



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 08:28 AM UTC

PDB ID : 1YM4 / pdb_00001ym4
Title : Crystal structure of human beta secretase complexed with NVP-AMK640
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 : 2.25 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

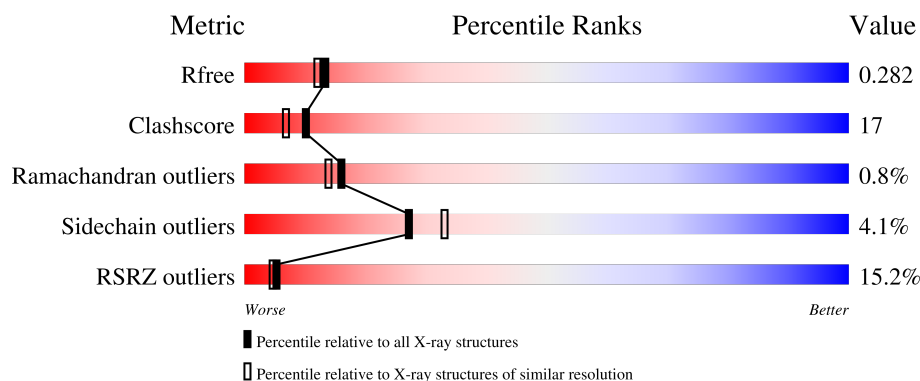
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	408	5% 68% 23% 7%
1	B	408	7% 66% 24% 8%
1	C	408	30% 50% 41% 7%
2	X	5	40% 40% 20%
2	Y	5	40% 20% 40% 20%

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Mol	Chain	Length	Quality of chain
2	Z	5	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9538 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	379	Total	C	N	O	S	0	0	0
			2975	1903	495	563	14			
1	B	377	Total	C	N	O	S	0	0	0
			2966	1898	493	561	14			
1	C	379	Total	C	N	O	S	0	0	0
			2975	1903	495	563	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-AMK640 INHIBITOR.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	X	5	Total	C	N	O	0	0	0
			45	29	6	10			
2	Y	5	Total	C	N	O	0	0	0
			45	29	6	10			
2	Z	5	Total	C	N	O	0	0	0
			45	29	6	10			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	203	Total	O	0	0
			203	203		

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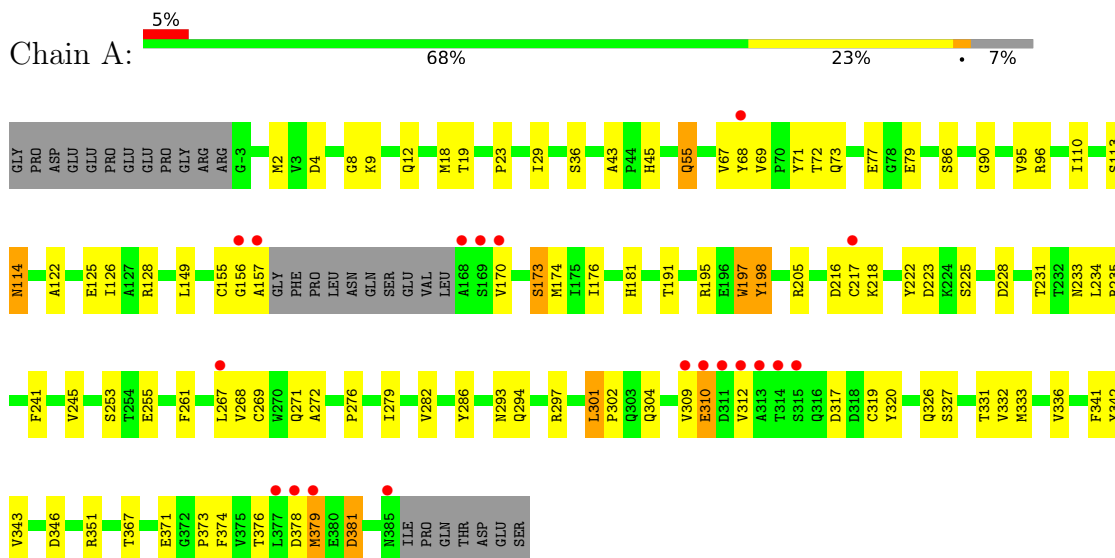
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	155	Total 155	O 155	0	0
3	C	117	Total 117	O 117	0	0
3	X	6	Total 6	O 6	0	0
3	Y	3	Total 3	O 3	0	0
3	Z	3	Total 3	O 3	0	0

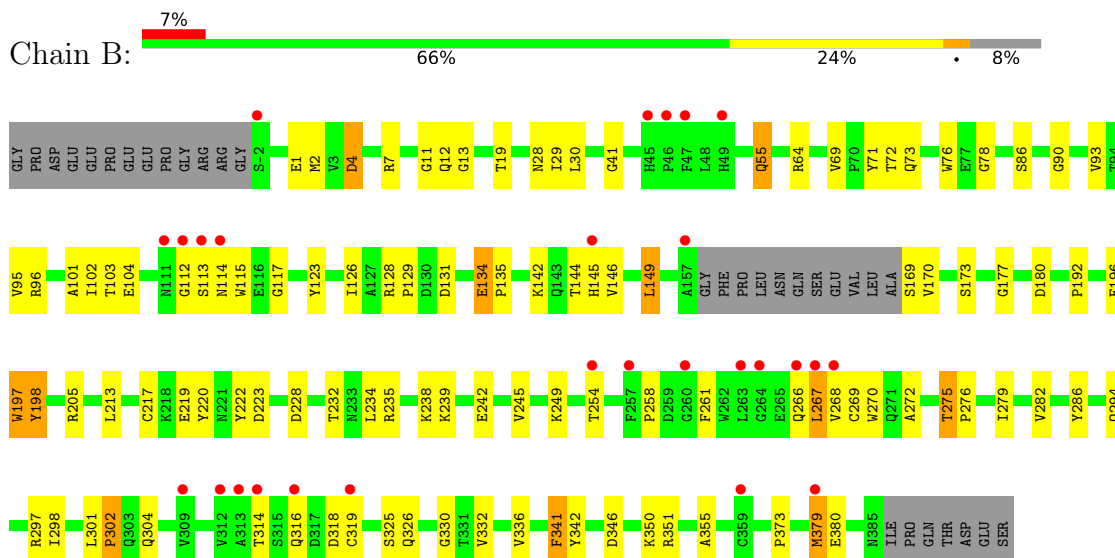
3 Residue-property plots [i](#)

