



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:57 AM UTC

PDB ID : 1SGZ / pdb_00001sgz
Title : Crystal Structure of Unbound Beta-Secretase Catalytic Domain.
Authors : Hong, L.; Tang, J.
Deposited on : 2004-02-24
Resolution : 2.00 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
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

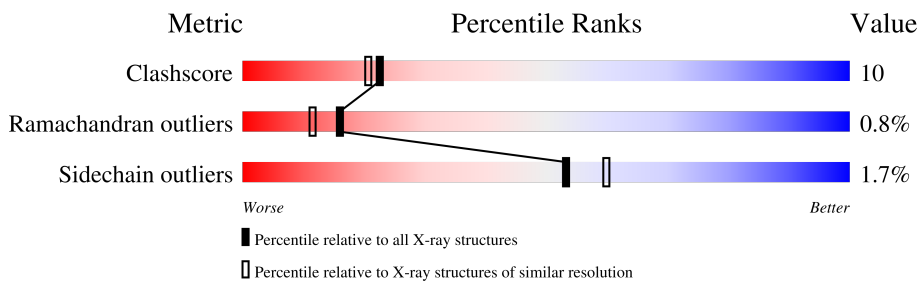
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

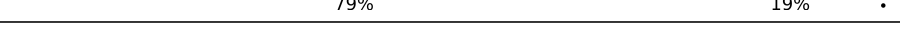
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	389	 78% 19% . .
1	B	389	 79% 17% .
1	C	389	 81% 16% .
1	D	389	 79% 19% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13122 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	389	Total	C	N	O	S	0	0	0
			3053	1953	507	579	14			
1	B	389	Total	C	N	O	S	0	0	0
			3053	1953	507	579	14			
1	C	389	Total	C	N	O	S	0	0	0
			3053	1953	507	579	14			
1	D	389	Total	C	N	O	S	0	0	0
			3053	1953	507	579	14			

- Molecule 2 is water.

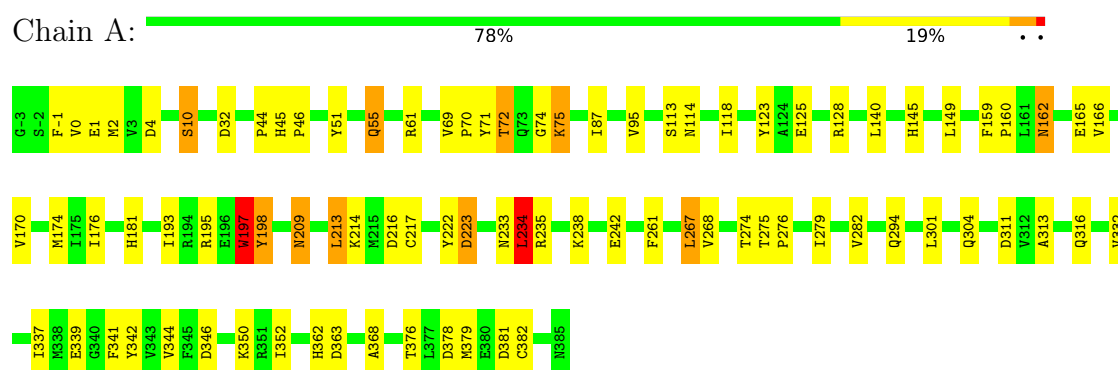
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	234	Total	O	0	0
			234	234		
2	B	242	Total	O	0	0
			242	242		
2	C	228	Total	O	0	0
			228	228		
2	D	206	Total	O	0	0
			206	206		

3 Residue-property plots

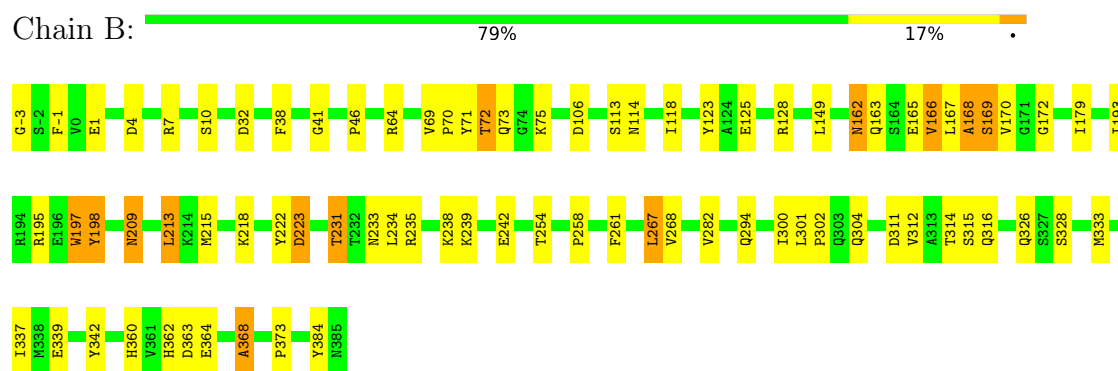
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

