



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 04:15 PM UTC

PDB ID : 1YM2 / pdb_00001ym2
Title : Crystal structure of human beta secretase complexed with NVP-AUR200
Authors : Hanessian, S.; Yun, H.; Hou, Y.; Yang, G.; Bayrakdarian, M.; Therrien, E.;
Moitessier, N.; Roggo, S.; Veenstra, S.
Deposited on : 2005-01-20
Resolution : 2.05 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	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
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)	:	2.49

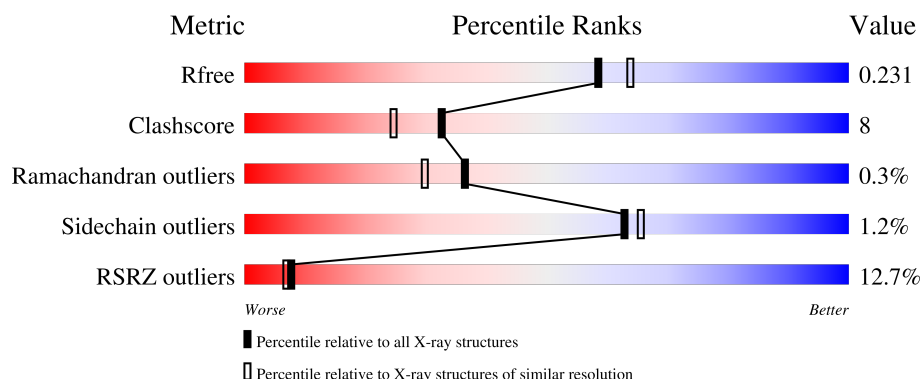
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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}	180053	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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	402	 11% 74% 18% • 6%
1	B	402	 16% 74% 18% • 6%
1	C	402	 9% 76% 17% 6%
2	X	6	 67% 17% 17%
2	Y	6	 67% 17% 17%

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Mol	Chain	Length	Quality of chain
2	Z	6	 A horizontal bar chart showing the quality of chain Z. The bar is divided into three segments: green (67%), yellow (17%), and red (17%). The percentages are labeled below each segment.

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9605 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 Beta-secretase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	376	Total	C	N	O	S	0	0	0
			2960	1895	492	559	14			
1	B	377	Total	C	N	O	S	0	0	0
			2966	1898	493	561	14			
1	C	376	Total	C	N	O	S	0	0	0
			2960	1895	492	559	14			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	GLY	-	expression tag	UNP P56817
A	-14	PRO	-	expression tag	UNP P56817
B	-15	GLY	-	expression tag	UNP P56817
B	-14	PRO	-	expression tag	UNP P56817
C	-15	GLY	-	expression tag	UNP P56817
C	-14	PRO	-	expression tag	UNP P56817

- Molecule 2 is a protein called NVP-AUR200 INHIBITOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	X	6	Total	C	N	O	S	0	0	0
			47	34	5	7	1			
2	Y	6	Total	C	N	O	S	0	0	0
			47	34	5	7	1			
2	Z	6	Total	C	N	O	S	0	0	0
			47	34	5	7	1			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	202	Total	O	0	0
			202	202		

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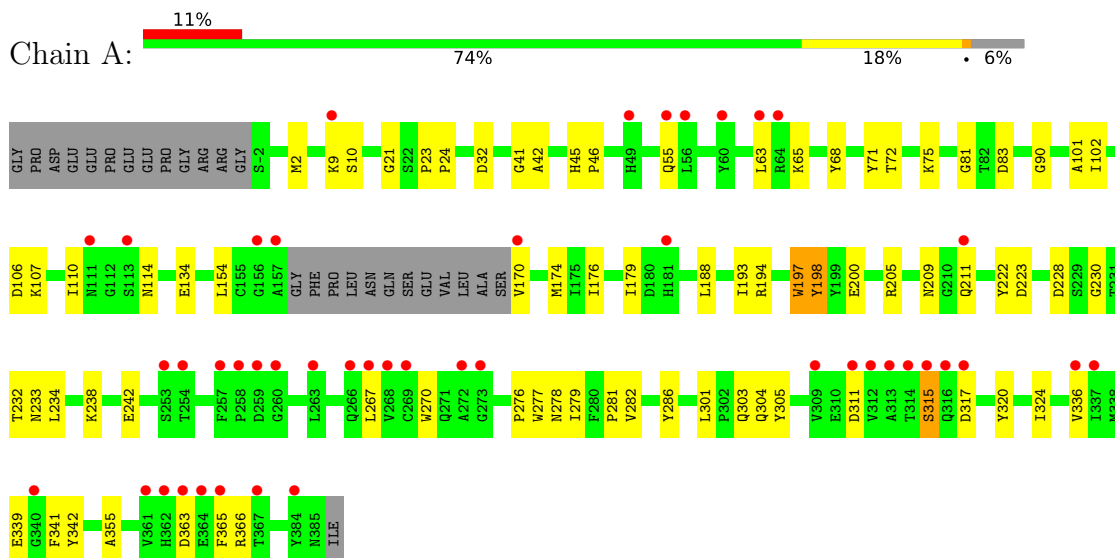
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	162	Total 162	O 162	0	0
3	C	203	Total 203	O 203	0	0
3	X	4	Total 4	O 4	0	0
3	Y	3	Total 3	O 3	0	0
3	Z	4	Total 4	O 4	0	0