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: Beta-secretase 1

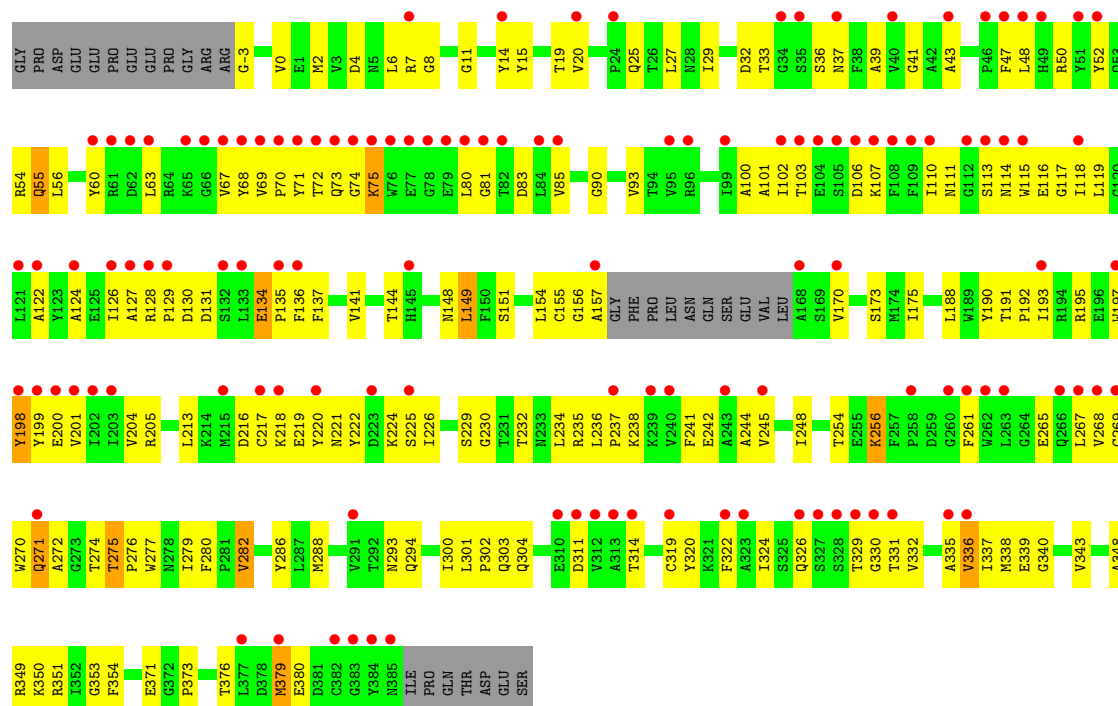


• Molecule 1: Beta-secretase 1



• Molecule 1: Beta-secretase 1

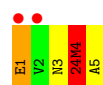
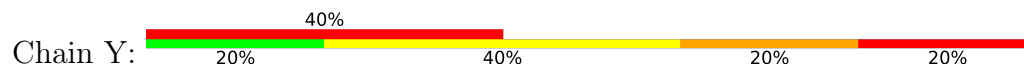




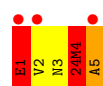
• Molecule 2: NVP-AMK640 INHIBITOR



• Molecule 2: NVP-AMK640 INHIBITOR



• Molecule 2: NVP-AMK640 INHIBITOR



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	223.68Å 107.75Å 61.48Å 90.00° 100.32° 90.00°	Depositor
Resolution (Å)	96.77 – 2.25 96.77 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.3 (96.77-2.25) 99.4 (96.77-2.25)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 2.25Å)	Xtriage
Refinement program	CNX 2002	Depositor
R, R_{free}	0.240 , 0.288 0.232 , 0.282	Depositor DCC
R_{free} test set	6850 reflections (10.12%)	wwPDB-VP
Wilson B-factor (Å ²)	36.7	Xtriage
Anisotropy	0.741	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 48.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9538	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 3.95% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 24M

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	0.59	1/3050 (0.0%)	1.00	14/4145 (0.3%)
1	B	0.51	0/3041	0.93	9/4133 (0.2%)
1	C	0.46	0/3050	0.91	10/4145 (0.2%)
2	X	1.70	0/28	1.38	0/34
2	Y	1.69	1/28 (3.6%)	1.39	0/34
2	Z	1.90	2/28 (7.1%)	1.29	0/34
All	All	0.54	4/9225 (0.0%)	0.95	33/12525 (0.3%)

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Z	5	ALA	C-O	5.62	1.34	1.23
1	A	333	MET	SD-CE	-5.54	1.65	1.79
2	Z	1	GLU	CD-OE2	5.34	1.35	1.25
2	Y	5	ALA	C-O	5.31	1.34	1.23

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	198	TYR	N-CA-C	-9.93	95.77	110.46
1	A	198	TYR	N-CA-C	-8.64	97.68	110.46
1	A	301	LEU	CA-C-N	-7.54	111.87	119.56
1	A	301	LEU	C-N-CA	-7.54	111.87	119.56
1	C	198	TYR	N-CA-C	-7.49	98.03	109.41
1	A	341	PHE	N-CA-C	7.18	119.83	109.14
1	C	280	PHE	CA-C-N	6.92	126.85	120.21
1	C	280	PHE	C-N-CA	6.92	126.85	120.21
1	C	0	VAL	N-CA-C	6.77	117.53	110.62
1	A	233	ASN	N-CA-C	6.70	119.59	110.35
1	A	191	THR	N-CA-C	-6.28	100.66	110.14
1	A	23	PRO	CA-C-N	6.06	126.38	119.83
1	A	23	PRO	C-N-CA	6.06	126.38	119.83
1	A	342	TYR	N-CA-C	-6.04	99.36	108.96
1	B	134	GLU	CA-C-N	5.97	125.88	119.85
1	B	134	GLU	C-N-CA	5.97	125.88	119.85
1	C	134	GLU	CA-C-N	5.85	125.80	119.78
1	C	134	GLU	C-N-CA	5.85	125.80	119.78
1	A	343	VAL	N-CA-C	5.75	115.88	107.37
1	C	275	THR	CA-C-N	5.56	126.79	119.84
1	C	275	THR	C-N-CA	5.56	126.79	119.84
1	A	45	HIS	CA-C-N	5.49	126.70	119.84
1	A	45	HIS	C-N-CA	5.49	126.70	119.84
1	A	43	ALA	CA-C-N	5.40	125.41	119.90
1	A	43	ALA	C-N-CA	5.40	125.41	119.90
1	B	275	THR	CA-C-N	5.38	126.57	119.84
1	B	275	THR	C-N-CA	5.38	126.57	119.84
1	C	43	ALA	CA-C-N	5.33	125.33	119.89
1	C	43	ALA	C-N-CA	5.33	125.33	119.89
1	B	341	PHE	N-CA-C	5.32	117.07	109.14
1	B	342	TYR	N-CA-C	-5.32	100.06	108.73
1	B	123	TYR	N-CA-C	5.22	117.59	110.55
1	B	302	PRO	N-CA-C	-5.20	107.36	113.86

