



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:07 PM UTC

PDB ID : 1I4E / pdb_00001i4e
Title : CRYSTAL STRUCTURE OF THE CASPASE-8/P35 COMPLEX
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Deposited on : 2001-02-20
Resolution : 3.00 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

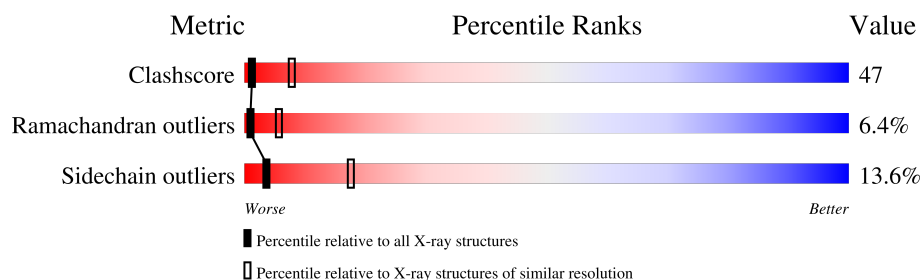
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)

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	299	
2	B	258	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4354 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 Early 35 kDa protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	294	Total	C	N	O	S	0	0	0
			2409	1543	393	462	11			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ACE	-	acetylation	UNP P08160

- Molecule 2 is a protein called Caspase-8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	243	Total	C	N	O	S	0	0	0
			1945	1228	333	368	16			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	2285	HIS	ASP	SEE REMARK 999	UNP Q14790

4 Data and refinement statistics

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	99.97Å 117.34Å 346.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.00 – 3.00	Depositor
% Data completeness (in resolution range)	99.1 (24.00-3.00)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.236 , 0.296	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4354	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.51	0/2455	0.97	14/3309 (0.4%)
2	B	0.46	0/1987	0.96	5/2682 (0.2%)
All	All	0.48	0/4442	0.97	19/5991 (0.3%)

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	158	GLY	N-CA-C	-8.12	104.81	114.48
1	A	119	LEU	N-CA-C	-6.68	105.00	113.01
2	B	2223	ASP	N-CA-C	6.65	116.64	107.73
1	A	121	SER	N-CA-C	6.57	120.61	111.74
2	B	2357	ILE	N-CA-C	6.24	116.64	106.72
1	A	125	THR	N-CA-C	-6.18	105.74	113.28
1	A	110	VAL	CB-CA-C	-6.00	104.05	112.14
2	B	2282	LYS	CA-C-N	5.66	125.61	119.78
2	B	2282	LYS	C-N-CA	5.66	125.61	119.78
1	A	283	HIS	N-CA-C	5.42	117.53	107.99
1	A	264	ILE	N-CA-C	5.37	115.09	108.53
1	A	95	TYR	N-CA-C	5.27	117.33	110.43
1	A	113	SER	N-CA-C	5.22	116.97	111.28
1	A	180	VAL	CA-C-N	5.21	126.35	119.84
1	A	180	VAL	C-N-CA	5.21	126.35	119.84
1	A	133	TYR	N-CA-C	5.17	119.06	112.34
1	A	3	VAL	N-CA-C	5.13	120.01	109.34
1	A	120	LYS	N-CA-C	-5.09	107.04	113.20
2	B	2256	SER	N-CA-C	-5.01	107.66	112.97

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	2409	0	2394	236	0
2	B	1945	0	1914	178	0
All	All	4354	0	4308	411	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 47.

