



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 3, 2025 – 12:34 PM EST

PDB ID : 9NPD / pdb_00009npd
Title : Crystal structure of the inactive conformation of a glycoside hydrolase (CapGH2b - E553Q Mutant) from the GH2 family in the space group P3121 at 3.05 Å
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Deposited on : 2025-03-11
Resolution : 3.05 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.46

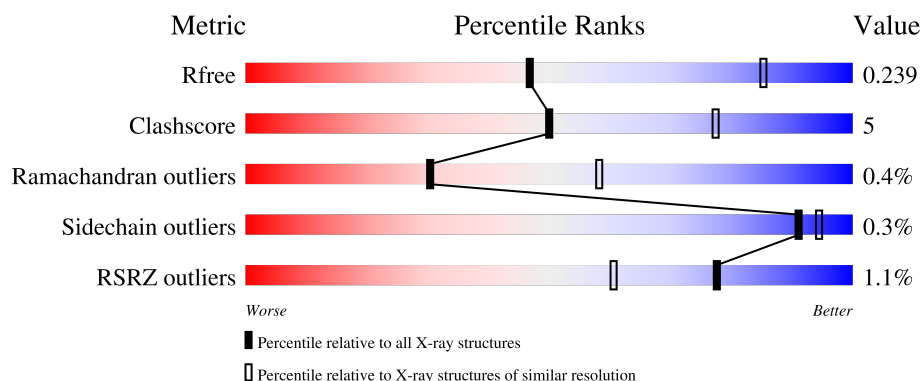
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.05 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}	164625	2258 (3.10-3.02)
Clashscore	180529	2399 (3.10-3.02)
Ramachandran outliers	177936	2269 (3.10-3.02)
Sidechain outliers	177891	2268 (3.10-3.02)
RSRZ outliers	164620	2258 (3.10-3.02)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	798	
1	B	798	
1	C	798	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 17910 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 Glycoside hydrolase family 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	737	Total	C	N	O	S	0	0	0
			5916	3780	1010	1096	30			
1	B	741	Total	C	N	O	S	0	0	0
			5953	3806	1019	1099	29			
1	C	734	Total	C	N	O	S	0	0	0
			5894	3763	1008	1094	29			

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is MALONATE ION (CCD ID: MLI) (formula: $C_3H_2O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			7	3	4		
4	B	1	Total	C	O	0	0
			7	3	4		

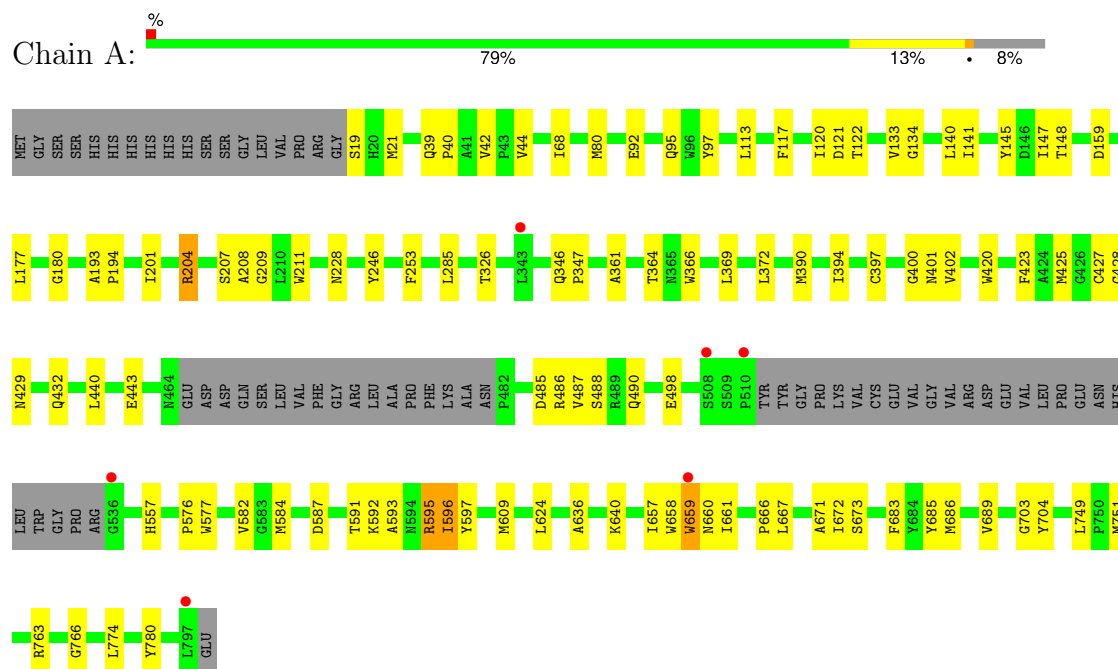
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	37	Total	O	0	0
			37	37		
5	B	16	Total	O	0	0
			16	16		
5	C	18	Total	O	0	0
			18	18		