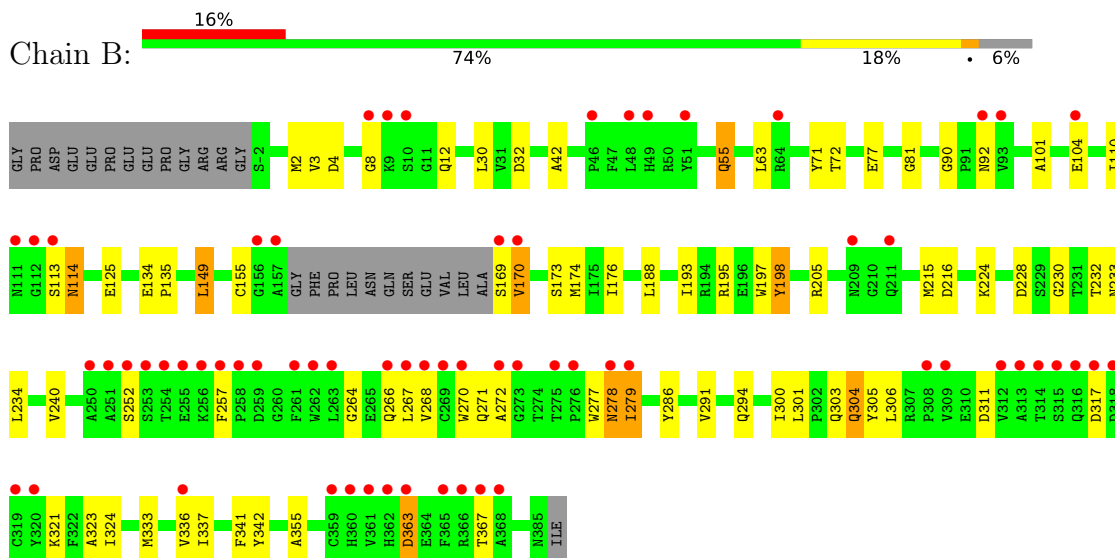
3 Residue-property plots

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.