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	X	4	24M	Mainchain,Peptide
2	Y	4	24M	Mainchain,Peptide
2	Z	4	24M	Mainchain,Peptide

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	2975	0	2886	76	0
1	B	2966	0	2878	81	1
1	C	2975	0	2886	153	0
2	X	45	0	42	4	0
2	Y	45	0	42	4	0
2	Z	45	0	42	8	0
3	A	203	0	0	9	0
3	B	155	0	0	14	1
3	C	117	0	0	26	0
3	X	6	0	0	0	0
3	Y	3	0	0	0	0
3	Z	3	0	0	2	0
All	All	9538	0	8776	306	2

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 17.

All (306) 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:B:4:ASP:H	1:B:173:SER:HB3	1.32	0.94
1:A:4:ASP:H	1:A:173:SER:HB3	1.31	0.94
1:A:267:LEU:HD22	1:A:309:VAL:HG21	1.49	0.94
1:B:254:THR:HG21	1:B:279:ILE:HB	1.54	0.89
1:B:319:CYS:SG	3:B:2067:HOH:O	2.32	0.87
1:C:73:GLN:HE21	2:Z:3:ASN:HB2	1.40	0.86
1:A:73:GLN:NE2	2:X:3:ASN:HD22	1.73	0.85
1:B:11:GLY:O	2:Y:1:GLU:HB3	1.78	0.83
1:C:4:ASP:H	1:C:173:SER:HB3	1.44	0.82
1:A:4:ASP:HB3	3:A:1171:HOH:O	1.79	0.81
1:A:2:MET:HG2	1:A:90:GLY:HA2	1.63	0.81
1:C:193:ILE:HB	1:C:350:LYS:HG2	1.61	0.81
1:B:4:ASP:N	1:B:173:SER:HB3	1.97	0.80
1:C:238:LYS:O	1:C:242:GLU:HG3	1.83	0.79
1:C:72:THR:HG21	3:Z:3022:HOH:O	1.82	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:128:ARG:HG3	3:C:3120:HOH:O	1.81	0.78
1:C:235:ARG:HB2	1:C:332:VAL:HB	1.66	0.78
1:C:11:GLY:O	2:Z:1:GLU:HB3	1.85	0.77
1:C:148:ASN:HA	3:C:3098:HOH:O	1.84	0.77
1:A:301:LEU:H	1:A:304:GLN:HE21	1.32	0.76
1:C:234:LEU:HB2	1:C:336:VAL:HG21	1.66	0.76
1:B:145:HIS:HA	3:B:2159:HOH:O	1.86	0.75
1:C:379:MET:HE3	1:C:380:GLU:HG2	1.69	0.75
1:C:55:GLN:H	1:C:55:GLN:HE21	1.33	0.74
1:C:204:VAL:HG11	3:C:3091:HOH:O	1.86	0.74
1:A:55:GLN:H	1:A:55:GLN:HE21	1.35	0.73
1:A:4:ASP:N	1:A:173:SER:HB3	2.06	0.71
1:B:2:MET:HG2	1:B:90:GLY:HA2	1.72	0.71
1:C:157:ALA:HB3	3:C:3075:HOH:O	1.90	0.71
1:B:238:LYS:O	1:B:242:GLU:HG3	1.91	0.71
1:A:241:PHE:O	1:A:245:VAL:HG23	1.91	0.70
1:A:8:GLY:C	1:A:170:VAL:HG12	2.16	0.70
1:A:55:GLN:H	1:A:55:GLN:NE2	1.87	0.70
1:C:301:LEU:H	1:C:304:GLN:HE21	1.37	0.69
1:A:197:TRP:CD1	1:A:198:TYR:H	2.10	0.69
1:C:213:LEU:HB3	1:C:220:TYR:OH	1.93	0.68
1:A:8:GLY:O	1:A:170:VAL:HG12	1.93	0.68
1:C:110:ILE:HB	1:C:113:SER:HB3	1.76	0.68
1:C:241:PHE:O	1:C:245:VAL:HG23	1.94	0.68
1:C:55:GLN:H	1:C:55:GLN:NE2	1.93	0.67
1:B:96:ARG:HD2	3:B:2137:HOH:O	1.95	0.67
1:C:63:LEU:HG	1:C:81:GLY:HA2	1.76	0.67
1:B:301:LEU:H	1:B:304:GLN:HE21	1.43	0.66
1:C:217:CYS:HA	1:C:220:TYR:CD1	2.30	0.66
1:B:64:ARG:HD2	3:B:2047:HOH:O	1.95	0.65
1:B:73:GLN:NE2	2:Y:3:ASN:HD22	1.95	0.65
1:B:341:PHE:HB3	1:B:355:ALA:O	1.97	0.65
1:C:137:PHE:CE2	3:C:3098:HOH:O	2.50	0.65
1:B:103:THR:O	1:B:104:GLU:HG3	1.97	0.65
1:B:197:TRP:CD1	1:B:198:TYR:H	2.15	0.65
1:C:69:VAL:HA	3:C:3120:HOH:O	1.97	0.64
1:A:301:LEU:H	1:A:304:GLN:NE2	1.94	0.64
1:A:267:LEU:HD13	1:A:319:CYS:HB3	1.79	0.64
1:B:301:LEU:H	1:B:304:GLN:NE2	1.96	0.64
1:C:70:PRO:HA	1:C:75:LYS:HB3	1.80	0.63
1:C:234:LEU:HB2	1:C:336:VAL:CG2	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:VAL:HG22	1:B:128:ARG:HB2	1.82	0.62
1:A:68:TYR:HD2	1:C:68:TYR:HD2	1.48	0.61
1:B:219:GLU:OE1	1:B:239:LYS:HD3	2.01	0.60
1:C:195:ARG:HB3	1:C:197:TRP:CD1	2.37	0.60
1:C:4:ASP:H	1:C:173:SER:CB	2.14	0.60
1:B:276:PRO:O	1:B:279:ILE:HG12	2.02	0.60
1:C:195:ARG:HA	3:C:3117:HOH:O	2.03	0.59
1:C:267:LEU:O	1:C:267:LEU:HD12	2.02	0.59
1:B:266:GLN:HB3	3:B:2152:HOH:O	2.02	0.59
1:C:222:TYR:O	1:C:330:GLY:HA2	2.03	0.58
1:C:256:LYS:HA	3:C:3052:HOH:O	2.02	0.58
1:C:282:VAL:HG22	1:C:300:ILE:O	2.03	0.58