All (411) 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:A:38:GLN:HA	1:A:160:GLU:HG3	1.37	1.04
2:B:2231:LYS:HB2	2:B:2232:PRO:HD3	1.40	1.04
2:B:2413:ARG:HG3	2:B:2419:THR:HG22	1.36	1.03
1:A:33:LYS:H	1:A:33:LYS:HD2	1.23	1.02
1:A:99:GLU:HG3	1:A:100:HIS:H	1.23	0.97
2:B:2339:GLN:HE21	2:B:2344:LYS:HZ2	1.07	0.94
1:A:60:ASN:HD21	1:A:62:ASN:HD22	1.16	0.90
1:A:200:VAL:HG22	1:A:278:LEU:HB3	1.52	0.89
2:B:2291:GLN:O	2:B:2295:ILE:HG13	1.73	0.88
2:B:2224:LYS:HG3	2:B:2472:LYS:HD3	1.56	0.87
1:A:13:GLN:HG3	1:A:14:THR:H	1.40	0.87
1:A:39:LEU:HD22	1:A:39:LEU:H	1.38	0.87
2:B:2439:ILE:HD11	2:B:2476:PHE:CE2	2.09	0.86
1:A:60:ASN:HD21	1:A:62:ASN:ND2	1.72	0.86
2:B:2339:GLN:HE21	2:B:2344:LYS:NZ	1.74	0.85
1:A:204:GLN:HE21	1:A:205:PHE:H	1.22	0.83
2:B:2425:LEU:O	2:B:2429:LEU:HB2	1.77	0.83
1:A:60:ASN:ND2	1:A:62:ASN:HD22	1.77	0.83
1:A:214:VAL:HG21	1:A:242:ILE:HG22	1.60	0.83
2:B:2447:ASN:HB3	2:B:2463:MET:HE1	1.58	0.82
1:A:99:GLU:HG3	1:A:100:HIS:N	1.94	0.82
2:B:2266:ASP:HB3	2:B:2422:ILE:HG21	1.62	0.81
1:A:53:ILE:O	1:A:94:LYS:HE3	1.81	0.81
1:A:227:GLU:HB2	1:A:246:LEU:HD21	1.62	0.80
1:A:44:LEU:HD23	1:A:45:MET:N	1.96	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2398:ASP:HA	2:B:2470:LEU:HD23	1.62	0.80
1:A:237:LYS:HG2	1:A:238:ASN:H	1.44	0.80
2:B:2414:ASN:HD22	2:B:2417:GLU:H	1.30	0.79
1:A:38:GLN:HA	1:A:160:GLU:CG	2.13	0.79
2:B:2251:VAL:HG13	2:B:2254:LEU:HB2	1.65	0.79
1:A:237:LYS:CG	1:A:238:ASN:H	1.96	0.78
2:B:2260:ARG:NH2	2:B:2263:THR:HG23	1.98	0.78
2:B:2289:VAL:HG23	2:B:2327:ASP:OD1	1.82	0.78
1:A:35:MET:HE2	1:A:167:LEU:HD12	1.64	0.78
1:A:104:SER:HB2	1:A:120:LYS:HD2	1.67	0.77
1:A:118:ILE:HG12	1:A:122:HIS:HB3	1.66	0.77
1:A:106:GLN:H	1:A:106:GLN:NE2	1.83	0.77
1:A:225:ASN:HD22	1:A:225:ASN:H	1.31	0.77
1:A:60:ASN:ND2	1:A:62:ASN:HB2	2.00	0.76
1:A:118:ILE:HG23	1:A:118:ILE:O	1.85	0.76
1:A:195:ASP:OD1	1:A:283:HIS:HD2	1.69	0.76
1:A:125:THR:HB	1:A:129:SER:HB3	1.68	0.75
1:A:181:PRO:HA	1:A:292:ASN:OD1	1.87	0.74
2:B:2228:MET:HE3	2:B:2233:ARG:HD2	1.69	0.74
1:A:60:ASN:HD22	1:A:62:ASN:HB2	1.51	0.73