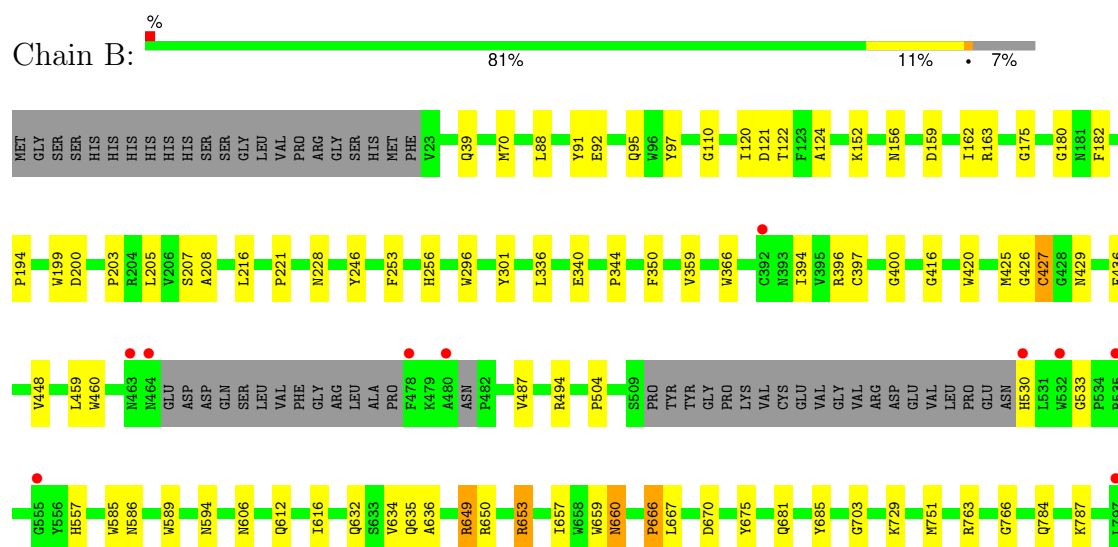
3 Residue-property plots [i](#)