1:C:232:THR:OG1	2:Z:2:VAL:HG22	2.03	0.58
1:A:156:GLY:O	1:A:170:VAL:HG23	2.04	0.58
1:B:4:ASP:H	1:B:173:SER:CB	2.12	0.58
1:C:242:GLU:HG2	3:C:3063:HOH:O	2.04	0.58
1:A:327:SER:HB2	3:A:1102:HOH:O	2.04	0.57
1:C:36:SER:OG	1:C:122:ALA:HB3	2.03	0.57
1:C:192:PRO:HD2	1:C:288:MET:O	2.04	0.57
1:C:41:GLY:HA2	1:C:102:ILE:HB	1.87	0.56
1:C:32:ASP:OD1	1:C:230:GLY:HA3	2.05	0.56
1:A:157:ALA:HB3	3:A:1122:HOH:O	2.05	0.56
1:A:267:LEU:HD22	1:A:309:VAL:CG2	2.31	0.56
1:A:73:GLN:HB3	2:X:3:ASN:HB2	1.87	0.56
1:C:74:GLY:HA2	1:C:107:LYS:HB2	1.88	0.56
1:A:297:ARG:HG2	1:A:374:PHE:CE1	2.41	0.56
1:C:69:VAL:HG21	3:C:3114:HOH:O	2.06	0.55
1:A:276:PRO:O	1:A:279:ILE:HG12	2.07	0.55
1:A:379:MET:HE2	1:A:379:MET:H	1.71	0.55
1:C:55:GLN:HG2	1:C:56:LEU:HD23	1.89	0.55
1:C:110:ILE:HD11	2:Z:2:VAL:HG12	1.88	0.55
1:B:169:SER:HB3	3:B:2147:HOH:O	2.08	0.54
1:C:29:ILE:HD12	1:C:117:GLY:HA3	1.88	0.54
1:A:73:GLN:HE21	2:X:3:ASN:HD22	1.52	0.54
1:B:93:VAL:HG11	1:B:144:THR:HG21	1.89	0.54
1:C:267:LEU:HB2	1:C:320:TYR:O	2.07	0.54
1:C:149:LEU:HD23	1:C:149:LEU:C	2.33	0.54
1:A:197:TRP:CG	1:A:198:TYR:H	2.25	0.54
1:A:261:PHE:CD1	1:A:268:VAL:HG23	2.43	0.54
1:B:197:TRP:CG	1:B:198:TYR:H	2.25	0.54
1:C:236:LEU:O	1:C:326:GLN:HA	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:GLY:HA2	1:B:102:ILE:HB	1.90	0.53
1:B:270:TRP:CE3	1:B:275:THR:HG23	2.43	0.53
1:C:193:ILE:HB	1:C:350:LYS:CG	2.37	0.53
1:C:230:GLY:O	2:Z:2:VAL:HG23	2.07	0.53
1:A:379:MET:H	1:A:379:MET:CE	2.21	0.53
1:A:235:ARG:HB2	1:A:332:VAL:HB	1.90	0.53
1:C:73:GLN:NE2	2:Z:3:ASN:HB2	2.18	0.53
1:A:216:ASP:C	1:A:218:LYS:H	2.17	0.53
1:C:71:TYR:HB2	1:C:74:GLY:O	2.08	0.52
1:C:47:PHE:CE2	1:C:111:ASN:HB2	2.44	0.52
1:C:195:ARG:HD3	3:C:3103:HOH:O	2.08	0.52
1:C:20:VAL:HG22	1:C:85:VAL:HG22	1.92	0.52
1:B:55:GLN:H	1:B:55:GLN:NE2	2.07	0.52
1:C:293:ASN:HA	1:C:376:THR:O	2.10	0.52
1:C:67:VAL:HG23	3:C:3093:HOH:O	2.09	0.52
1:C:113:SER:HB2	1:C:115:TRP:NE1	2.24	0.52
1:A:155:CYS:O	1:A:170:VAL:HG22	2.10	0.51
1:B:217:CYS:HA	1:B:220:TYR:CD1	2.46	0.51
1:C:126:ILE:HG23	1:C:197:TRP:HB2	1.91	0.51
1:B:232:THR:O	1:B:336:VAL:HG13	2.10	0.51
1:C:322:PHE:CE2	1:C:324:ILE:HB	2.46	0.51
1:C:379:MET:HE2	1:C:380:GLU:H	1.74	0.51
1:B:254:THR:CG2	1:B:279:ILE:HB	2.36	0.51
1:C:20:VAL:HG22	1:C:85:VAL:HG13	1.91	0.51
1:A:8:GLY:CA	1:A:170:VAL:HG12	2.41	0.51
1:B:78:GLY:HA3	1:B:101:ALA:O	2.11	0.51
1:C:197:TRP:CZ2	1:C:224:LYS:HD3	2.46	0.51
1:C:379:MET:HE2	1:C:379:MET:H	1.76	0.51
1:C:107:LYS:N	3:C:3055:HOH:O	2.23	0.51
1:C:199:TYR:HB2	3:C:3088:HOH:O	2.11	0.50
1:B:113:SER:HB2	1:B:115:TRP:NE1	2.26	0.50
1:B:234:LEU:HB2	1:B:336:VAL:HG21	1.92	0.50
1:C:110:ILE:HG22	3:C:3081:HOH:O	2.10	0.50
1:C:137:PHE:O	1:C:141:VAL:HG23	2.11	0.50
1:B:301:LEU:HB3	1:B:302:PRO:HD2	1.93	0.50
1:B:7:ARG:HG2	3:B:2150:HOH:O	2.11	0.50
1:C:200:GLU:HA	1:C:225:SER:O	2.11	0.50
1:C:294:GLN:HG2	1:C:373:PRO:HB2	1.93	0.50
1:A:234:LEU:N	1:A:336:VAL:HG21	2.27	0.50
1:C:301:LEU:H	1:C:304:GLN:NE2	2.08	0.50
1:B:29:ILE:HD12	1:B:117:GLY:HA3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:LEU:HB2	1:B:336:VAL:CG2	2.42	0.49
1:B:261:PHE:CD1	1:B:268:VAL:HG23	2.47	0.49
1:B:326:GLN:HG2	3:B:2154:HOH:O	2.12	0.49
1:B:126:ILE:HG23	1:B:197:TRP:HB2	1.94	0.49
1:A:68:TYR:HD2	1:C:68:TYR:CD2	2.28	0.49
1:C:224:LYS:HG3	3:C:3111:HOH:O	2.13	0.49
1:A:181:HIS:ND1	1:B:64:ARG:NH1	2.61	0.49
1:A:253:SER:C	1:A:255:GLU:H	2.20	0.49
1:B:268:VAL:O	1:B:319:CYS:HA	2.12	0.49
1:C:70:PRO:HD2	3:C:3120:HOH:O	2.13	0.49