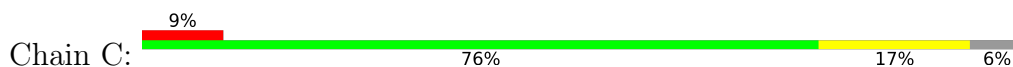
- Molecule 1: Beta-secretase 1

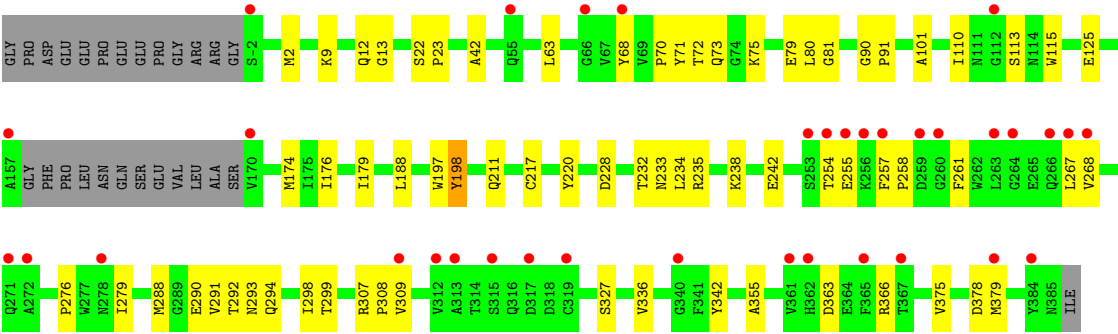


- Molecule 1: Beta-secretase 1



- Molecule 1: Beta-secretase 1





● Molecule 2: NVP-AUR200 INHIBITOR



● Molecule 2: NVP-AUR200 INHIBITOR



● Molecule 2: NVP-AUR200 INHIBITOR



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	82.26Å 103.26Å 100.62Å 90.00° 104.12° 90.00°	Depositor
Resolution (Å)	47.05 – 2.05 47.05 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.7 (47.05-2.05) 99.9 (47.05-2.05)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.87 (at 2.05Å)	Xtriage
Refinement program	CNX 2002	Depositor
R, R_{free}	0.212 , 0.237 0.208 , 0.231	Depositor DCC
R_{free} test set	10253 reflections (10.04%)	wwPDB-VP
Wilson B-factor (Å ²)	43.4	Xtriage
Anisotropy	0.224	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 43.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9605	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.75% 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: 24O, LYT, ACE

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	0.30	0/3035	0.86	7/4125 (0.2%)
1	B	0.30	0/3041	0.85	7/4133 (0.2%)
1	C	0.30	0/3035	0.88	6/4125 (0.1%)
2	X	1.14	0/22	1.49	0/27
2	Y	0.88	0/22	1.49	0/27
2	Z	0.94	0/22	1.46	0/27
All	All	0.31	0/9177	0.87	20/12464 (0.2%)

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
2	X	0	2
2	Y	0	2
2	Z	0	2
All	All	0	6

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	TYR	N-CA-C	-8.62	98.10	110.59
1	B	198	TYR	N-CA-C	-8.49	97.20	110.36
1	C	198	TYR	N-CA-C	-7.68	98.46	110.36
1	A	234	LEU	N-CA-C	-6.97	96.28	108.20
1	B	234	LEU	N-CA-C	-6.74	96.67	108.20
1	C	234	LEU	N-CA-C	-6.71	96.73	108.20
1	A	341	PHE	N-CA-C	6.22	118.41	109.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	290	GLU	N-CA-C	-6.08	104.77	111.82
1	B	193	ILE	N-CA-C	-6.04	98.31	107.73
1	A	233	ASN	N-CA-C	6.03	118.67	110.35
1	A	193	ILE	N-CA-C	-6.00	98.37	107.73
1	B	341	PHE	N-CA-C	5.93	117.97	109.14
1	C	233	ASN	N-CA-C	5.82	118.38	110.35
1	C	293	ASN	N-CA-C	-5.47	105.83	112.88
1	B	216	ASP	N-CA-C	-5.44	101.59	109.59
1	C	298	ILE	N-CA-C	-5.43	100.51	108.11
1	B	342	TYR	N-CA-C	-5.39	99.95	108.73
1	A	134	GLU	CA-C-N	5.10	125.00	119.85
1	A	134	GLU	C-N-CA	5.10	125.00	119.85
1	B	233	ASN	N-CA-C	5.03	118.16	110.36