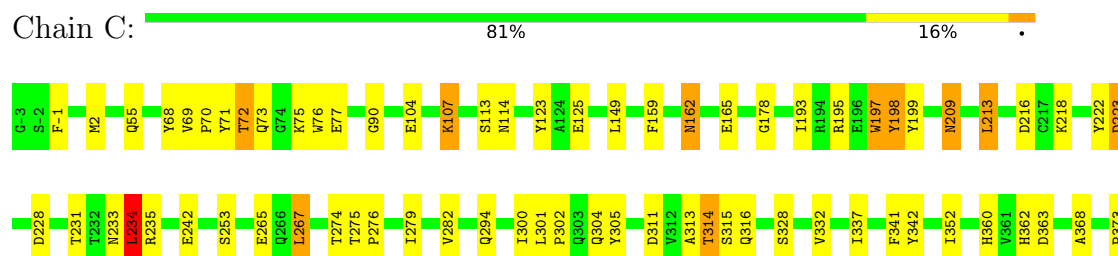
• Molecule 1: Beta-secretase

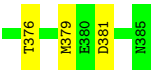


• Molecule 1: Beta-secretase

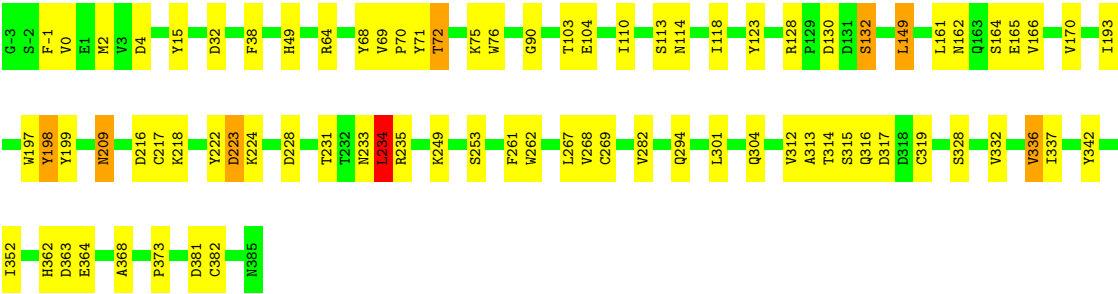
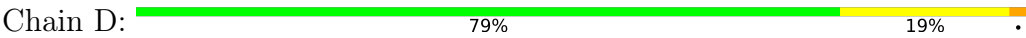


• Molecule 1: Beta-secretase





● Molecule 1: Beta-secretase



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	86.16Å 130.81Å 88.65Å 90.00° 97.27° 90.00°	Depositor
Resolution (Å)	42.70 – 2.00	Depositor
% Data completeness (in resolution range)	94.6 (42.70-2.00)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.196 , 0.228	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13122	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	0.53	0/3131	1.03	17/4256 (0.4%)
1	B	0.54	1/3131 (0.0%)	1.01	14/4256 (0.3%)
1	C	0.51	0/3131	1.02	15/4256 (0.4%)
1	D	0.49	0/3131	1.01	12/4256 (0.3%)
All	All	0.52	1/12524 (0.0%)	1.01	58/17024 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	333	MET	SD-CE	-6.42	1.63	1.79