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

• Molecule 1: Glycoside hydrolase family 2

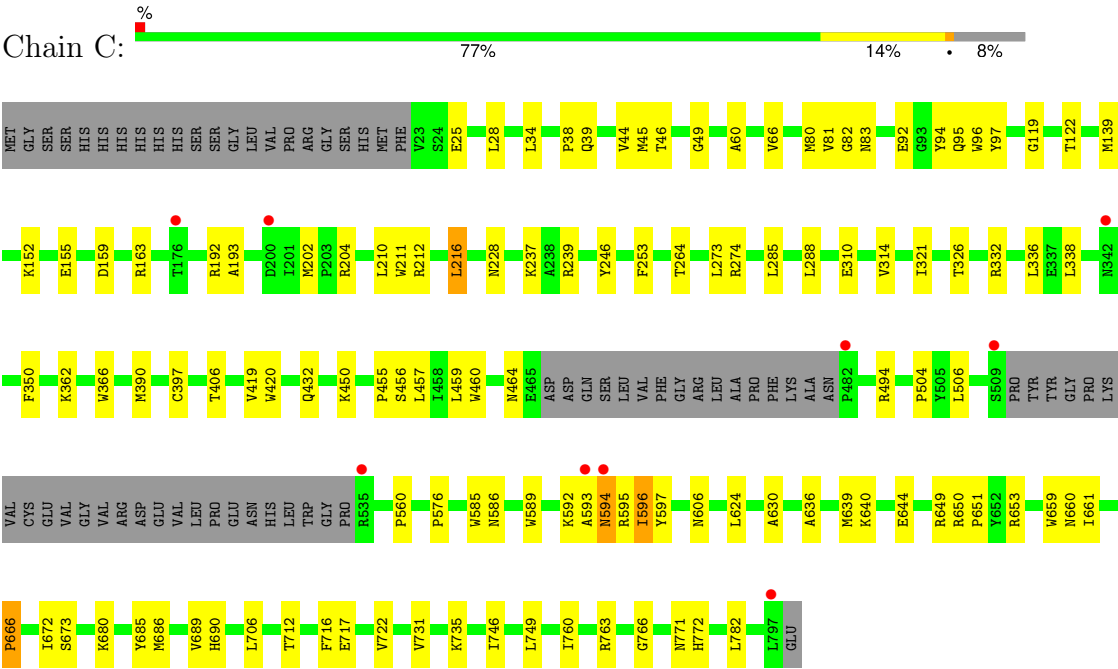


• Molecule 1: Glycoside hydrolase family 2



GLU

● Molecule 1: Glycoside hydrolase family 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	222.91Å 222.91Å 151.36Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.02 – 3.05 49.02 – 3.05	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.02-3.05) 99.8 (49.02-3.05)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.20 (at 3.07Å)	Xtriage
Refinement program	PHENIX (1.21.2_5419: ???)	Depositor
R, R_{free}	0.217 , 0.238 0.219 , 0.239	Depositor DCC
R_{free} test set	4130 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	87.9	Xtriage
Anisotropy	0.532	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 60.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	17910	wwPDB-VP
Average B, all atoms (Å ²)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.10% 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, 0.333 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: PO4, MLI, ACT

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	0.33	0/6071	0.52	3/8244 (0.0%)
1	B	0.29	1/6109 (0.0%)	0.44	2/8294 (0.0%)
1	C	0.31	0/6046	0.47	1/8209 (0.0%)
All	All	0.31	1/18226 (0.0%)	0.48	6/24747 (0.0%)

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	4
1	B	0	4
1	C	0	3
All	All	0	11

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	660	ASN	C-N	-8.11	1.23	1.33

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	593	ALA	N-CA-C	-7.12	104.47	113.02
1	C	593	ALA	N-CA-C	-6.90	103.16	112.26
1	B	660	ASN	CA-C-N	5.79	130.24	120.29
1	B	660	ASN	C-N-CA	5.79	130.24	120.29
1	A	201	ILE	N-CA-C	-5.63	107.79	113.20
1	A	209	GLY	CA-C-O	-5.04	118.94	122.22

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	121	ASP	Peptide
1	A	204	ARG	Sidechain
1	A	595	ARG	Sidechain
1	A	659	TRP	Peptide
1	B	121	ASP	Peptide
1	B	649	ARG	Sidechain
1	B	650	ARG	Sidechain
1	B	653	ARG	Sidechain
1	C	163	ARG	Sidechain
1	C	192	ARG	Sidechain
1	C	204	ARG	Sidechain

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	5916	0	5737	63	0
1	B	5953	0	5777	55	0
1	C	5894	0	5719	74	0
2	A	15	0	0	0	0
2	B	10	0	0	0	0
2	C	25	0	0	0	0
3	A	8	0	6	1	0
3	B	4	0	3	0	0
4	B	14	0	4	1	0
5	A	37	0	0	0	0
5	B	16	0	0	0	0
5	C	18	0	0	0	0
All	All	17910	0	17246	183	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 5.