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	X	4	24O	Peptide,Mainchain
2	Y	4	24O	Peptide,Mainchain
2	Z	4	24O	Peptide,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	2960	0	2873	46	0
1	B	2966	0	2878	52	0
1	C	2960	0	2873	45	0
2	X	47	0	53	4	0
2	Y	47	0	53	2	0
2	Z	47	0	53	3	0
3	A	202	0	0	5	0
3	B	162	0	0	2	0
3	C	203	0	0	2	0
3	X	4	0	0	0	0
3	Y	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	Z	4	0	0	0	0
All	All	9605	0	8783	140	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 (140) 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:288:MET:HE1	1:C:379:MET:HE3	1.49	0.90
1:C:258:PRO:HD2	1:C:268:VAL:HG12	1.55	0.88
1:A:110:ILE:HD11	2:X:2:LEU:HD13	1.56	0.85
1:B:2:MET:HG2	1:B:90:GLY:HA2	1.60	0.84
1:A:366:ARG:HA	1:C:211:GLN:HE22	1.45	0.81
1:B:252:SER:HA	1:B:279:ILE:HD12	1.67	0.77
1:C:174:MET:HE3	1:C:176:ILE:HD11	1.68	0.76
1:A:2:MET:HG2	1:A:90:GLY:HA2	1.71	0.72
1:A:110:ILE:HD11	2:X:2:LEU:CD1	2.22	0.69
1:B:267:LEU:H	1:B:267:LEU:HD23	1.59	0.66
1:B:169:SER:HB3	3:B:2141:HOH:O	1.96	0.65
1:B:4:ASP:H	1:B:173:SER:HB3	1.61	0.65
1:A:276:PRO:O	1:A:279:ILE:HG12	1.97	0.64
1:B:155:CYS:O	1:B:170:VAL:HG22	1.98	0.64
1:B:215:MET:HE1	1:B:240:VAL:HA	1.80	0.63
1:C:276:PRO:O	1:C:279:ILE:HG12	1.98	0.63
1:A:9:LYS:HG2	3:A:1191:HOH:O	1.98	0.62
1:B:149:LEU:HD12	1:B:149:LEU:C	2.24	0.62
1:B:197:TRP:CG	1:B:198:TYR:H	2.18	0.61
1:B:270:TRP:O	1:B:317:ASP:HB3	1.99	0.61
1:A:174:MET:HE3	1:A:176:ILE:HD11	1.83	0.61
1:B:77:GLU:HG2	1:B:104:GLU:HB2	1.84	0.60
1:A:197:TRP:CG	1:A:198:TYR:H	2.21	0.59
1:B:278:ASN:HD22	1:B:279:ILE:N	1.98	0.59
1:A:110:ILE:CD1	2:X:2:LEU:HD13	2.30	0.59
1:B:300:ILE:HG21	1:B:337:ILE:HD13	1.85	0.59
1:C:197:TRP:CG	1:C:198:TYR:H	2.22	0.57
1:A:270:TRP:O	1:A:317:ASP:HB3	2.03	0.57
1:B:12:GLN:NE2	1:B:113:SER:HA	2.19	0.57
1:C:188:LEU:HD23	1:C:355:ALA:HB2	1.86	0.56
1:B:8:GLY:C	1:B:170:VAL:HG12	2.30	0.56
1:C:267:LEU:HD22	1:C:309:VAL:HG21	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:301:LEU:HD11	1:B:367:THR:HA	1.86	0.56
1:B:197:TRP:CD1	1:B:198:TYR:H	2.24	0.56
1:C:363:ASP:HB3	1:C:366:ARG:O	2.06	0.55
1:C:254:THR:HG21	1:C:279:ILE:HG21	1.88	0.55
1:B:303:GLN:NE2	1:B:363:ASP:HB3	2.21	0.55
1:C:238:LYS:O	1:C:242:GLU:HG3	2.08	0.54
1:A:10:SER:HB3	1:A:339:GLU:OE1	2.07	0.53
1:B:55:GLN:H	1:B:55:GLN:CD	2.17	0.53