1:A:378:ASP:HB3	1:A:381:ASP:OD2	2.13	0.49
1:C:225:SER:HA	1:C:331:THR:O	2.13	0.49
1:C:154:LEU:O	1:C:339:GLU:HA	2.12	0.48
1:C:33:THR:HB	3:C:3088:HOH:O	2.13	0.48
1:B:258:PRO:HB2	1:B:266:GLN:OE1	2.13	0.48
1:C:198:TYR:OH	2:Z:5:ALA:HB3	2.14	0.48
1:A:174:MET:HE3	1:A:176:ILE:HD11	1.95	0.48
1:A:73:GLN:HE22	2:X:3:ASN:HD22	1.57	0.48
1:A:294:GLN:HG3	1:A:373:PRO:HB2	1.94	0.48
1:B:235:ARG:NH2	3:B:2133:HOH:O	2.46	0.48
1:C:148:ASN:HB3	1:C:348:ALA:HB2	1.96	0.48
1:A:268:VAL:HG12	1:A:269:CYS:N	2.29	0.48
1:B:12:GLN:OE1	1:B:113:SER:HA	2.13	0.48
1:C:8:GLY:HA2	1:C:15:TYR:CE2	2.49	0.48
1:A:294:GLN:HG2	3:A:1148:HOH:O	2.13	0.48
1:C:119:LEU:HD11	1:C:136:PHE:CD2	2.49	0.48
1:C:188:LEU:HD23	1:C:354:PHE:O	2.14	0.48
1:A:125:GLU:HB2	3:A:1188:HOH:O	2.14	0.47
1:B:197:TRP:CD1	1:B:197:TRP:N	2.82	0.47
1:C:55:GLN:HE21	1:C:55:GLN:N	2.09	0.47
1:C:225:SER:OG	1:C:331:THR:HB	2.14	0.47
1:C:301:LEU:HB3	1:C:302:PRO:HD2	1.96	0.47
3:A:1190:HOH:O	1:C:238:LYS:HD3	2.13	0.47
1:A:205:ARG:HB3	1:A:286:TYR:HB2	1.96	0.47
1:C:37:ASN:HD21	1:C:127:ALA:HA	1.80	0.47
1:C:113:SER:HG	1:C:115:TRP:CD1	2.32	0.47
1:C:261:PHE:CD1	1:C:268:VAL:HG23	2.49	0.47
1:C:39:ALA:HB2	1:C:100:ALA:HB3	1.97	0.47
1:B:149:LEU:C	1:B:149:LEU:HD23	2.40	0.47
1:C:217:CYS:N	3:C:3115:HOH:O	2.47	0.46
1:C:371:GLU:HG2	3:C:3105:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:SER:O	1:A:114:ASN:CB	2.63	0.46
1:C:2:MET:HG2	1:C:90:GLY:HA2	1.97	0.46
1:B:222:TYR:HA	1:B:223:ASP:HA	1.59	0.46
1:A:149:LEU:HD23	1:A:149:LEU:C	2.41	0.46
1:A:222:TYR:HA	1:A:223:ASP:HA	1.64	0.46
1:C:14:TYR:CG	1:C:154:LEU:HD22	2.50	0.46
1:B:249:LYS:NZ	3:B:2125:HOH:O	2.46	0.46
1:B:7:ARG:HG2	3:B:2084:HOH:O	2.16	0.46
1:B:379:MET:CE	1:B:380:GLU:HG2	2.46	0.46
1:C:101:ALA:O	1:C:103:THR:HG23	2.16	0.46
1:C:4:ASP:N	1:C:173:SER:HB3	2.22	0.46
1:C:48:LEU:HD22	1:C:116:GLU:HB3	1.97	0.46
1:A:12:GLN:OE1	1:A:113:SER:HA	2.16	0.46
1:A:122:ALA:CB	1:A:126:ILE:HD11	2.46	0.45
1:A:234:LEU:HB2	1:A:336:VAL:HG21	1.97	0.45
1:C:219:GLU:O	1:C:237:PRO:HG3	2.15	0.45
1:C:237:PRO:HB2	3:C:3084:HOH:O	2.15	0.45
1:B:228:ASP:OD2	2:Y:4:24M:H192	2.16	0.45
1:A:225:SER:OG	1:A:331:THR:HB	2.16	0.45
1:B:28:ASN:HB2	1:B:115:TRP:HA	1.98	0.45
1:A:79:GLU:HB3	3:A:1163:HOH:O	2.17	0.45
1:C:197:TRP:CD1	1:C:198:TYR:H	2.34	0.45
1:C:311:ASP:HB3	1:C:314:THR:OG1	2.16	0.45
1:A:267:LEU:HB2	1:A:320:TYR:O	2.16	0.45
1:B:128:ARG:HA	1:B:129:PRO:C	2.41	0.45
1:C:-3:GLY:N	3:C:3109:HOH:O	2.50	0.45
1:B:73:GLN:HE22	2:Y:3:ASN:HD22	1.64	0.45
1:B:235:ARG:HB2	1:B:332:VAL:HB	1.99	0.45
1:A:68:TYR:CD2	1:C:68:TYR:HD2	2.31	0.44
1:B:268:VAL:HG12	1:B:269:CYS:N	2.32	0.44
1:B:192:PRO:HB3	3:B:2121:HOH:O	2.17	0.44
1:C:267:LEU:HD13	1:C:319:CYS:HB3	1.98	0.44
1:C:276:PRO:O	1:C:279:ILE:HG12	2.18	0.44
1:A:9:LYS:HB2	1:A:12:GLN:HB2	1.99	0.44
1:A:36:SER:OG	1:A:122:ALA:HB3	2.16	0.44
1:B:196:GLU:OE2	1:B:350:LYS:HE3	2.17	0.44
1:B:269:CYS:HA	1:B:318:ASP:O	2.17	0.44
1:B:298:ILE:HB	1:B:341:PHE:CZ	2.51	0.44
1:C:93:VAL:HG11	1:C:144:THR:HG21	1.99	0.44
1:C:106:ASP:HA	3:C:3055:HOH:O	2.18	0.44
1:A:19:THR:OG1	1:A:86:SER:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:VAL:HB	1:B:76:TRP:CZ2	2.53	0.44
1:C:19:THR:HA	1:C:25:GLN:O	2.18	0.44
1:C:32:ASP:OD1	2:Z:4:24M:C36	2.66	0.44
1:C:47:PHE:CZ	1:C:111:ASN:HB2	2.52	0.44
1:C:226:ILE:CG1	1:C:332:VAL:HG22	2.47	0.44
1:A:96:ARG:NE	3:A:1031:HOH:O	2.33	0.43
1:B:134:GLU:HA	1:B:135:PRO:HD3	1.84	0.43
1:C:271:GLN:HB2	1:C:274:THR:CG2	2.48	0.43
1:B:197:TRP:CG	1:B:198:TYR:N	2.86	0.43