All (183) 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:390:MET:HE1	1:C:686:MET:HB3	1.81	0.62
1:A:595:ARG:O	1:A:596:ILE:C	2.43	0.60
1:B:366:TRP:HB3	1:B:397:CYS:HA	1.83	0.59
1:C:28:LEU:HD13	1:C:216:LEU:HD23	1.84	0.59
1:A:486:ARG:HD2	1:C:494:ARG:CZ	2.32	0.59
1:C:390:MET:HE3	1:C:690:HIS:CG	2.38	0.59
1:B:784:GLN:HA	1:B:787:LYS:HD3	1.85	0.58
1:B:612:GLN:HB3	1:B:634:VAL:HG11	1.86	0.57
1:C:459:LEU:HD12	1:C:504:PRO:HG2	1.85	0.57
1:B:426:GLY:O	1:B:427:CYS:C	2.47	0.56
1:B:340:GLU:HA	1:B:344:PRO:HB3	1.87	0.56
1:B:459:LEU:HD12	1:B:504:PRO:HG2	1.87	0.56
1:C:310:GLU:HB2	1:C:326:THR:HG23	1.86	0.56
1:C:390:MET:HE3	1:C:690:HIS:ND1	2.21	0.56
1:A:180:GLY:HA3	1:C:285:LEU:HD12	1.87	0.56
1:B:666:PRO:HD3	1:B:675:TYR:CD2	2.41	0.55
1:B:88:LEU:HD13	1:B:205:LEU:HD11	1.88	0.55
1:A:366:TRP:HB3	1:A:397:CYS:HA	1.88	0.55
1:C:763:ARG:HE	1:C:766:GLY:HA2	1.72	0.55
1:C:228:ASN:HB3	1:C:246:TYR:HB2	1.89	0.54
1:A:703:GLY:HA2	1:A:751:MET:HG2	1.89	0.54
1:A:19:SER:HB2	1:A:326:THR:HB	1.90	0.54
1:B:436:PHE:HE2	1:B:487:VAL:HG21	1.73	0.54
1:C:636:ALA:HB1	1:C:685:TYR:CG	2.42	0.54
1:C:722:VAL:HG23	1:C:731:VAL:HB	1.90	0.53
1:C:97:TYR:HE1	1:C:159:ASP:HB3	1.72	0.53
1:A:432:GLN:O	1:C:494:ARG:HD3	2.09	0.53
1:A:425:MET:HE2	1:A:487:VAL:HG11	1.91	0.52
1:A:177:LEU:HD13	1:A:429:ASN:HD22	1.73	0.52
1:A:394:ILE:HD13	1:A:657:ILE:HD11	1.92	0.52
1:A:285:LEU:HD12	1:B:180:GLY:HA3	1.91	0.52
1:B:120:ILE:O	1:B:122:THR:HA	2.10	0.52
1:C:39:GLN:HB2	1:C:95:GLN:HG3	1.91	0.52
1:C:264:THR:HG22	1:C:274:ARG:HG3	1.91	0.52
1:A:68:ILE:HG12	1:A:372:LEU:HD13	1.92	0.52
1:A:211:TRP:CH2	1:A:402:VAL:HG11	2.45	0.52
1:A:661:ILE:O	1:A:673:SER:HB3	2.09	0.52
1:A:39:GLN:HB2	1:A:95:GLN:HG3	1.92	0.51
1:C:586:ASN:HD21	1:C:589:TRP:CD1	2.28	0.51
1:A:113:LEU:H	1:A:148:THR:HG23	1.76	0.51
1:A:576:PRO:HD3	1:A:624:LEU:HD13	1.92	0.51
1:A:636:ALA:HB1	1:A:685:TYR:CG	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:557:HIS:HA	1:B:670:ASP:HA	1.93	0.51
1:A:390:MET:HE1	1:A:686:MET:C	2.36	0.50
1:C:314:VAL:HG12	1:C:321:ILE:HA	1.93	0.50
1:A:120:ILE:O	1:A:122:THR:HA	2.12	0.50