1:C:257:PHE:HD2	1:C:268:VAL:HG11	1.73	0.52
1:A:65:LYS:NZ	1:A:65:LYS:HB3	2.23	0.52
1:A:63:LEU:HG	1:A:81:GLY:HA2	1.91	0.52
1:C:228:ASP:OD2	2:Z:4:24O:H552	2.09	0.51
1:A:55:GLN:H	1:A:55:GLN:CD	2.17	0.51
1:B:30:LEU:HD11	2:Y:2:LEU:HD21	1.92	0.51
1:C:197:TRP:CD1	1:C:198:TYR:H	2.29	0.50
1:B:264:GLY:O	1:B:321:LYS:HE3	2.12	0.50
1:C:179:ILE:HG23	1:C:342:TYR:HE2	1.77	0.50
1:A:363:ASP:HB3	1:A:366:ARG:O	2.12	0.50
1:B:333:MET:HE2	1:B:337:ILE:HG21	1.94	0.50
1:C:261:PHE:CD1	1:C:268:VAL:HG13	2.47	0.50
1:C:292:THR:HG21	1:C:378:ASP:HB3	1.94	0.50
1:C:110:ILE:HD11	2:Z:2:LEU:HD13	1.93	0.49
1:C:125:GLU:HG3	3:C:3114:HOH:O	2.12	0.49
1:C:217:CYS:HA	1:C:220:TYR:CD1	2.47	0.49
1:B:55:GLN:H	1:B:55:GLN:NE2	2.11	0.49
1:B:277:TRP:HZ3	1:B:306:LEU:HD12	1.78	0.49
1:A:232:THR:O	1:A:336:VAL:HG13	2.13	0.48
1:A:41:GLY:HA2	1:A:102:ILE:HB	1.95	0.48
1:A:197:TRP:CD1	1:A:198:TYR:H	2.31	0.48
1:C:91:PRO:HD3	1:C:176:ILE:HB	1.96	0.48
1:B:305:TYR:HB2	1:B:324:ILE:HG13	1.95	0.48
1:A:32:ASP:OD1	1:A:230:GLY:HA3	2.14	0.47
1:A:222:TYR:HA	1:A:223:ASP:HA	1.68	0.47
1:A:9:LYS:HD2	3:A:1154:HOH:O	2.13	0.47
1:A:188:LEU:HD23	1:A:355:ALA:HB2	1.97	0.47
1:B:2:MET:CG	1:B:90:GLY:HA2	2.38	0.47
1:B:205:ARG:HB3	1:B:286:TYR:HB2	1.96	0.47
1:A:228:ASP:OD2	2:X:4:24O:H552	2.14	0.47
1:C:2:MET:HG2	1:C:90:GLY:HA2	1.96	0.47
1:A:304:GLN:O	1:A:336:VAL:HB	2.15	0.46
1:C:68:TYR:HE1	1:C:75:LYS:HD3	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:ASP:OD2	1:A:107:LYS:HG3	2.16	0.46
1:A:311:ASP:HB3	1:A:315:SER:HA	1.97	0.46
1:A:179:ILE:HG23	1:A:342:TYR:HE2	1.81	0.45
1:B:232:THR:O	1:B:336:VAL:HG13	2.17	0.45
1:B:278:ASN:HD22	1:B:279:ILE:H	1.63	0.45
1:C:68:TYR:OH	1:C:70:PRO:HB3	2.16	0.45
1:C:73:GLN:NE2	1:C:73:GLN:HA	2.32	0.45
1:B:323:ALA:HB1	1:B:336:VAL:HG11	1.99	0.45
1:A:366:ARG:HA	1:C:211:GLN:NE2	2.25	0.44
1:C:73:GLN:HA	1:C:73:GLN:HE21	1.83	0.44
1:B:267:LEU:HD23	1:B:267:LEU:N	2.30	0.44
1:A:170:VAL:HG12	3:A:1186:HOH:O	2.17	0.44
1:C:307:ARG:HA	1:C:308:PRO:HD3	1.84	0.44
3:A:1152:HOH:O	1:C:299:THR:HG21	2.17	0.44
1:C:13:GLY:HA2	3:C:3146:HOH:O	2.18	0.44
1:B:228:ASP:OD2	2:Y:4:24O:H552	2.18	0.43
1:C:267:LEU:HD22	1:C:309:VAL:CG2	2.47	0.43
1:A:68:TYR:CG	1:B:3:VAL:HG11	2.53	0.43
1:B:42:ALA:CB	1:B:101:ALA:HB1	2.48	0.43
1:A:209:ASN:ND2	1:A:281:PRO:HB3	2.34	0.43
1:A:282:VAL:HG12	1:A:301:LEU:HD23	2.01	0.43