1:B:222:TYR:O	1:B:330:GLY:HA2	2.18	0.43
1:A:71:TYR:O	1:A:72:THR:C	2.61	0.43
1:A:110:ILE:HB	1:A:113:SER:HB3	2.00	0.43
1:C:193:ILE:HG13	1:C:351:ARG:N	2.33	0.43
1:C:216:ASP:OD1	1:C:218:LYS:HB2	2.18	0.43
1:C:379:MET:H	1:C:379:MET:CE	2.31	0.43
1:B:71:TYR:HE2	1:B:76:TRP:NE1	2.16	0.43
1:B:294:GLN:CG	1:B:373:PRO:HB2	2.48	0.43
1:C:52:TYR:OH	1:C:83:ASP:OD2	2.28	0.43
1:B:286:TYR:CZ	1:B:297:ARG:HD3	2.54	0.43
1:C:216:ASP:HA	3:C:3066:HOH:O	2.18	0.43
1:A:253:SER:C	1:A:255:GLU:N	2.76	0.43
1:A:293:ASN:HA	1:A:376:THR:O	2.19	0.43
1:C:27:LEU:HA	1:C:50:ARG:NH2	2.33	0.43
1:A:195:ARG:HD3	3:A:1110:HOH:O	2.18	0.43
1:B:346:ASP:HB3	1:B:351:ARG:HG3	2.01	0.43
1:A:228:ASP:OD2	1:A:231:THR:OG1	2.28	0.42
1:A:301:LEU:O	1:A:302:PRO:C	2.60	0.42
1:B:142:LYS:HB3	3:B:2109:HOH:O	2.17	0.42
1:B:314:THR:C	1:B:316:GLN:N	2.77	0.42
1:C:221:ASN:HB3	3:C:3013:HOH:O	2.19	0.42
1:C:269:CYS:HA	1:C:319:CYS:HA	2.01	0.42
1:C:349:ARG:O	1:C:350:LYS:C	2.62	0.42
1:C:197:TRP:CD2	1:C:198:TYR:HD2	2.37	0.42
1:A:197:TRP:CD1	1:A:197:TRP:N	2.87	0.42
1:B:113:SER:O	1:B:114:ASN:CB	2.66	0.42
1:C:201:VAL:O	1:C:225:SER:HB2	2.19	0.42
1:C:32:ASP:CB	1:C:118:ILE:HD11	2.49	0.42
1:C:270:TRP:CE3	1:C:275:THR:HG23	2.55	0.42
1:C:271:GLN:H	1:C:271:GLN:HG2	1.64	0.42
1:C:128:ARG:HA	1:C:129:PRO:C	2.44	0.42
1:C:151:SER:OG	1:C:175:ILE:HB	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:244:ALA:O	1:C:248:ILE:HG13	2.18	0.42
1:A:197:TRP:CG	1:A:198:TYR:N	2.87	0.42
1:B:205:ARG:HB3	1:B:286:TYR:HB2	2.01	0.42
1:C:33:THR:HG23	1:C:229:SER:OG	2.19	0.42
1:B:294:GLN:HG3	1:B:373:PRO:HB2	2.02	0.42
1:C:124:ALA:HA	1:C:127:ALA:HB2	2.01	0.42
1:A:379:MET:SD	1:A:379:MET:N	2.89	0.42
1:C:37:ASN:HD21	1:C:128:ARG:H	1.67	0.42
1:B:180:ASP:OD2	1:B:180:ASP:C	2.62	0.42
1:C:113:SER:O	1:C:114:ASN:HB3	2.20	0.42
1:C:277:TRP:CZ3	1:C:303:GLN:HG3	2.55	0.42
1:C:37:ASN:HB3	3:C:3114:HOH:O	2.20	0.41
1:C:205:ARG:HB3	1:C:286:TYR:HB2	2.01	0.41
1:C:39:ALA:CB	1:C:100:ALA:HB3	2.50	0.41
1:C:304:GLN:HB3	1:C:336:VAL:O	2.20	0.41
1:C:338:MET:C	1:C:340:GLY:H	2.28	0.41
1:A:269:CYS:SG	1:A:312:VAL:HG23	2.61	0.41
1:B:19:THR:OG1	1:B:86:SER:HB2	2.20	0.41
1:C:294:GLN:CG	1:C:373:PRO:HB2	2.51	0.41
1:A:67:VAL:O	1:A:77:GLU:HG3	2.21	0.41
1:A:241:PHE:CG	1:A:326:GLN:HB3	2.55	0.41
1:A:271:GLN:O	1:A:272:ALA:C	2.63	0.41
1:A:346:ASP:HB3	1:A:351:ARG:HG3	2.02	0.41
1:B:267:LEU:HD13	1:B:319:CYS:HB3	2.01	0.41
1:B:146:VAL:HG13	1:B:177:GLY:HA3	2.03	0.41
1:B:254:THR:HG22	3:B:2051:HOH:O	2.20	0.41
1:C:191:THR:HG23	1:C:191:THR:O	2.21	0.41
1:C:332:VAL:HG11	3:Z:3094:HOH:O	2.20	0.41
1:A:18:MET:SD	1:A:29:ILE:HG13	2.60	0.41
1:C:54:ARG:HD2	1:C:60:TYR:CZ	2.56	0.41
1:C:193:ILE:HG13	1:C:351:ARG:CA	2.50	0.41
1:C:6:LEU:O	1:C:7:ARG:HG3	2.21	0.41
1:B:13:GLY:HA3	1:B:30:LEU:HD11	2.03	0.40
1:C:67:VAL:O	1:C:67:VAL:HG13	2.21	0.40
1:A:69:VAL:HG22	1:A:128:ARG:HB2	2.02	0.40
1:C:113:SER:O	1:C:114:ASN:CB	2.69	0.40
1:B:268:VAL:HG12	1:B:269:CYS:H	1.86	0.40
1:C:190:TYR:HA	1:C:353:GLY:HA2	2.02	0.40
1:C:335:ALA:C	1:C:337:ILE:N	2.78	0.40
1:A:297:ARG:HH21	1:A:371:GLU:CD	2.29	0.40
1:C:134:GLU:HA	1:C:135:PRO:HD3	1.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:155:CYS:O	1:C:170:VAL:HG22	2.22	0.40
1:C:71:TYR:C	1:C:73:GLN:N	2.78	0.40
1:C:270:TRP:CE2	1:C:276:PRO:HD2	2.57	0.40
1:C:322:PHE:CZ	1:C:324:ILE:HB	2.56	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:GLY:CA	1:B:112:GLY:CA[2_556]	2.16	0.04
3:B:2152:HOH:O	3:B:2152:HOH:O[2_556]	2.18	0.02