2:B:2431:GLU:O	2:B:2434:PRO:HD2	1.87	0.73
1:A:134:GLU:N	1:A:134:GLU:OE1	2.22	0.72
1:A:71:VAL:HG22	1:A:279:TYR:HD2	1.54	0.72
1:A:225:ASN:H	1:A:225:ASN:ND2	1.86	0.72
1:A:104:SER:CB	1:A:120:LYS:HD2	2.20	0.72
1:A:61:ASN:HD21	1:A:165:GLN:CG	2.02	0.71
1:A:39:LEU:HD22	1:A:39:LEU:N	2.05	0.71
1:A:237:LYS:HG2	1:A:238:ASN:N	2.04	0.71
1:A:77:GLN:HE22	1:A:239:LYS:NZ	1.89	0.71
1:A:145:ARG:O	1:A:147:ASP:N	2.24	0.71
1:A:60:ASN:HA	1:A:164:ASN:ND2	2.05	0.71
1:A:35:MET:CE	1:A:167:LEU:HD12	2.20	0.71
2:B:2400:LEU:HD21	2:B:2439:ILE:HG21	1.73	0.71
1:A:97:LYS:HB2	1:A:97:LYS:NZ	2.04	0.71
2:B:2394:PRO:HG2	2:B:2397:ALA:HB2	1.73	0.71
2:B:2314:ILE:HG21	2:B:2323:ILE:HG21	1.72	0.71
2:B:2271:THR:HG22	2:B:2281:ILE:HG21	1.72	0.70
2:B:2289:VAL:HG13	2:B:2331:ALA:HB2	1.74	0.70
2:B:2294:GLU:O	2:B:2298:ILE:HG13	1.92	0.70
1:A:33:LYS:H	1:A:33:LYS:CD	1.96	0.69
2:B:2304:HIS:H	2:B:2347:SER:HB3	1.56	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:ILE:N	1:A:179:ILE:HD12	2.07	0.69
2:B:2251:VAL:CG2	2:B:2254:LEU:HD13	2.23	0.69
1:A:34:ILE:HD12	1:A:34:ILE:H	1.56	0.69
1:A:211:GLU:O	1:A:215:GLN:HB2	1.93	0.69
1:A:217:LEU:HB3	1:A:285:VAL:HG21	1.73	0.69
2:B:2274:PHE:O	2:B:2279:PHE:HB2	1.93	0.69
2:B:2270:LEU:HD23	2:B:2426:CYS:SG	2.33	0.68
1:A:38:GLN:CA	1:A:160:GLU:HG3	2.20	0.68
1:A:204:GLN:HE21	1:A:205:PHE:N	1.90	0.68
1:A:98:ASP:OD1	1:A:99:GLU:N	2.27	0.68
2:B:2270:LEU:HD11	2:B:2422:ILE:HD12	1.76	0.68
1:A:87:ASP:OD1	2:B:2260:ARG:HD2	1.94	0.68
2:B:2413:ARG:HG3	2:B:2419:THR:CG2	2.20	0.68
1:A:16:ILE:HD11	1:A:182:PHE:HE1	1.59	0.67
1:A:122:HIS:CE1	1:A:125:THR:HG21	2.30	0.66
1:A:125:THR:HB	1:A:129:SER:CB	2.25	0.66
2:B:2372:GLU:O	2:B:2373:THR:HG23	1.95	0.66
1:A:130:ILE:O	1:A:134:GLU:OE1	2.13	0.66
1:A:125:THR:O	1:A:129:SER:HB3	1.96	0.66
2:B:2253:LYS:HG3	2:B:2254:LEU:HD12	1.76	0.66
1:A:241:MET:HG2	1:A:270:ILE:HG23	1.78	0.66
1:A:237:LYS:CG	1:A:238:ASN:N	2.60	0.65
2:B:2338:SER:O	2:B:2341:THR:HG23	1.97	0.65
1:A:93:ILE:HG13	1:A:93:ILE:O	1.95	0.65
1:A:108:GLY:HA2	1:A:150:VAL:HG23	1.79	0.65
1:A:145:ARG:C	1:A:147:ASP:H	2.05	0.65