1:C:375:VAL:HG13	1:C:375:VAL:O	2.19	0.43
1:A:21:GLY:HA2	1:A:83:ASP:OD1	2.19	0.43
1:A:205:ARG:HB3	1:A:286:TYR:HB2	2.01	0.43
1:C:291:VAL:HB	1:C:294:GLN:HG3	2.01	0.43
1:B:197:TRP:CG	1:B:198:TYR:N	2.84	0.43
1:C:71:TYR:O	1:C:72:THR:C	2.61	0.43
1:C:63:LEU:HG	1:C:81:GLY:HA2	2.01	0.43
1:B:125:GLU:OE2	1:B:195:ARG:NH2	2.37	0.42
1:C:9:LYS:HZ2	1:C:12:GLN:HG3	1.84	0.42
1:A:194:ARG:HB3	1:A:200:GLU:HG2	2.01	0.42
1:A:154:LEU:O	1:A:339:GLU:HA	2.19	0.42
1:C:197:TRP:CG	1:C:198:TYR:N	2.87	0.42
1:B:174:MET:HE3	1:B:176:ILE:HD11	2.02	0.42
1:A:267:LEU:HD12	1:A:320:TYR:O	2.19	0.42
1:B:188:LEU:HD23	1:B:355:ALA:HB2	2.01	0.42
1:A:23:PRO:HA	1:A:24:PRO:HD3	1.87	0.42
1:B:257:PHE:HD2	1:B:268:VAL:HG21	1.85	0.42
1:B:277:TRP:CZ3	1:B:306:LEU:HD12	2.55	0.42
1:B:71:TYR:O	1:B:72:THR:C	2.63	0.42
1:A:238:LYS:O	1:A:242:GLU:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:ASN:C	1:B:92:ASN:HD22	2.27	0.41
1:B:134:GLU:HA	1:B:135:PRO:HD3	1.90	0.41
1:B:110:ILE:HB	1:B:113:SER:HB3	2.02	0.41
1:B:113:SER:O	1:B:114:ASN:CB	2.68	0.41
1:C:232:THR:O	1:C:336:VAL:HG13	2.20	0.41
1:B:271:GLN:O	1:B:272:ALA:C	2.64	0.41
1:A:305:TYR:HB2	1:A:324:ILE:HG13	2.02	0.41
1:B:278:ASN:HD22	1:B:278:ASN:N	2.18	0.41
1:C:235:ARG:HB3	1:C:327:SER:HB2	2.01	0.41
1:B:224:LYS:HE2	3:B:2111:HOH:O	2.19	0.41
1:C:113:SER:HG	1:C:115:TRP:CD1	2.38	0.41
1:C:255:GLU:OE1	1:C:276:PRO:HG3	2.20	0.41
1:A:75:LYS:NZ	3:A:1092:HOH:O	2.54	0.41
1:A:278:ASN:HA	1:A:365:PHE:HZ	1.85	0.41
1:A:42:ALA:CB	1:A:101:ALA:HB1	2.51	0.41
1:B:301:LEU:H	1:B:304:GLN:NE2	2.19	0.41
1:C:22:SER:HA	1:C:23:PRO:C	2.45	0.41
1:A:71:TYR:O	1:A:72:THR:C	2.64	0.40
1:B:63:LEU:HG	1:B:81:GLY:HA2	2.04	0.40
1:B:291:VAL:HG23	1:B:294:GLN:HB3	2.03	0.40
1:C:42:ALA:CB	1:C:101:ALA:HB1	2.50	0.40
1:C:110:ILE:CD1	2:Z:2:LEU:HD13	2.52	0.40
1:A:277:TRP:CZ3	1:A:303:GLN:HA	2.56	0.40
1:B:32:ASP:OD1	1:B:230:GLY:HA3	2.22	0.40
1:C:63:LEU:HD12	1:C:80:LEU:HB3	2.03	0.40
1:A:45:HIS:HA	1:A:46:PRO:HD3	1.96	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	372/402 (92%)	353 (95%)	18 (5%)	1 (0%)	36	30
1	B	373/402 (93%)	352 (94%)	19 (5%)	2 (0%)	24	16
1	C	372/402 (92%)	356 (96%)	16 (4%)	0	100	100
2	X	3/6 (50%)	2 (67%)	1 (33%)	0	100	100
2	Y	3/6 (50%)	2 (67%)	1 (33%)	0	100	100
2	Z	3/6 (50%)	2 (67%)	1 (33%)	0	100	100
All	All	1126/1224 (92%)	1067 (95%)	56 (5%)	3 (0%)	36	30

