PTQ	C7-C8-C9	-3.27	108.41	114.05
2	D	2001	PTQ	C7-C8-C9	-3.27	108.41	114.05
2	A	2001	PTQ	C7-S1-C1	6.24	109.54	100.28

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 79 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2001	PTQ	20	0
2	B	2001	PTQ	20	0
2	C	2001	PTQ	20	0
2	D	2001	PTQ	19	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.