2:B:2241:ASN:HD22	2:B:2316:SER:CB	2.09	0.65
2:B:2227:GLN:O	2:B:2308:ASP:HB3	1.96	0.64
2:B:2323:ILE:HD11	2:B:2357:ILE:CG2	2.27	0.64
2:B:2413:ARG:CG	2:B:2419:THR:HG22	2.20	0.64
1:A:61:ASN:HD21	1:A:165:GLN:HG2	1.62	0.64
1:A:127:LYS:O	1:A:131:GLU:HB2	1.97	0.64
2:B:2299:TYR:HA	2:B:2302:MET:HE3	1.79	0.64
1:A:115:PHE:CE1	1:A:138:LEU:HD13	2.33	0.64
1:A:17:ARG:HG3	1:A:199:TYR:HD1	1.62	0.64
2:B:2266:ASP:OD1	2:B:2419:THR:HG23	1.96	0.64
1:A:236:SER:HB3	1:A:237:LYS:NZ	2.14	0.63
1:A:61:ASN:OD1	1:A:164:ASN:N	2.31	0.63
1:A:118:ILE:HG13	1:A:122:HIS:H	1.63	0.63
2:B:2288:THR:HG22	2:B:2326:THR:HB	1.79	0.63
1:A:33:LYS:HD2	1:A:33:LYS:N	2.05	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2371:VAL:HG22	2:B:2373:THR:OG1	1.98	0.62
2:B:2407:ASN:O	2:B:2408:ASN:HB2	1.99	0.62
1:A:249:THR:HG21	1:A:259:LYS:HE2	1.81	0.62
2:B:2251:VAL:HG21	2:B:2254:LEU:HD13	1.79	0.62
2:B:2253:LYS:HG3	2:B:2254:LEU:CD1	2.29	0.62
1:A:93:ILE:O	1:A:94:LYS:HB2	1.97	0.62
1:A:108:GLY:H	1:A:149:TYR:HA	1.65	0.62
1:A:179:ILE:HG13	1:A:294:ILE:HG13	1.83	0.61
1:A:207:GLY:O	1:A:211:GLU:HG3	2.00	0.61
2:B:2323:ILE:HD11	2:B:2357:ILE:HD13	1.80	0.61
2:B:2439:ILE:HD11	2:B:2476:PHE:HE2	1.60	0.61
2:B:2298:ILE:C	2:B:2300:GLN:H	2.08	0.61
2:B:2260:ARG:HD3	2:B:2317:HIS:HD2	1.65	0.61
2:B:2447:ASN:ND2	2:B:2464:PRO:HB2	2.16	0.61
2:B:2414:ASN:ND2	2:B:2417:GLU:H	1.98	0.61
1:A:59:LYS:O	1:A:164:ASN:HA	2.01	0.61
1:A:241:MET:CG	1:A:270:ILE:HG23	2.31	0.61
1:A:35:MET:HG2	1:A:155:LEU:HD21	1.83	0.61
1:A:77:GLN:HE22	1:A:239:LYS:HZ3	1.50	0.60
1:A:114:LYS:O	1:A:117:LYS:HD3	2.02	0.60
1:A:185:GLU:O	1:A:186:ILE:C	2.43	0.60
2:B:2281:ILE:HG22	2:B:2283:PRO:HD3	1.82	0.60
2:B:2332:PRO:HB2	2:B:2335:GLU:HG3	1.84	0.60
2:B:2323:ILE:HD11	2:B:2357:ILE:HG21	1.82	0.60
1:A:130:ILE:HD12	1:A:131:GLU:N	2.16	0.60
2:B:2260:ARG:HH21	2:B:2263:THR:HG23	1.67	0.60
2:B:2432:ARG:HG3	2:B:2432:ARG:HH11	1.65	0.60
2:B:2246:LYS:HD3	2:B:2250:LYS:HE3	1.84	0.60
1:A:87:ASP:HB3	2:B:2317:HIS:HA	1.84	0.59
1:A:178:VAL:C	1:A:179:ILE:HD12	2.27	0.59
2:B:2231:LYS:HB2	2:B:2232:PRO:CD	2.22	0.59