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	311	ASP
1	A	315	SER
1	B	363	ASP

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	321/342 (94%)	318 (99%)	3 (1%)	70	75
1	B	322/342 (94%)	314 (98%)	8 (2%)	42	39
1	C	321/342 (94%)	320 (100%)	1 (0%)	86	90
2	X	3/3 (100%)	3 (100%)	0	100	100
2	Y	3/3 (100%)	3 (100%)	0	100	100
2	Z	3/3 (100%)	3 (100%)	0	100	100
All	All	973/1035 (94%)	961 (99%)	12 (1%)	63	65

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	114	ASN
1	A	197	TRP

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Mol	Chain	Res	Type
1	A	211	GLN
1	B	55	GLN
1	B	114	ASN
1	B	149	LEU
1	B	170	VAL
1	B	266	GLN
1	B	278	ASN
1	B	279	ILE
1	B	304	GLN
1	C	79	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	HIS
1	A	114	ASN
1	A	278	ASN
1	A	316	GLN
1	A	326	GLN
1	A	362	HIS
1	A	385	ASN
1	B	12	GLN
1	B	55	GLN
1	B	73	GLN
1	B	89	HIS
1	B	92	ASN
1	B	114	ASN
1	B	181	HIS
1	B	233	ASN
1	B	271	GLN
1	B	278	ASN
1	B	293	ASN
1	B	304	GLN
1	B	326	GLN
1	B	385	ASN
1	C	53	GLN
1	C	73	GLN
1	C	89	HIS
1	C	114	ASN
1	C	211	GLN
1	C	233	ASN
1	C	271	GLN

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Mol	Chain	Res	Type
1	C	326	GLN
1	C	362	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues 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
2	24O	X	4	2	16,16,17	0.83	0	11,22,24	2.77	6 (54%)
2	24O	Z	4	2	16,16,17	0.75	0	11,22,24	2.63	5 (45%)
2	24O	Y	4	2	16,16,17	0.76	0	11,22,24	2.70	6 (54%)

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	24O	X	4	2	-	1/13/26/28	0/1/1/1
2	24O	Z	4	2	-	1/13/26/28	0/1/1/1
2	24O	Y	4	2	-	1/13/26/28	0/1/1/1

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	4	24O	C55-C54-C51	7.03	114.60	108.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Y	4	24O	C55-C54-C51	6.83	114.43	108.80
2	Z	4	24O	C55-C54-C51	6.67	114.30	108.80
2	X	4	24O	C95-C92-CA	-3.04	109.21	115.76
2	Z	4	24O	C95-C92-CA	-2.96	109.39	115.76
2	X	4	24O	O-C-C49	-2.92	118.62	125.19
2	Y	4	24O	C95-C92-CA	-2.83	109.66	115.76
2	Y	4	24O	O-C-C49	-2.73	119.04	125.19
2	Y	4	24O	C55-C47-C49	2.52	108.84	104.58
2	Z	4	24O	C55-C47-C49	2.43	108.71	104.58
2	X	4	24O	C55-C47-C49	2.42	108.67	104.58
2	Z	4	24O	O-C-C49	-2.39	119.82	125.19
2	X	4	24O	O58-C54-C51	-2.27	122.64	125.53
2	Y	4	24O	O58-C54-C55	-2.25	122.67	125.53
2	Z	4	24O	O58-C54-C51	-2.22	122.71	125.53
2	X	4	24O	O58-C54-C55	-2.18	122.75	125.53
2	Y	4	24O	O58-C54-C51	-2.07	122.90	125.53

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	X	4	24O	O-C-C49-C47
2	Y	4	24O	O-C-C49-C47
2	Z	4	24O	O-C-C49-C47

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	X	4	24O	1	0
2	Z	4	24O	1	0
2	Y	4	24O	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	376/402 (93%)	0.68	45 (11%) 9 8	30, 44, 74, 107	0
1	B	377/402 (93%)	0.90	65 (17%) 4 3	28, 46, 90, 113	0
1	C	376/402 (93%)	0.54	35 (9%) 14 14	30, 44, 69, 79	0
2	X	3/6 (50%)	0.30	0 100 100	37, 37, 40, 45	0
2	Y	3/6 (50%)	0.28	0 100 100	36, 36, 41, 43	0
2	Z	3/6 (50%)	0.33	0 100 100	38, 38, 40, 44	0
All	All	1138/1224 (92%)	0.70	145 (12%) 8 7	28, 45, 77, 113	0