1:C:338:LEU:HD13	1:C:350:PHE:HB3	1.94	0.50
1:A:80:MET:HB3	1:A:666:PRO:HG2	1.93	0.50
1:B:39:GLN:HB2	1:B:95:GLN:HG3	1.93	0.50
1:B:396:ARG:HG3	1:B:420:TRP:CG	2.47	0.50
1:A:361:ALA:HB1	1:A:394:ILE:HG21	1.93	0.50
1:B:97:TYR:HE1	1:B:159:ASP:HB3	1.76	0.50
1:A:117:PHE:CG	1:A:120:ILE:HD11	2.47	0.49
1:B:636:ALA:HB1	1:B:685:TYR:CG	2.48	0.49
1:B:703:GLY:HA2	1:B:751:MET:HB2	1.94	0.49
1:A:587:ASP:O	1:A:591:THR:HG23	2.13	0.49
1:C:650:ARG:N	1:C:651:PRO:HD2	2.28	0.49
1:A:228:ASN:HB3	1:A:246:TYR:HB2	1.94	0.49
1:C:594:ASN:C	1:C:596:ILE:H	2.20	0.49
1:C:273:LEU:HD23	1:C:288:LEU:HD23	1.95	0.48
1:A:763:ARG:HH11	1:A:766:GLY:HA2	1.77	0.48
1:C:366:TRP:HB3	1:C:397:CYS:HA	1.94	0.48
1:A:193:ALA:HB2	1:A:402:VAL:HG22	1.96	0.48
1:A:141:ILE:HG21	1:A:443:GLU:HA	1.96	0.48
1:B:616:ILE:HG13	1:B:634:VAL:HG13	1.96	0.48
1:C:644:GLU:HG3	1:C:689:VAL:HG21	1.95	0.48
1:A:364:THR:HG22	1:A:658:TRP:CH2	2.49	0.47
1:B:296:TRP:CZ2	1:B:416:GLY:HA2	2.49	0.47
1:B:336:LEU:HD11	1:B:350:PHE:CD1	2.49	0.47
1:B:253:PHE:CZ	1:C:92:GLU:HB2	2.50	0.47
1:B:632:GLN:HB3	1:B:681:GLN:HB2	1.96	0.47
1:C:706:LEU:HG	1:C:746:ILE:HD12	1.97	0.47
1:A:92:GLU:HB2	1:C:253:PHE:CZ	2.49	0.46
1:A:592:LYS:HD2	1:A:667:LEU:HD23	1.97	0.46
1:A:253:PHE:CZ	1:B:92:GLU:HB2	2.51	0.46
1:B:194:PRO:HD2	1:B:400:GLY:HA2	1.96	0.46
1:A:595:ARG:O	1:A:597:TYR:N	2.49	0.46
1:B:203:PRO:HD3	1:B:667:LEU:HD11	1.96	0.46
1:C:760:ILE:HD11	1:C:771:ASN:HB3	1.97	0.46
1:A:659:TRP:CD1	1:A:660:ASN:HB3	2.51	0.45
1:B:207:SER:OG	1:B:208:ALA:N	2.49	0.45
1:B:88:LEU:HB3	4:B:805:MLI:H12	1.98	0.45
1:C:459:LEU:HD11	1:C:506:LEU:HG	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:253:PHE:HA	1:B:256:HIS:ND1	2.32	0.45
1:C:406:THR:HG23	1:C:450:LYS:HE2	1.98	0.45
1:A:133:VAL:HG11	1:A:147:ILE:HG22	1.98	0.45
1:C:640:LYS:HE2	1:C:772:HIS:CE1	2.52	0.45
1:C:717:GLU:HB2	1:C:735:LYS:NZ	2.30	0.45
1:A:498:GLU:HG2	1:B:175:GLY:HA3	1.98	0.45
1:C:46:THR:HG23	1:C:49:GLY:H	1.82	0.45
1:C:630:ALA:HB2	1:C:782:LEU:HD11	1.99	0.45
1:A:207:SER:OG	1:A:208:ALA:N	2.50	0.45
1:C:595:ARG:O	1:C:597:TYR:N	2.49	0.45