2:B:2406:VAL:HG13	2:B:2463:MET:O	2.02	0.59
2:B:2339:GLN:NE2	2:B:2344:LYS:HZ2	1.88	0.58
1:A:13:GLN:CG	1:A:14:THR:H	2.10	0.58
1:A:214:VAL:HG12	1:A:244:LYS:HG3	1.85	0.58
2:B:2357:ILE:HB	2:B:2403:MET:CE	2.33	0.58
1:A:179:ILE:HG22	1:A:179:ILE:O	2.03	0.58
2:B:2339:GLN:NE2	2:B:2344:LYS:NZ	2.50	0.58
1:A:43:VAL:HG12	1:A:155:LEU:O	2.02	0.58
2:B:2357:ILE:HB	2:B:2403:MET:HE1	1.85	0.58
2:B:2322:ILE:C	2:B:2322:ILE:HD12	2.29	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:ASN:HB3	1:A:110:VAL:HG23	1.86	0.57
2:B:2357:ILE:HD12	2:B:2403:MET:HE1	1.86	0.57
2:B:2306:ASN:O	2:B:2307:MET:HE2	2.04	0.57
1:A:8:GLU:O	1:A:11:VAL:HG12	2.04	0.57
1:A:74:GLN:O	1:A:77:GLN:HG3	2.05	0.57
1:A:24:GLN:H	1:A:24:GLN:NE2	2.03	0.57
2:B:2226:TYR:CE1	2:B:2472:LYS:HG3	2.40	0.57
2:B:2270:LEU:HD13	2:B:2313:CYS:SG	2.44	0.57
1:A:115:PHE:HE1	1:A:138:LEU:HD13	1.68	0.57
2:B:2248:ARG:HD3	2:B:2257:ILE:O	2.05	0.57
2:B:2343:LEU:HG	2:B:2395:ASP:OD1	2.04	0.56
2:B:2229:LYS:O	2:B:2230:SER:C	2.49	0.56
2:B:2237:LEU:HD21	2:B:2299:TYR:CD2	2.40	0.56
2:B:2251:VAL:HG11	2:B:2254:LEU:HD22	1.87	0.56
1:A:75:PHE:CZ	1:A:270:ILE:HG13	2.40	0.56
1:A:61:ASN:HD21	1:A:165:GLN:HG3	1.67	0.56
2:B:2250:LYS:O	2:B:2252:PRO:HD3	2.06	0.56
2:B:2366:GLN:NE2	2:B:2409:CYS:SG	2.79	0.56
1:A:102:SER:HB3	1:A:120:LYS:NZ	2.21	0.56
2:B:2241:ASN:HD22	2:B:2316:SER:HB2	1.71	0.56
1:A:21:VAL:HB	1:A:25:THR:HG22	1.87	0.55
1:A:237:LYS:HD2	1:A:237:LYS:N	2.21	0.55
2:B:2260:ARG:HH21	2:B:2263:THR:CG2	2.19	0.55
1:A:127:LYS:HA	1:A:130:ILE:HG13	1.89	0.55
2:B:2248:ARG:HG3	2:B:2257:ILE:HG22	1.89	0.55
1:A:134:GLU:O	1:A:139:PRO:HD3	2.06	0.55
2:B:2248:ARG:NH2	2:B:2259:ASP:OD1	2.39	0.55
1:A:176:ASN:N	1:A:176:ASN:HD22	2.03	0.55
1:A:53:ILE:HD12	1:A:169:PHE:HB3	1.88	0.55
1:A:106:GLN:NE2	1:A:106:GLN:N	2.54	0.55
1:A:43:VAL:CG1	1:A:155:LEU:HB2	2.36	0.55
1:A:164:ASN:N	1:A:164:ASN:HD22	2.04	0.55
1:A:195:ASP:OD1	1:A:283:HIS:CD2	2.55	0.54
2:B:2445:GLU:O	2:B:2448:TYR:HB3	2.06	0.54
1:A:107:ASN:O	1:A:110:VAL:HG23	2.07	0.54
1:A:4:ILE:C	1:A:6:PRO:HD2	2.32	0.54
2:B:2248:ARG:HG2	2:B:2255:HIS:O	2.08	0.54