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	198	TYR	N-CA-C	-9.58	96.70	110.59
1	C	234	LEU	N-CA-C	-9.14	94.43	108.96
1	B	233	ASN	N-CA-C	9.01	122.16	110.53
1	D	234	LEU	N-CA-C	-9.00	94.64	108.96
1	A	233	ASN	N-CA-C	8.85	121.95	110.53
1	A	234	LEU	N-CA-C	-8.13	96.03	108.96
1	B	198	TYR	N-CA-C	-7.96	98.03	110.36
1	D	316	GLN	N-CA-C	-7.80	103.76	113.28
1	B	234	LEU	N-CA-C	-7.79	96.57	108.96
1	A	198	TYR	N-CA-C	-7.71	98.40	110.36
1	C	233	ASN	N-CA-C	7.70	121.75	110.59
1	A	342	TYR	N-CA-C	-7.69	96.70	109.46
1	C	198	TYR	N-CA-C	-7.49	98.75	110.36
1	D	233	ASN	N-CA-C	7.24	119.86	110.53
1	D	123	TYR	N-CA-C	7.20	120.27	110.55
1	D	342	TYR	N-CA-C	-7.14	97.08	108.73
1	B	123	TYR	N-CA-C	7.06	120.08	110.55
1	B	193	ILE	N-CA-C	-7.03	98.14	108.54
1	A	193	ILE	N-CA-C	-6.68	98.65	108.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	341	PHE	N-CA-C	6.66	119.30	109.24
1	D	328	SER	N-CA-C	-6.42	104.69	113.30
1	C	342	TYR	N-CA-C	-6.27	98.50	108.73
1	B	342	TYR	N-CA-C	-6.22	98.60	108.73
1	C	123	TYR	N-CA-C	6.21	118.93	110.55
1	A	123	TYR	N-CA-C	6.12	118.82	110.55
1	B	213	LEU	N-CA-C	-6.08	105.12	112.54
1	D	253	SER	N-CA-C	5.98	120.18	113.01
1	A	10	SER	N-CA-C	5.97	117.79	111.28
1	A	316	GLN	N-CA-C	-5.90	106.00	112.72
1	D	368	ALA	N-CA-C	-5.81	103.26	110.41
1	C	328	SER	N-CA-C	-5.80	105.53	113.30
1	C	213	LEU	N-CA-C	-5.72	105.56	112.54
1	A	368	ALA	N-CA-C	-5.68	102.99	110.43
1	B	328	SER	N-CA-C	-5.62	105.77	113.30
1	C	197	TRP	N-CA-C	-5.56	98.96	110.80
1	D	216	ASP	N-CA-C	-5.56	101.81	110.10
1	A	341	PHE	N-CA-C	5.44	117.46	109.24
1	B	197	TRP	N-CA-C	-5.43	99.22	110.80
1	C	253	SER	N-CA-C	5.39	119.34	112.87
1	A	214	LYS	N-CA-C	5.37	118.84	111.54
1	D	38	PHE	N-CA-C	-5.29	99.16	108.20
1	A	197	TRP	N-CA-C	-5.23	99.66	110.80
1	A	216	ASP	N-CA-C	-5.21	102.19	109.96
1	A	87	ILE	CA-C-N	5.21	126.35	119.84
1	A	87	ILE	C-N-CA	5.21	126.35	119.84
1	C	314	THR	N-CA-C	-5.21	106.52	112.92
1	C	216	ASP	N-CA-C	-5.18	102.38	110.10
1	B	368	ALA	N-CA-C	-5.16	104.07	110.41
1	B	38	PHE	N-CA-C	-5.15	100.34	108.73
1	C	316	GLN	N-CA-C	-5.08	106.83	112.57
1	C	305	TYR	N-CA-C	5.08	119.35	113.20
1	B	41	GLY	N-CA-C	-5.07	105.43	111.36
1	A	213	LEU	N-CA-C	-5.04	106.39	112.54
1	B	302	PRO	N-CA-C	-5.04	107.30	113.84
1	B	316	GLN	N-CA-C	-5.03	106.39	112.88
1	D	193	ILE	N-CA-C	-5.03	99.88	107.73
1	A	181	HIS	N-CA-C	5.02	118.50	112.38
1	C	193	ILE	N-CA-C	-5.00	100.42	107.98

There are no chirality outliers.

There are no planarity outliers.

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	3053	0	2968	64	0
1	B	3053	0	2968	66	0
1	C	3053	0	2968	54	0
1	D	3053	0	2968	63	0
2	A	234	0	0	8	0
2	B	242	0	0	11	0
2	C	228	0	0	2	0
2	D	206	0	0	4	0
All	All	13122	0	11872	240	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 10.