1:B:70:MET:HE1	1:B:91:TYR:CE1	2.52	0.45
1:C:457:LEU:HD21	1:C:460:TRP:CZ2	2.52	0.45
1:C:661:ILE:O	1:C:673:SER:HB3	2.16	0.45
1:A:97:TYR:HE1	1:A:159:ASP:HB3	1.82	0.44
1:B:124:ALA:HB2	1:B:162:ILE:HG12	1.99	0.44
1:A:427:CYS:SG	1:A:428:GLY:N	2.89	0.44
1:C:80:MET:HB3	1:C:666:PRO:HG2	1.99	0.44
1:B:585:TRP:CE2	1:B:606:ASN:HB3	2.52	0.44
1:C:202:MET:HB3	1:C:202:MET:HE3	1.74	0.44
1:C:390:MET:CE	1:C:690:HIS:CE1	3.00	0.44
1:A:204:ARG:HB2	1:A:596:ILE:HG23	2.00	0.44
1:A:364:THR:HG22	1:A:658:TRP:CZ2	2.53	0.44
1:C:390:MET:CE	1:C:690:HIS:ND1	2.80	0.44
1:B:199:TRP:CD1	1:B:200:ASP:H	2.36	0.43
1:C:722:VAL:HG21	1:C:749:LEU:HD13	1.99	0.43
1:B:659:TRP:HA	1:B:659:TRP:CE3	2.53	0.43
1:C:661:ILE:HG13	1:C:672:ILE:HD11	2.01	0.43
1:A:423:PHE:O	1:A:425:MET:N	2.52	0.43
1:A:557:HIS:HB3	1:A:609:MET:HG2	2.00	0.43
1:A:485:ASP:HB3	1:A:488:SER:OG	2.19	0.43
1:B:301:TYR:CE1	1:B:359:VAL:HG13	2.54	0.43
1:B:182:PHE:HB2	1:B:427:CYS:HB2	1.99	0.43
1:A:194:PRO:HD2	1:A:400:GLY:HA2	2.01	0.43
1:A:640:LYS:HG3	1:A:689:VAL:HG11	2.00	0.43
1:A:660:ASN:ND2	1:A:671:ALA:HB2	2.34	0.43
1:C:34:LEU:HB2	1:C:60:ALA:HB2	2.00	0.42
1:C:336:LEU:HD11	1:C:350:PHE:CD1	2.54	0.42
1:C:592:LYS:HD3	1:C:592:LYS:HA	1.87	0.42
1:A:577:TRP:HA	1:A:584:MET:O	2.19	0.42
1:C:362:LYS:HD2	1:C:690:HIS:CD2	2.54	0.42
1:B:152:LYS:HG2	1:B:156:ASN:OD1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:763:ARG:HE	1:B:766:GLY:HA2	1.84	0.42
1:C:576:PRO:HD3	1:C:624:LEU:HD13	2.00	0.42
1:A:672:ILE:HD12	1:A:683:PHE:HA	2.01	0.42
1:C:139:MET:CE	1:C:193:ALA:H	2.32	0.42
1:C:659:TRP:HA	1:C:660:ASN:HA	1.84	0.42
1:B:182:PHE:HD2	1:B:427:CYS:HB3	1.83	0.42
1:C:152:LYS:HE3	1:C:155:GLU:O	2.20	0.42
1:B:228:ASN:HB3	1:B:246:TYR:HB2	2.01	0.42
1:C:119:GLY:O	1:C:210:LEU:HA	2.20	0.42
1:C:649:ARG:HB2	1:C:653:ARG:HG2	2.02	0.42
1:B:216:LEU:HD23	1:B:216:LEU:HA	1.93	0.42
1:A:113:LEU:H	1:A:148:THR:CG2	2.33	0.41
1:A:577:TRP:CD1	1:A:582:VAL:HA	2.55	0.41
1:C:122:THR:OG1	1:C:139:MET:HB2	2.19	0.41
1:B:530:HIS:CD2	1:B:533:GLY:HA2	2.54	0.41
1:C:66:VAL:HG11	1:C:96:TRP:CD2	2.54	0.41
1:C:585:TRP:CE2	1:C:606:ASN:HB3	2.55	0.41