1:A:95:TYR:CZ	1:A:120:LYS:HG2	2.42	0.54
1:A:106:GLN:N	1:A:106:GLN:CD	2.66	0.54
2:B:2248:ARG:HA	2:B:2254:LEU:O	2.08	0.54
1:A:5:PHE:N	1:A:6:PRO:CD	2.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:SER:HB3	1:A:33:LYS:HA	1.89	0.53
1:A:239:LYS:HB3	1:A:241:MET:HE2	1.90	0.53
2:B:2224:LYS:CG	2:B:2472:LYS:HD3	2.34	0.53
1:A:237:LYS:CD	1:A:238:ASN:H	2.21	0.53
1:A:71:VAL:HG22	1:A:279:TYR:CD2	2.38	0.53
1:A:50:SER:OG	1:A:178:VAL:HA	2.08	0.53
1:A:60:ASN:ND2	1:A:62:ASN:H	2.06	0.53
1:A:250:THR:HG22	1:A:260:TYR:HD1	1.73	0.53
1:A:118:ILE:O	1:A:118:ILE:CG2	2.53	0.53
2:B:2450:VAL:HG11	2:B:2464:PRO:HD3	1.90	0.53
1:A:50:SER:CB	1:A:177:LYS:O	2.56	0.53
1:A:100:HIS:O	1:A:156:LYS:HB2	2.09	0.53
2:B:2236:CYS:HB3	2:B:2281:ILE:HD13	1.91	0.53
2:B:2243:ASN:O	2:B:2326:THR:HG23	2.08	0.53
2:B:2433:CYS:N	2:B:2434:PRO:CD	2.72	0.53
1:A:50:SER:HB3	1:A:177:LYS:O	2.08	0.52
2:B:2412:TYR:N	2:B:2462:GLN:OE1	2.42	0.52
2:B:2290:GLU:O	2:B:2294:GLU:HG3	2.08	0.52
2:B:2450:VAL:CG1	2:B:2462:GLN:HB3	2.39	0.52
1:A:253:SER:HB2	2:B:2417:GLU:OE2	2.10	0.52
2:B:2240:ASN:OD1	2:B:2263:THR:HG22	2.09	0.52
1:A:201:ASP:OD2	1:A:201:ASP:C	2.53	0.52
2:B:2320:LYS:O	2:B:2322:ILE:HG23	2.09	0.52
2:B:2239:ILE:HD13	2:B:2292:ILE:HG12	1.91	0.52
2:B:2260:ARG:O	2:B:2263:THR:OG1	2.28	0.52
2:B:2228:MET:HE2	2:B:2476:PHE:HD1	1.74	0.52
1:A:53:ILE:HD13	1:A:171:TYR:HB3	1.92	0.51
1:A:176:ASN:N	1:A:176:ASN:ND2	2.58	0.51
1:A:44:LEU:HD23	1:A:44:LEU:C	2.35	0.51
2:B:2276:GLU:O	2:B:2478:SER:HB2	2.11	0.51
2:B:2284:HIS:O	2:B:2285:HIS:O	2.29	0.51
2:B:2265:LEU:O	2:B:2269:ALA:HB2	2.11	0.51
2:B:2399:PHE:O	2:B:2468:PHE:HA	2.10	0.51
2:B:2458:ASN:C	2:B:2459:MET:HG3	2.35	0.51
1:A:264:ILE:HG13	1:A:265:PHE:CD2	2.46	0.51
1:A:107:ASN:O	1:A:108:GLY:C	2.54	0.51
2:B:2431:GLU:C	2:B:2431:GLU:CD	2.79	0.51
1:A:71:VAL:HG11	1:A:197:VAL:CG1	2.41	0.51
2:B:2251:VAL:HG22	2:B:2254:LEU:HD13	1.93	0.51
1:A:47:PHE:CE1	1:A:151:ALA:HB3	2.45	0.51
1:A:4:ILE:HG22	1:A:4:ILE:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:GLN:O	1:A:33:LYS:HE2	2.11	0.50