All (240) 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:70:PRO:HA	1:B:75:LYS:HB3	1.43	1.00
1:B:162:ASN:ND2	1:B:165:GLU:H	1.70	0.89
1:D:267:LEU:H	1:D:267:LEU:HD23	1.39	0.86
1:C:70:PRO:HA	1:C:75:LYS:HB3	1.59	0.84
1:D:110:ILE:HB	1:D:113:SER:HB3	1.60	0.83
1:C:162:ASN:ND2	1:C:165:GLU:H	1.75	0.83
1:C:235:ARG:HG3	1:C:332:VAL:HB	1.58	0.83
1:C:162:ASN:C	1:C:162:ASN:HD22	1.86	0.83
1:D:130:ASP:OD2	1:D:132:SER:HB3	1.81	0.80
1:A:162:ASN:C	1:A:162:ASN:HD22	1.90	0.78
1:D:70:PRO:HA	1:D:75:LYS:HB3	1.64	0.78
1:B:162:ASN:O	1:B:166:VAL:HG23	1.83	0.76
1:A:162:ASN:ND2	1:A:165:GLU:H	1.84	0.76
1:C:73:GLN:O	1:C:107:LYS:HD3	1.87	0.74
1:A:235:ARG:HG3	1:A:332:VAL:HB	1.69	0.73
1:C:162:ASN:HD22	1:C:165:GLU:H	1.37	0.72
1:D:267:LEU:H	1:D:267:LEU:CD2	2.04	0.71
1:B:162:ASN:HD21	1:B:165:GLU:H	1.38	0.71
1:A:70:PRO:HA	1:A:75:LYS:HB3	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:301:LEU:H	1:D:304:GLN:HE21	1.39	0.70
1:D:69:VAL:HA	1:D:128:ARG:HH12	1.55	0.70
1:A:301:LEU:H	1:A:304:GLN:NE2	1.90	0.70
1:A:125:GLU:OE2	1:A:195:ARG:NH1	2.25	0.69
1:B:222:TYR:O	1:B:223:ASP:HB3	1.93	0.69
1:B:162:ASN:C	1:B:162:ASN:HD22	2.01	0.68
1:D:4:ASP:OD2	1:D:170:VAL:HG11	1.93	0.68
1:C:311:ASP:OD2	1:C:315:SER:HB2	1.95	0.67
1:A:301:LEU:H	1:A:304:GLN:HE21	1.40	0.67
1:C:113:SER:O	1:C:114:ASN:HB2	1.95	0.67
1:D:162:ASN:O	1:D:166:VAL:HG23	1.95	0.66
1:A:145:HIS:CE1	1:B:311:ASP:OD2	2.50	0.64
1:D:301:LEU:H	1:D:304:GLN:NE2	1.96	0.64
1:C:162:ASN:ND2	1:C:165:GLU:N	2.46	0.64
1:D:32:ASP:OD2	1:D:118:ILE:HD11	1.98	0.64
1:A:234:LEU:HG	1:A:337:ILE:HD11	1.82	0.62
1:D:69:VAL:HA	1:D:128:ARG:NH1	2.13	0.62
1:B:167:LEU:O	1:B:169:SER:N	2.32	0.62
1:A:145:HIS:HE1	1:B:311:ASP:OD2	1.83	0.61
1:C:55:GLN:NE2	2:C:503:HOH:O	2.33	0.61
1:A:209:ASN:HD22	1:A:282:VAL:HG22	1.65	0.61
1:D:312:VAL:HG23	1:D:313:ALA:H	1.64	0.60
1:D:4:ASP:CG	1:D:170:VAL:HG11	2.26	0.60
1:B:7:ARG:HD3	1:B:169:SER:OG	2.01	0.60
1:C:301:LEU:H	1:C:304:GLN:HE21	1.50	0.60
1:D:267:LEU:HD23	1:D:267:LEU:N	2.14	0.60
1:A:71:TYR:CE2	1:A:75:LYS:HA	2.38	0.59
1:B:64:ARG:HD2	2:B:568:HOH:O	2.02	0.59
1:C:162:ASN:ND2	1:C:162:ASN:C	2.58	0.59
1:C:267:LEU:HD23	1:C:267:LEU:H	1.68	0.59
1:B:71:TYR:CE2	1:B:75:LYS:HA	2.38	0.59
1:B:362:HIS:HD2	1:B:363:ASP:O	1.86	0.59
1:D:2:MET:HG2	1:D:90:GLY:HA2	1.84	0.58
1:C:362:HIS:HD2	1:C:363:ASP:O	1.86	0.58
1:D:312:VAL:HG23	1:D:313:ALA:N	2.17	0.58
1:C:70:PRO:HA	1:C:75:LYS:CB	2.30	0.58
1:D:70:PRO:HA	1:D:75:LYS:CB	2.31	0.58
1:B:197:TRP:CG	1:B:198:TYR:H	2.22	0.58
1:B:70:PRO:HA	1:B:75:LYS:CB	2.28	0.58
1:C:2:MET:HG2	1:C:90:GLY:HA2	1.86	0.57
1:D:315:SER:OG	1:D:317:ASP:HB2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:SER:O	1:B:114:ASN:HB2	2.04	0.57