1:A:486:ARG:HG2	3:A:805:ACT:H3	2.02	0.41
1:B:420:TRP:C	1:B:420:TRP:CD1	2.98	0.41
1:A:40:PRO:HG2	1:A:42:VAL:O	2.21	0.41
1:A:704:TYR:HB2	1:A:749:LEU:HB2	2.02	0.41
1:C:717:GLU:HB2	1:C:735:LYS:HZ1	1.84	0.41
1:A:44:VAL:HB	1:A:95:GLN:HE22	1.85	0.41
1:B:425:MET:HE3	1:B:425:MET:HB2	1.90	0.41
1:B:586:ASN:HD21	1:B:589:TRP:CD1	2.39	0.41
1:C:211:TRP:H	1:C:211:TRP:CD1	2.39	0.41
1:C:712:THR:HG21	1:C:716:PHE:HE1	1.84	0.41
1:A:774:LEU:HD21	1:A:780:TYR:CZ	2.56	0.41
1:B:95:GLN:HG2	1:B:163:ARG:HA	2.03	0.41
1:B:110:GLY:HA3	1:B:221:PRO:HG3	2.03	0.41
1:C:119:GLY:N	1:C:212:ARG:HB2	2.35	0.41
1:A:420:TRP:C	1:A:420:TRP:CD1	2.99	0.41
1:C:25:GLU:HA	1:C:216:LEU:O	2.20	0.41
1:C:237:LYS:C	1:C:239:ARG:H	2.29	0.41
1:C:332:ARG:HH21	1:C:455:PRO:HA	1.84	0.41
1:A:366:TRP:CZ2	1:A:369:LEU:HD21	2.56	0.41
1:A:401:ASN:CG	1:A:402:VAL:H	2.29	0.40
1:B:653:ARG:HH11	1:B:653:ARG:HG3	1.86	0.40
1:C:336:LEU:HB2	1:C:504:PRO:HG3	2.04	0.40
1:A:134:GLY:HA3	1:A:145:TYR:CE1	2.57	0.40
1:B:649:ARG:HH21	1:B:653:ARG:HH12	1.70	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:390:MET:HE3	1:C:690:HIS:CE1	2.56	0.40
1:B:448:VAL:HA	1:B:460:TRP:CH2	2.56	0.40
1:B:557:HIS:O	1:B:635:GLN:HB2	2.22	0.40
1:B:729:LYS:HE3	1:B:729:LYS:HB3	1.90	0.40
1:C:639:MET:HB3	1:C:686:MET:SD	2.61	0.40
1:B:394:ILE:HD13	1:B:657:ILE:HD11	2.03	0.40
1:C:38:PRO:HG3	1:C:94:TYR:CZ	2.55	0.40
1:C:139:MET:HE1	1:C:193:ALA:H	1.86	0.40
1:A:21:MET:HE3	1:A:21:MET:HB3	2.01	0.40
1:A:346:GLN:HG2	1:A:347:PRO:HD2	2.03	0.40
1:A:440:LEU:CD2	1:A:487:VAL:HG13	2.51	0.40
1:B:494:ARG:HD3	1:C:432:GLN:O	2.21	0.40
1:B:659:TRP:CG	1:B:660:ASN:H	2.39	0.40
1:C:44:VAL:HG23	1:C:45:MET:H	1.86	0.40
1:C:81:VAL:HG22	1:C:82:GLY:H	1.87	0.40
1:C:419:VAL:HG23	1:C:456:SER:HB2	2.02	0.40
1:C:420:TRP:C	1:C:420:TRP:CD1	3.00	0.40
1:C:560:PRO:HA	1:C:680:LYS:HE2	2.04	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	731/798 (92%)	700 (96%)	29 (4%)	2 (0%)	37	64
1	B	733/798 (92%)	700 (96%)	30 (4%)	3 (0%)	30	58
1	C	728/798 (91%)	690 (95%)	35 (5%)	3 (0%)	30	58
All	All	2192/2394 (92%)	2090 (95%)	94 (4%)	8 (0%)	30	58