1:A:16:ILE:HD11	1:A:182:PHE:CE1	2.44	0.50
1:A:200:VAL:CG2	1:A:278:LEU:HB3	2.34	0.50
2:B:2391:ARG:H	2:B:2391:ARG:HD3	1.77	0.50
1:A:75:PHE:CD2	1:A:270:ILE:HD11	2.47	0.50
1:A:115:PHE:CD1	1:A:138:LEU:HD22	2.47	0.50
1:A:123:ASP:C	1:A:125:THR:H	2.20	0.50
2:B:2393:ILE:HB	2:B:2394:PRO:HD2	1.94	0.49
1:A:224:LYS:O	1:A:227:GLU:HG2	2.12	0.49
2:B:2413:ARG:HB3	2:B:2413:ARG:NH1	2.27	0.49
2:B:2439:ILE:HD11	2:B:2476:PHE:CZ	2.46	0.49
1:A:13:GLN:HG3	1:A:14:THR:N	2.18	0.49
1:A:28:LEU:O	1:A:168:SER:HA	2.12	0.49
1:A:39:LEU:N	1:A:39:LEU:CD2	2.74	0.49
2:B:2260:ARG:NH1	2:B:2413:ARG:HD3	2.27	0.49
2:B:2369:ILE:C	2:B:2369:ILE:HD12	2.38	0.49
2:B:2391:ARG:H	2:B:2391:ARG:CD	2.25	0.49
1:A:60:ASN:ND2	1:A:62:ASN:CB	2.73	0.49
2:B:2440:LEU:HD21	2:B:2468:PHE:CZ	2.47	0.49
2:B:2275:GLU:OE2	2:B:2275:GLU:HA	2.13	0.49
1:A:114:LYS:O	1:A:116:ALA:N	2.46	0.49
1:A:230:LEU:HD12	1:A:230:LEU:N	2.28	0.49
1:A:54:ARG:O	1:A:55:SER:HB3	2.12	0.49
1:A:179:ILE:N	1:A:179:ILE:CD1	2.75	0.49
1:A:13:GLN:CG	1:A:14:THR:N	2.75	0.49
2:B:2432:ARG:HG3	2:B:2432:ARG:NH1	2.27	0.49
1:A:104:SER:HB3	1:A:120:LYS:HD2	1.95	0.49
1:A:22:ASP:OD1	1:A:22:ASP:C	2.55	0.48
2:B:2400:LEU:HD21	2:B:2439:ILE:CG2	2.43	0.48
1:A:107:ASN:O	1:A:109:SER:N	2.46	0.48
1:A:107:ASN:HA	1:A:149:TYR:CD2	2.48	0.48
1:A:32:ASN:ND2	1:A:35:MET:HG3	2.28	0.48
1:A:299:LYS:C	1:A:299:LYS:HD2	2.38	0.48
1:A:2:CYS:O	1:A:3:VAL:O	2.32	0.48
2:B:2323:ILE:HD11	2:B:2357:ILE:HG23	1.95	0.48
1:A:251:GLU:OE1	1:A:251:GLU:N	2.40	0.48
1:A:182:PHE:CZ	1:A:280:VAL:HG11	2.49	0.48
1:A:82:TYR:HB2	1:A:262:TRP:CZ2	2.49	0.48
1:A:138:LEU:N	1:A:139:PRO:HD2	2.29	0.47
1:A:274:LYS:O	1:A:276:LYS:HG2	2.14	0.47
2:B:2319:ASP:O	2:B:2320:LYS:C	2.56	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2398:ASP:OD2	2:B:2471:ARG:NH1	2.47	0.47
1:A:145:ARG:C	1:A:147:ASP:N	2.69	0.47
1:A:219:LEU:HD12	1:A:229:VAL:HG13	1.96	0.47
2:B:2319:ASP:O	2:B:2322:ILE:HG13	2.14	0.47
1:A:248:PHE:CD1	1:A:248:PHE:O	2.66	0.47
2:B:2448:TYR:O	2:B:2451:SER:OG	2.29	0.47
1:A:81:ASP:C	1:A:81:ASP:OD1	2.57	0.47
1:A:217:LEU:HB3	1:A:285:VAL:CG2	2.44	0.47