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	375/408 (92%)	349 (93%)	24 (6%)	2 (0%)	24	24
1	B	373/408 (91%)	347 (93%)	24 (6%)	2 (0%)	24	24
1	C	375/408 (92%)	336 (90%)	34 (9%)	5 (1%)	9	6
2	X	2/5 (40%)	1 (50%)	1 (50%)	0	100	100
2	Y	2/5 (40%)	2 (100%)	0	0	100	100
2	Z	2/5 (40%)	2 (100%)	0	0	100	100
All	All	1129/1239 (91%)	1037 (92%)	83 (7%)	9 (1%)	16	14

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	310	GLU
1	A	217	CYS
1	B	272	ALA

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Mol	Chain	Res	Type
1	C	80	LEU
1	C	156	GLY
1	C	265	GLU
1	C	272	ALA
1	B	131	ASP
1	C	131	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	322/348 (92%)	311 (97%)	11 (3%)	32	40
1	B	322/348 (92%)	308 (96%)	14 (4%)	26	31
1	C	322/348 (92%)	310 (96%)	12 (4%)	30	37
2	X	3/3 (100%)	2 (67%)	1 (33%)	0	0
2	Y	3/3 (100%)	2 (67%)	1 (33%)	0	0
2	Z	3/3 (100%)	2 (67%)	1 (33%)	0	0
All	All	975/1053 (93%)	935 (96%)	40 (4%)	27	33

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	GLN
1	A	95	VAL
1	A	114	ASN
1	A	173	SER
1	A	197	TRP
1	A	282	VAL
1	A	310	GLU
1	A	317	ASP
1	A	367	THR
1	A	379	MET
1	A	381	ASP
1	B	1	GLU

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Mol	Chain	Res	Type
1	B	4	ASP
1	B	55	GLN
1	B	72	THR
1	B	95	VAL
1	B	149	LEU
1	B	170	VAL
1	B	197	TRP
1	B	213	LEU
1	B	245	VAL
1	B	267	LEU
1	B	282	VAL
1	B	325	SER
1	B	379	MET
1	C	55	GLN
1	C	75	LYS
1	C	130	ASP
1	C	149	LEU
1	C	254	THR
1	C	256	LYS
1	C	271	GLN
1	C	282	VAL
1	C	329	THR
1	C	336	VAL
1	C	343	VAL
1	C	379	MET
2	X	1	GLU
2	Y	1	GLU
2	Z	1	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	GLN
1	A	73	GLN
1	A	89	HIS
1	A	98	ASN
1	A	114	ASN
1	A	233	ASN
1	A	266	GLN
1	A	293	ASN
1	A	304	GLN
1	B	55	GLN

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Mol	Chain	Res	Type
1	B	73	GLN
1	B	98	ASN
1	B	111	ASN
1	B	304	GLN
1	B	326	GLN
1	C	55	GLN
1	C	73	GLN
1	C	111	ASN
1	C	271	GLN
1	C	293	ASN
1	C	304	GLN

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	24M	Y	4	2	15,15,16	0.79	1 (6%)	12,20,22	1.60	3 (25%)
2	24M	Z	4	2	15,15,16	0.60	0	12,20,22	1.75	4 (33%)
2	24M	X	4	2	15,15,16	0.72	0	12,20,22	1.55	3 (25%)

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	24M	Y	4	2	-	1/13/24/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	24M	Z	4	2	-	0/13/24/26	0/1/1/1
2	24M	X	4	2	-	1/13/24/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Y	4	24M	C9-C5	2.07	1.56	1.53

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Z	4	24M	C19-C9-C11	3.84	107.45	102.76
2	X	4	24M	C39-C36-CA	-3.40	108.44	115.76
2	Y	4	24M	C39-C36-CA	-3.27	108.73	115.76
2	Z	4	24M	C39-C36-CA	-3.08	109.12	115.76
2	Y	4	24M	C19-C9-C11	3.06	106.50	102.76
2	Y	4	24M	O-C-C11	-2.49	119.59	125.19
2	X	4	24M	C19-C9-C11	2.47	105.78	102.76
2	Z	4	24M	O-C-C11	-2.43	119.72	125.19
2	X	4	24M	O-C-C11	-2.29	120.04	125.19
2	Z	4	24M	C13-C11-C9	2.02	107.36	103.26

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	X	4	24M	O-C-C11-C9
2	Y	4	24M	O-C-C11-C9

There are no ring outliers.