1:D:0:VAL:HG12	2:D:514:HOH:O	2.04	0.57
1:D:261:PHE:CD1	1:D:268:VAL:HG23	2.39	0.57
1:C:77:GLU:HG2	1:C:104:GLU:HB2	1.85	0.57
1:B:125:GLU:OE2	1:B:195:ARG:NH1	2.38	0.57
1:B:222:TYR:O	1:B:223:ASP:CB	2.53	0.57
1:B:7:ARG:HG2	1:B:169:SER:HA	1.86	0.57
1:B:231:THR:HG22	2:B:409:HOH:O	2.04	0.57
1:C:73:GLN:HG2	1:C:107:LYS:HE3	1.87	0.56
1:C:234:LEU:HG	1:C:337:ILE:HD11	1.87	0.56
1:B:69:VAL:HG22	1:B:128:ARG:HG3	1.87	0.56
1:A:162:ASN:C	1:A:162:ASN:ND2	2.63	0.56
1:C:107:LYS:NZ	1:C:107:LYS:HB3	2.20	0.56
1:C:209:ASN:ND2	1:C:282:VAL:H	2.03	0.56
1:D:314:THR:HG22	2:D:467:HOH:O	2.06	0.56
1:A:166:VAL:CG1	2:A:531:HOH:O	2.54	0.55
1:C:267:LEU:HD23	1:C:267:LEU:N	2.22	0.55
1:A:197:TRP:CG	1:A:198:TYR:H	2.25	0.55
1:B:113:SER:OG	2:B:586:HOH:O	2.18	0.54
1:C:301:LEU:H	1:C:304:GLN:NE2	2.05	0.54
1:A:294:GLN:O	1:A:379:MET:HE1	2.07	0.54
1:D:197:TRP:CG	1:D:198:TYR:H	2.26	0.54
1:D:75:LYS:HD2	1:D:75:LYS:C	2.32	0.54
1:D:161:LEU:HB2	1:D:166:VAL:HG22	1.90	0.54
1:C:197:TRP:CG	1:C:198:TYR:H	2.26	0.53
1:D:234:LEU:HG	1:D:337:ILE:HD11	1.89	0.53
1:B:238:LYS:HE2	1:B:242:GLU:OE2	2.08	0.53
1:B:301:LEU:H	1:B:304:GLN:HE21	1.57	0.53
1:D:249:LYS:HE2	1:D:262:TRP:CD1	2.44	0.53
1:A:209:ASN:ND2	1:A:282:VAL:H	2.06	0.53
1:A:311:ASP:C	1:A:313:ALA:N	2.66	0.53
1:C:69:VAL:HG21	1:C:76:TRP:CZ2	2.43	0.53
1:D:15:TYR:OH	1:D:114:ASN:ND2	2.39	0.52
1:B:162:ASN:ND2	1:B:162:ASN:C	2.68	0.52
1:C:222:TYR:O	1:C:223:ASP:CB	2.58	0.52
1:C:294:GLN:O	1:C:379:MET:HE1	2.09	0.52
1:C:360:HIS:HE2	1:C:368:ALA:H	1.58	0.52
1:B:170:VAL:HG12	1:B:170:VAL:O	2.10	0.52
1:A:261:PHE:CD1	1:A:268:VAL:HG23	2.45	0.52
1:A:55:GLN:CD	2:A:477:HOH:O	2.53	0.51
1:A:113:SER:O	1:A:114:ASN:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:218:LYS:HG2	1:C:381:ASP:O	2.10	0.51
1:A:10:SER:HB3	1:A:339:GLU:OE1	2.10	0.51
1:B:106:ASP:CG	1:C:107:LYS:HE2	2.35	0.51
1:C:276:PRO:O	1:C:279:ILE:HG12	2.11	0.51
1:A:222:TYR:O	1:A:223:ASP:CB	2.59	0.51
1:B:46:PRO:HG3	1:C:265:GLU:CD	2.35	0.51
1:D:222:TYR:O	1:D:223:ASP:CB	2.59	0.51
1:A:197:TRP:CD1	1:A:198:TYR:H	2.29	0.51
1:B:1:GLU:HG2	2:B:524:HOH:O	2.10	0.51
1:B:32:ASP:OD2	1:B:118:ILE:HD11	2.11	0.51
1:B:197:TRP:CD1	1:B:198:TYR:H	2.27	0.51
1:B:149:LEU:C	1:B:149:LEU:HD23	2.35	0.51
1:B:301:LEU:H	1:B:304:GLN:NE2	2.09	0.51
1:D:235:ARG:HG3	1:D:332:VAL:HB	1.92	0.50
1:B:364:GLU:HG3	2:B:622:HOH:O	2.11	0.50
1:D:294:GLN:HG3	1:D:373:PRO:HB2	1.94	0.50
1:A:311:ASP:C	1:A:313:ALA:H	2.19	0.50
1:D:149:LEU:C	1:D:149:LEU:HD23	2.37	0.50
1:A:74:GLY:O	1:A:75:LYS:HB3	2.12	0.50
1:C:149:LEU:HD23	1:C:149:LEU:C	2.37	0.50
1:C:71:TYR:CE2	1:C:75:LYS:HA	2.46	0.49
1:C:162:ASN:HD21	1:C:165:GLU:N	2.10	0.49