All (145) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	267	LEU	6.3
1	A	365	PHE	6.1
1	B	314	THR	5.7
1	B	312	VAL	5.6
1	A	267	LEU	5.6
1	B	258	PRO	5.5
1	B	170	VAL	5.3
1	A	361	VAL	5.2
1	A	157	ALA	5.1
1	B	315	SER	4.7
1	C	361	VAL	4.7
1	A	314	THR	4.5
1	B	367	THR	4.4
1	A	312	VAL	4.4
1	A	263	LEU	4.2
1	B	268	VAL	4.1
1	A	55	GLN	4.0
1	A	257	PHE	4.0
1	A	170	VAL	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	263	LEU	3.9
1	A	309	VAL	3.8
1	B	273	GLY	3.8
1	B	156	GLY	3.8
1	B	313	ALA	3.8
1	A	313	ALA	3.7
1	B	257	PHE	3.7
1	B	309	VAL	3.7
1	A	317	ASP	3.5
1	A	49	HIS	3.5
1	B	270	TRP	3.4
1	B	361	VAL	3.4
1	B	262	TRP	3.4
1	C	365	PHE	3.4
1	B	253	SER	3.4
1	A	272	ALA	3.3
1	B	362	HIS	3.3
1	A	311	ASP	3.3
1	C	-2	SER	3.3
1	C	157	ALA	3.3
1	A	260	GLY	3.2
1	C	267	LEU	3.1
1	A	340	GLY	3.1
1	B	263	LEU	3.1
1	B	317	ASP	3.1
1	A	315	SER	3.1
1	A	364	GLU	3.1
1	B	93	VAL	3.0
1	C	55	GLN	3.0
1	A	259	ASP	3.0
1	B	363	ASP	3.0
1	A	156	GLY	3.0
1	A	258	PRO	3.0
1	B	360	HIS	3.0
1	B	10	SER	2.9
1	C	255	GLU	2.9
1	B	254	THR	2.9
1	C	254	THR	2.9
1	B	320	TYR	2.9
1	B	157	ALA	2.9
1	C	260	GLY	2.9
1	B	336	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	181	HIS	2.7
1	B	261	PHE	2.7
1	C	272	ALA	2.7
1	C	384	TYR	2.7
1	B	266	GLN	2.7
1	B	276	PRO	2.7
1	B	9	LYS	2.7
1	A	362	HIS	2.6
1	B	278	ASN	2.6
1	C	362	HIS	2.6
1	B	269	CYS	2.6
1	B	250	ALA	2.6
1	B	366	ARG	2.6
1	B	316	GLN	2.5
1	A	273	GLY	2.5
1	B	92	ASN	2.5
1	B	48	LEU	2.5
1	B	104	GLU	2.5
1	B	365	PHE	2.5
1	C	340	GLY	2.5
1	A	363	ASP	2.5
1	A	56	LEU	2.5
1	A	337	ILE	2.5
1	B	319	CYS	2.5
1	B	252	SER	2.5
1	C	170	VAL	2.4
1	C	257	PHE	2.4
1	C	315	SER	2.4
1	C	367	THR	2.4
1	B	251	ALA	2.4
1	B	272	ALA	2.4
1	A	316	GLN	2.4
1	C	259	ASP	2.4
1	B	368	ALA	2.4
1	B	359	CYS	2.4
1	A	60	TYR	2.3
1	B	51	TYR	2.3
1	A	336	VAL	2.3
1	A	254	THR	2.3
1	B	209	ASN	2.3
1	B	8	GLY	2.3
1	C	312	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	211	GLN	2.3
1	C	313	ALA	2.3
1	C	112	GLY	2.3
1	B	113	SER	2.3
1	A	211	GLN	2.3
1	A	266	GLN	2.2
1	C	309	VAL	2.2
1	A	9	LYS	2.2
1	C	68	TYR	2.2
1	B	256	LYS	2.2
1	B	259	ASP	2.2
1	A	367	THR	2.2
1	B	308	PRO	2.2
1	C	268	VAL	2.2
1	B	255	GLU	2.1
1	B	112	GLY	2.1
1	C	266	GLN	2.1
1	B	49	HIS	2.1
1	A	64	ARG	2.1
1	A	113	SER	2.1
1	B	318	ASP	2.1
1	C	317	ASP	2.1
1	C	66	GLY	2.1
1	B	64	ARG	2.1
1	A	269	CYS	2.1
1	C	253	SER	2.1
1	C	319	CYS	2.1
1	B	111	ASN	2.1
1	B	46	PRO	2.1
1	B	279	ILE	2.1
1	C	264	GLY	2.1
1	A	268	VAL	2.1
1	B	169	SER	2.1
1	A	111	ASN	2.1
1	C	278	ASN	2.1
1	C	256	LYS	2.1
1	A	253	SER	2.1
1	A	63	LEU	2.0
1	C	379	MET	2.0
1	C	271	GLN	2.0
1	B	275	THR	2.0
1	A	384	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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($\text{\AA}^2$)	Q<0.9
2	24O	X	4	16/17	0.97	0.07	35,37,37,37	0
2	24O	Y	4	16/17	0.97	0.06	34,36,38,39	0
2	24O	Z	4	16/17	0.97	0.08	35,37,38,39	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.