2 monomers are involved in 2 short contacts:

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	379/408 (92%)	0.18	19 (5%) 34 33	22, 36, 65, 104	0
1	B	377/408 (92%)	0.51	27 (7%) 21 20	28, 43, 75, 105	0
1	C	379/408 (92%)	1.53	123 (32%) 1 0	29, 59, 83, 112	0
2	X	4/5 (80%)	0.51	0 100 100	26, 31, 43, 53	0
2	Y	4/5 (80%)	1.81	2 (50%) 0 0	52, 54, 60, 81	0
2	Z	4/5 (80%)	2.52	3 (75%) 0 0	53, 59, 65, 75	0
All	All	1147/1239 (92%)	0.75	174 (15%) 5 5	22, 44, 78, 112	0

All (174) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	314	THR	5.6
1	B	113	SER	5.0
1	B	312	VAL	5.0
1	C	68	TYR	4.9
1	A	312	VAL	4.7
2	Z	5	ALA	4.7
1	A	379	MET	4.6
1	B	112	GLY	4.5
1	C	67	VAL	4.4
1	C	312	VAL	4.4
1	B	379	MET	4.3
1	C	261	PHE	4.3
1	A	170	VAL	4.1
1	B	157	ALA	4.0
1	C	385	ASN	3.9
1	C	268	VAL	3.9
1	C	327	SER	3.8
1	A	313	ALA	3.8
1	C	7	ARG	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	111	ASN	3.7
1	C	157	ALA	3.7
1	C	81	GLY	3.7
1	C	197	TRP	3.6
1	C	128	ARG	3.6
1	C	269	CYS	3.6
1	A	314	THR	3.6
1	C	262	TRP	3.6
1	C	110	ILE	3.5
1	C	260	GLY	3.5
1	B	267	LEU	3.5
1	C	263	LEU	3.5
1	C	311	ASP	3.5
1	C	115	TRP	3.4
1	B	47	PHE	3.4
1	B	309	VAL	3.4
1	C	168	ALA	3.4
1	C	76	TRP	3.3
1	C	328	SER	3.3
1	C	382	CYS	3.3
1	C	60	TYR	3.3
1	A	168	ALA	3.3
1	C	193	ILE	3.3
1	C	69	VAL	3.3
1	C	379	MET	3.2
1	C	78	GLY	3.2
1	C	72	THR	3.2
1	A	68	TYR	3.2
1	B	313	ALA	3.2
1	C	199	TYR	3.2
1	C	20	VAL	3.2
1	C	71	TYR	3.2
1	C	267	LEU	3.2
1	C	132	SER	3.1
1	C	66	GLY	3.1
1	C	330	GLY	3.1
1	C	384	TYR	3.1
1	B	264	GLY	3.1
1	C	34	GLY	3.1
1	C	313	ALA	3.1
1	C	113	SER	3.0
1	C	124	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	336	VAL	3.0
1	B	49	HIS	3.0
1	B	314	THR	3.0
1	C	225	SER	3.0
1	A	310	GLU	3.0
1	C	70	PRO	3.0
1	C	127	ALA	3.0
1	C	73	GLN	3.0
1	C	329	THR	3.0
1	C	129	PRO	3.0
1	C	331	THR	2.9
1	A	377	LEU	2.9
1	C	202	ILE	2.9
1	C	266	GLN	2.9
1	C	240	VAL	2.9
1	C	133	LEU	2.8
1	C	99	ILE	2.8
1	B	-2	SER	2.8
1	B	145	HIS	2.8
1	A	157	ALA	2.8
1	C	126	ILE	2.8
1	C	109	PHE	2.8
1	A	156	GLY	2.7
1	C	77	GLU	2.7
1	C	47	PHE	2.7
1	C	82	THR	2.7
1	C	48	LEU	2.7
1	C	326	GLN	2.7
1	A	315	SER	2.7
1	C	80	LEU	2.7
1	C	198	TYR	2.7
1	C	383	GLY	2.7
1	C	105	SER	2.7
1	C	51	TYR	2.6
1	C	220	TYR	2.6
1	B	257	PHE	2.6
1	C	203	ILE	2.6
1	B	46	PRO	2.6
1	C	96	ARG	2.6
1	C	37	ASN	2.6
1	C	62	ASP	2.6
1	C	106	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	103	THR	2.6
1	C	145	HIS	2.6
1	B	114	ASN	2.5
1	C	258	PRO	2.5
1	C	310	GLU	2.5
1	C	61	ARG	2.5
1	C	243	ALA	2.5
1	C	271	GLN	2.5
1	B	263	LEU	2.5
1	C	79	GLU	2.5
1	C	114	ASN	2.5
1	C	74	GLY	2.5
1	C	245	VAL	2.4
1	C	49	HIS	2.4
1	C	223	ASP	2.4
2	Y	1	GLU	2.4
1	C	95	VAL	2.4
1	A	378	ASP	2.4
2	Z	1	GLU	2.4
1	B	260	GLY	2.4
1	A	311	ASP	2.4
1	C	218	LYS	2.4
1	C	322	PHE	2.4
1	A	267	LEU	2.4
1	C	323	ALA	2.3
1	C	108	PHE	2.3
1	C	84	LEU	2.3
1	C	52	TYR	2.3
1	A	309	VAL	2.3
1	B	266	GLN	2.3
1	C	170	VAL	2.3
1	C	122	ALA	2.3
1	C	136	PHE	2.3
1	C	291	VAL	2.3
1	C	75	LYS	2.3
1	A	385	ASN	2.3
1	A	169	SER	2.3
1	B	45	HIS	2.3
1	C	104	GLU	2.3
1	C	335	ALA	2.2
1	B	316	GLN	2.2
1	C	237	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	65	LYS	2.2
1	C	46	PRO	2.2
1	C	135	PRO	2.2
1	C	215	MET	2.2
1	A	217	CYS	2.2
1	C	112	GLY	2.2
1	C	102	ILE	2.2
1	C	40	VAL	2.2
1	C	239	LYS	2.2
1	B	319	CYS	2.2
1	C	121	LEU	2.1
1	C	201	VAL	2.1
1	C	200	GLU	2.1
1	C	319	CYS	2.1
1	C	43	ALA	2.1
1	C	377	LEU	2.1
1	B	268	VAL	2.1
1	C	85	VAL	2.1
1	C	63	LEU	2.1
1	C	14	TYR	2.1
1	C	24	PRO	2.1
1	C	35	SER	2.1
1	C	107	LYS	2.0
1	C	217	CYS	2.0
2	Y	2	VAL	2.0
2	Z	2	VAL	2.0
1	B	254	THR	2.0
1	B	359	CYS	2.0
1	C	118	ILE	2.0

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

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	24M	Z	4	15/16	0.86	0.15	53,58,65,67	0
2	24M	Y	4	15/16	0.89	0.13	45,48,52,54	0
2	24M	X	4	15/16	0.94	0.08	24,28,32,32	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.