1:D:64:ARG:NH1	2:D:490:HOH:O	2.45	0.49
1:A:166:VAL:HG12	2:A:531:HOH:O	2.11	0.49
1:D:128:ARG:HG3	1:D:128:ARG:HH11	1.78	0.49
1:D:70:PRO:HD2	1:D:128:ARG:HH12	1.77	0.49
1:D:71:TYR:O	1:D:72:THR:C	2.55	0.49
1:D:69:VAL:O	1:D:75:LYS:HB2	2.12	0.48
1:B:364:GLU:O	1:B:364:GLU:HG2	2.13	0.48
1:C:376:THR:HB	1:C:379:MET:SD	2.54	0.48
1:D:304:GLN:O	1:D:336:VAL:HG13	2.14	0.48
1:A:70:PRO:HA	1:A:75:LYS:CB	2.43	0.48
1:C:68:TYR:CZ	1:C:70:PRO:HB3	2.48	0.48
1:D:128:ARG:NH1	1:D:128:ARG:HG3	2.28	0.48
1:D:362:HIS:HD2	1:D:363:ASP:O	1.96	0.48
1:B:209:ASN:HD22	1:B:282:VAL:HG22	1.78	0.48
1:B:209:ASN:ND2	1:B:282:VAL:H	2.11	0.48
1:D:209:ASN:ND2	1:D:282:VAL:H	2.11	0.48
1:B:326:GLN:HG2	2:B:460:HOH:O	2.13	0.47
1:A:149:LEU:HB2	1:A:346:ASP:HA	1.97	0.47
1:D:-1:PHE:HB3	1:D:2:MET:HE3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:269:CYS:HG	1:D:319:CYS:CB	2.23	0.47
1:B:162:ASN:HD21	1:B:165:GLU:N	2.10	0.47
1:C:242:GLU:HG2	2:C:597:HOH:O	2.15	0.47
1:A:-1:PHE:HB3	1:A:2:MET:HE3	1.97	0.47
1:D:162:ASN:OD1	1:D:165:GLU:CD	2.59	0.46
1:A:159:PHE:HB2	1:A:160:PRO:HD2	1.97	0.46
1:B:71:TYR:O	1:B:72:THR:C	2.58	0.46
1:B:10:SER:HB3	1:B:339:GLU:OE1	2.16	0.46
1:B:261:PHE:CD1	1:B:268:VAL:HG23	2.51	0.46
1:A:71:TYR:O	1:A:72:THR:C	2.59	0.46
1:D:68:TYR:CZ	1:D:70:PRO:HB3	2.50	0.46
1:A:162:ASN:HD22	1:A:165:GLU:H	1.62	0.46
1:B:311:ASP:OD2	1:B:315:SER:OG	2.33	0.46
1:A:267:LEU:HD22	2:A:608:HOH:O	2.15	0.46
1:B:-3:GLY:HA2	1:B:179:ILE:O	2.16	0.46
1:B:168:ALA:O	1:B:169:SER:O	2.34	0.46
1:B:169:SER:HB3	2:B:598:HOH:O	2.14	0.46
1:D:218:LYS:HG3	1:D:381:ASP:O	2.15	0.46
1:B:300:ILE:HD13	1:B:337:ILE:HD12	1.96	0.45
1:B:-1:PHE:N	1:B:-1:PHE:CD1	2.84	0.45
1:B:215:MET:HE1	1:B:239:LYS:HB3	1.99	0.45
1:D:199:TYR:HB3	1:D:352:ILE:HD11	1.99	0.45
1:A:0:VAL:HG12	2:A:583:HOH:O	2.16	0.45
1:C:71:TYR:O	1:C:72:THR:C	2.59	0.45
1:D:228:ASP:OD2	1:D:231:THR:OG1	2.33	0.45
1:A:162:ASN:HD21	1:A:165:GLU:H	1.60	0.45
1:D:69:VAL:HG22	1:D:128:ARG:HG3	1.97	0.45
1:C:222:TYR:O	1:C:223:ASP:HB3	2.17	0.45
1:C:197:TRP:CD1	1:C:198:TYR:H	2.33	0.45
1:D:162:ASN:ND2	1:D:164:SER:HB3	2.31	0.45
1:B:231:THR:HG21	1:B:235:ARG:HD2	1.99	0.45
1:B:384:TYR:HB2	2:B:625:HOH:O	2.17	0.45
1:B:209:ASN:HD22	1:B:209:ASN:HA	1.59	0.44
1:B:314:THR:HG23	1:C:314:THR:HG22	2.00	0.44
1:D:198:TYR:CE2	1:D:224:LYS:HE3	2.52	0.44
1:A:217:CYS:CB	1:A:382:CYS:HG	2.22	0.44
1:D:364:GLU:O	1:D:364:GLU:HG2	2.16	0.44
1:A:213:LEU:HD12	1:A:213:LEU:HA	1.79	0.44
1:B:267:LEU:CD2	1:B:267:LEU:H	2.30	0.44
1:B:300:ILE:HD13	1:B:337:ILE:CD1	2.48	0.44
1:B:360:HIS:HE2	1:B:368:ALA:H	1.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:PRO:HB2	2:B:563:HOH:O	2.17	0.44
1:A:174:MET:HE3	1:A:176:ILE:HD11	1.99	0.44