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	596	ILE
1	A	490	GLN
1	B	594	ASN
1	B	427	CYS
1	C	594	ASN
1	B	666	PRO
1	C	596	ILE
1	C	666	PRO

5.3.2 Protein sidechains [i](#)

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	637/689 (92%)	636 (100%)	1 (0%)	92	95
1	B	639/689 (93%)	638 (100%)	1 (0%)	92	95
1	C	634/689 (92%)	631 (100%)	3 (0%)	86	91
All	All	1910/2067 (92%)	1905 (100%)	5 (0%)	91	94

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	140	LEU
1	B	429	ASN
1	C	83	ASN
1	C	216	LEU
1	C	464	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	421	GLN
1	A	429	ASN
1	A	483	ASN
1	A	575	ASN
1	A	635	GLN

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Mol	Chain	Res	Type
1	A	681	GLN
1	A	711	ASN
1	A	742	GLN
1	B	351	GLN
1	B	421	GLN
1	B	429	ASN
1	B	464	ASN
1	B	635	GLN
1	B	730	GLN
1	C	129	ASN
1	C	271	GLN
1	C	349	GLN
1	C	421	GLN
1	C	575	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

15 ligands 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
3	ACT	A	805	-	3,3,3	1.04	0	3,3,3	0.78	0
4	MLI	B	804	-	6,6,6	1.59	1 (16%)	7,7,7	1.19	0
2	PO4	C	805	-	4,4,4	1.59	1 (25%)	6,6,6	0.49	0
2	PO4	B	802	-	4,4,4	1.55	1 (25%)	6,6,6	0.48	0
2	PO4	A	801	-	4,4,4	0.80	0	6,6,6	0.44	0
4	MLI	B	805	-	6,6,6	1.55	1 (16%)	7,7,7	1.30	1 (14%)
2	PO4	C	801	-	4,4,4	1.57	1 (25%)	6,6,6	0.48	0
2	PO4	C	802	-	4,4,4	1.57	1 (25%)	6,6,6	0.51	0
3	ACT	B	803	-	3,3,3	1.12	0	3,3,3	1.23	0
2	PO4	A	803	-	4,4,4	1.48	1 (25%)	6,6,6	0.61	0
2	PO4	C	804	-	4,4,4	1.57	1 (25%)	6,6,6	0.49	0
3	ACT	A	804	-	3,3,3	1.12	0	3,3,3	1.22	0
2	PO4	B	801	-	4,4,4	1.50	1 (25%)	6,6,6	0.56	0
2	PO4	A	802	-	4,4,4	1.59	1 (25%)	6,6,6	0.50	0
2	PO4	C	803	-	4,4,4	1.56	1 (25%)	6,6,6	0.48	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MLI	B	805	-	-	2/4/4/4	-
4	MLI	B	804	-	-	0/4/4/4	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	805	PO4	P-O1	2.77	1.57	1.50
2	A	802	PO4	P-O1	2.75	1.57	1.50
2	C	804	PO4	P-O1	2.74	1.57	1.50
2	C	802	PO4	P-O1	2.73	1.57	1.50
2	B	802	PO4	P-O1	2.69	1.56	1.50
2	C	801	PO4	P-O1	2.69	1.56	1.50
2	C	803	PO4	P-O1	2.69	1.56	1.50
2	B	801	PO4	P-O1	2.55	1.56	1.50
2	A	803	PO4	P-O1	2.51	1.56	1.50
4	B	804	MLI	C1-C3	2.37	1.54	1.51
4	B	805	MLI	C1-C3	2.33	1.54	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	805	MLI	O6-C2-C1	-2.26	115.67	122.11

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	805	MLI	C3-C1-C2-O6
4	B	805	MLI	C3-C1-C2-O7

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	805	ACT	1	0
4	B	805	MLI	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, 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	737/798 (92%)	-0.25	6 (0%) 82 66	66, 92, 136, 155	0
1	B	741/798 (92%)	-0.16	10 (1%) 74 56	69, 104, 151, 174	0
1	C	734/798 (91%)	-0.15	9 (1%) 76 58	70, 103, 133, 178	0
All	All	2212/2394 (92%)	-0.19	25 (1%) 77 60	66, 100, 140, 178	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	510	PRO	4.7
1	A	797	LEU	4.5
1	C	797	LEU	3.8
1	B	532	TRP	3.6
1	B	555	GLY	3.2
1	B	797	LEU	3.2
1	C	593	ALA	2.9
1	C	509	SER	2.8
1	B	480	ALA	2.8
1	B	392	CYS	2.7
1	C	594	ASN	2.6
1	A	343	LEU	2.6
1	C	482	PRO	2.6
1	A	508	SER	2.5
1	B	463	ASN	2.4
1	B	478	PHE	2.3
1	B	530	HIS	2.3
1	C	535	ARG	2.3
1	C	342	ASN	2.2
1	C	176	THR	2.2
1	A	536	GLY	2.1
1	B	464	ASN	2.1
1	B	535	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	200	ASP	2.0
1	A	659	TRP	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 oligosaccharides 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. 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	B-factors(Å ²)	Q<0.9
2	PO4	C	804	5/5	0.37	0.10	157,171,185,190	0
3	ACT	A	805	4/4	0.51	0.20	113,128,148,157	0
2	PO4	A	803	5/5	0.54	0.10	153,158,198,260	0
2	PO4	C	803	5/5	0.56	0.10	145,149,166,178	0
2	PO4	B	802	5/5	0.57	0.08	162,164,171,189	0
2	PO4	C	801	5/5	0.74	0.10	99,111,124,136	0
2	PO4	A	802	5/5	0.75	0.12	91,113,123,131	0
2	PO4	C	805	5/5	0.78	0.16	136,148,162,169	0
3	ACT	B	803	4/4	0.79	0.20	93,98,105,106	0
3	ACT	A	804	4/4	0.85	0.22	103,107,110,112	0
2	PO4	A	801	5/5	0.86	0.09	79,98,105,112	0
4	MLI	B	804	7/7	0.86	0.10	93,95,108,111	0
2	PO4	B	801	5/5	0.89	0.09	91,95,104,113	0
4	MLI	B	805	7/7	0.92	0.20	83,84,91,95	0
2	PO4	C	802	5/5	0.94	0.08	98,99,110,110	0

6.5 Other polymers [i](#)

There are no such residues in this entry.