1:D:209:ASN:HD22	1:D:209:ASN:HA	1.56	0.44
1:A:276:PRO:O	1:A:279:ILE:HG12	2.18	0.43
1:C:274:THR:O	1:C:275:THR:C	2.62	0.43
1:D:209:ASN:HD22	1:D:282:VAL:HG22	1.82	0.43
1:D:222:TYR:O	1:D:223:ASP:HB3	2.19	0.43
1:B:294:GLN:HG2	1:B:373:PRO:HB2	2.00	0.43
1:A:44:PRO:HD3	1:A:51:TYR:CZ	2.54	0.43
1:A:267:LEU:H	1:A:267:LEU:CD2	2.32	0.43
1:C:294:GLN:CG	1:C:373:PRO:HB2	2.49	0.42
1:A:45:HIS:CG	1:A:46:PRO:HD2	2.54	0.42
1:A:311:ASP:OD2	1:A:313:ALA:HB3	2.19	0.42
1:D:103:THR:O	1:D:104:GLU:HG3	2.19	0.42
1:A:32:ASP:OD2	1:A:118:ILE:HD11	2.20	0.42
1:C:300:ILE:HD13	1:C:337:ILE:CD1	2.50	0.42
1:B:4:ASP:HA	1:B:172:GLY:O	2.19	0.42
1:B:213:LEU:HA	1:B:213:LEU:HD12	1.80	0.42
1:A:1:GLU:O	1:A:1:GLU:HG2	2.19	0.42
1:A:166:VAL:HG11	2:A:531:HOH:O	2.17	0.42
1:A:311:ASP:O	1:A:313:ALA:N	2.52	0.42
1:A:362:HIS:HD2	1:A:363:ASP:O	2.01	0.42
1:C:228:ASP:OD2	1:C:231:THR:OG1	2.37	0.42
1:C:-1:PHE:CZ	1:C:178:GLY:HA3	2.54	0.42
1:D:217:CYS:HG	1:D:382:CYS:CB	2.27	0.42
1:A:4:ASP:OD2	1:A:170:VAL:HG11	2.20	0.42
1:A:350:LYS:NZ	2:A:613:HOH:O	2.53	0.42
1:B:163:GLN:HA	1:B:163:GLN:NE2	2.35	0.42
1:B:312:VAL:O	1:C:314:THR:HG23	2.19	0.42
1:C:125:GLU:OE1	1:C:195:ARG:NH1	2.53	0.42
1:A:234:LEU:HG	1:A:337:ILE:CD1	2.49	0.42
1:B:218:LYS:HB3	2:B:625:HOH:O	2.20	0.41
1:A:344:VAL:O	1:A:352:ILE:HA	2.20	0.41
1:D:166:VAL:O	1:D:166:VAL:HG12	2.19	0.41
1:A:274:THR:O	1:A:275:THR:C	2.64	0.41
1:C:301:LEU:HB3	1:C:302:PRO:HD2	2.02	0.41
1:A:45:HIS:ND1	1:A:46:PRO:HD2	2.36	0.41
1:A:238:LYS:HE2	1:A:242:GLU:OE2	2.21	0.41
1:B:197:TRP:CG	1:B:198:TYR:N	2.87	0.41
1:C:199:TYR:HB3	1:C:352:ILE:HD11	2.03	0.41
1:A:235:ARG:CG	1:A:332:VAL:HB	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:71:TYR:CE2	1:D:75:LYS:HA	2.54	0.41
1:C:209:ASN:HD22	1:C:282:VAL:HG22	1.85	0.41
1:D:49:HIS:HB2	2:D:561:HOH:O	2.21	0.41
1:A:376:THR:HB	1:A:379:MET:SD	2.61	0.40
1:D:69:VAL:HG21	1:D:76:TRP:CZ2	2.56	0.40
1:A:69:VAL:HG22	1:A:128:ARG:HG3	2.04	0.40
1:A:95:VAL:HG11	1:A:140:LEU:HD12	2.03	0.40
1:B:73:GLN:HG2	1:B:73:GLN:O	2.21	0.40
1:D:2:MET:CG	1:D:90:GLY:HA2	2.51	0.40
1:A:55:GLN:NE2	2:A:477:HOH:O	2.53	0.40
1:B:254:THR:HG23	2:B:478:HOH:O	2.21	0.40
1:A:74:GLY:O	1:A:75:LYS:CB	2.69	0.40
1:A:378:ASP:O	1:A:381:ASP:HB2	2.21	0.40
1:D:75:LYS:C	1:D:75:LYS:CD	2.93	0.40
1:A:61:ARG:HD3	1:C:159:PHE:CG	2.57	0.40
1:C:107:LYS:HB3	1:C:107:LYS:HZ2	1.85	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	387/389 (100%)	369 (95%)	15 (4%)	3 (1%)	16	11
1	B	387/389 (100%)	369 (95%)	14 (4%)	4 (1%)	12	8
1	C	387/389 (100%)	372 (96%)	12 (3%)	3 (1%)	16	11
1	D	387/389 (100%)	371 (96%)	14 (4%)	2 (0%)	24	21
All	All	1548/1556 (100%)	1481 (96%)	55 (4%)	12 (1%)	16	11

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	223	ASP
1	B	72	THR
1	B	169	SER
1	B	223	ASP
1	C	223	ASP
1	D	72	THR
1	D	223	ASP
1	C	72	THR
1	B	168	ALA
1	C	313	ALA
1	A	75	LYS
1	A	72	THR

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	331/331 (100%)	325 (98%)	6 (2%)	51	58
1	B	331/331 (100%)	326 (98%)	5 (2%)	57	64
1	C	331/331 (100%)	325 (98%)	6 (2%)	51	58
1	D	331/331 (100%)	326 (98%)	5 (2%)	57	64
All	All	1324/1324 (100%)	1302 (98%)	22 (2%)	53	60

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	GLN
1	A	162	ASN
1	A	197	TRP
1	A	209	ASN
1	A	234	LEU
1	A	267	LEU
1	B	162	ASN
1	B	166	VAL
1	B	209	ASN
1	B	231	THR

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Mol	Chain	Res	Type
1	B	267	LEU
1	C	107	LYS
1	C	162	ASN
1	C	209	ASN
1	C	213	LEU
1	C	234	LEU
1	C	267	LEU
1	D	132	SER
1	D	149	LEU
1	D	209	ASN
1	D	234	LEU
1	D	336	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	49	HIS
1	A	55	GLN
1	A	73	GLN
1	A	89	HIS
1	A	111	ASN
1	A	145	HIS
1	A	162	ASN
1	A	209	ASN
1	A	293	ASN
1	A	304	GLN
1	A	362	HIS
1	A	385	ASN
1	B	28	ASN
1	B	73	GLN
1	B	92	ASN
1	B	111	ASN
1	B	114	ASN
1	B	162	ASN
1	B	163	GLN
1	B	209	ASN
1	B	233	ASN
1	B	294	GLN
1	B	304	GLN
1	B	362	HIS
1	B	385	ASN

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Mol	Chain	Res	Type
1	C	28	ASN
1	C	55	GLN
1	C	73	GLN
1	C	111	ASN
1	C	114	ASN
1	C	162	ASN
1	C	209	ASN
1	C	266	GLN
1	C	304	GLN
1	C	362	HIS
1	C	385	ASN
1	D	28	ASN
1	D	89	HIS
1	D	111	ASN
1	D	114	ASN
1	D	181	HIS
1	D	209	ASN
1	D	304	GLN
1	D	362	HIS

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 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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.