1:A:35:MET:HG2	1:A:155:LEU:CD2	2.45	0.47
1:A:102:SER:C	1:A:120:LYS:HZ1	2.23	0.47
1:A:118:ILE:C	1:A:120:LYS:N	2.73	0.47
1:A:123:ASP:O	1:A:125:THR:N	2.47	0.47
1:A:277:VAL:HG12	1:A:278:LEU:N	2.29	0.47
2:B:2358:GLN:HE21	2:B:2419:THR:CB	2.28	0.47
1:A:39:LEU:HD23	1:A:157:PRO:HA	1.95	0.47
1:A:71:VAL:HG11	1:A:197:VAL:HG13	1.96	0.47
2:B:2241:ASN:HD22	2:B:2316:SER:HB3	1.80	0.47
2:B:2321:GLY:HA2	2:B:2361:GLN:HE22	1.79	0.47
1:A:180:VAL:HG21	1:A:200:VAL:HG11	1.97	0.47
2:B:2241:ASN:HB2	2:B:2316:SER:HB2	1.96	0.46
1:A:12:SER:O	1:A:33:LYS:HG3	2.16	0.46
2:B:2329:GLN:NE2	2:B:2330:GLU:N	2.62	0.46
2:B:2314:ILE:CG2	2:B:2323:ILE:HG21	2.45	0.46
1:A:269:PHE:N	1:A:269:PHE:CD1	2.83	0.46
1:A:299:LYS:HD2	1:A:299:LYS:OXT	2.15	0.46
1:A:154:VAL:O	1:A:156:LYS:HG3	2.15	0.46
2:B:2288:THR:O	2:B:2289:VAL:C	2.59	0.46
1:A:249:THR:CG2	1:A:259:LYS:HB2	2.46	0.46
2:B:2452:ASN:O	2:B:2453:LYS:C	2.59	0.46
2:B:2305:SER:C	2:B:2307:MET:H	2.22	0.46
2:B:2306:ASN:ND2	2:B:2306:ASN:H	2.14	0.46
1:A:61:ASN:C	1:A:63:LEU:N	2.71	0.45
1:A:246:LEU:C	1:A:246:LEU:HD23	2.41	0.45
1:A:61:ASN:OD1	1:A:61:ASN:N	2.48	0.45
1:A:177:LYS:HD2	1:A:177:LYS:N	2.31	0.45
1:A:240:SER:OG	1:A:271:TYR:HB3	2.16	0.45
1:A:97:LYS:HB2	1:A:97:LYS:HZ1	1.78	0.45
1:A:114:LYS:O	1:A:115:PHE:C	2.58	0.45
2:B:2400:LEU:CD2	2:B:2439:ILE:HG21	2.43	0.45
1:A:106:GLN:H	1:A:106:GLN:CD	2.25	0.45
1:A:120:LYS:HE3	1:A:120:LYS:HB3	1.76	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:LYS:HA	1:A:130:ILE:CG1	2.46	0.45
2:B:2401:LEU:HD11	2:B:2403:MET:HE3	1.98	0.45
2:B:2438:ASP:OD1	2:B:2441:THR:OG1	2.31	0.45
1:A:206:ASP:O	1:A:206:ASP:CG	2.60	0.45
2:B:2298:ILE:C	2:B:2300:GLN:N	2.74	0.45
1:A:61:ASN:ND2	1:A:165:GLN:HG3	2.30	0.45
1:A:75:PHE:CE1	1:A:281:LYS:HB2	2.52	0.45
2:B:2314:ILE:HG21	2:B:2323:ILE:HD13	1.98	0.45
2:B:2358:GLN:HA	2:B:2404:ALA:HB2	1.98	0.45
2:B:2358:GLN:NE2	2:B:2419:THR:HB	2.32	0.45
2:B:2398:ASP:CA	2:B:2470:LEU:HD23	2.40	0.45
2:B:2429:LEU:HD23	2:B:2442:ILE:HD13	1.99	0.45
1:A:13:GLN:NE2	1:A:68:LYS:NZ	2.65	0.44
1:A:135:LYS:HD3	1:A:136:TYR:CE2	2.52	0.44
1:A:186:ILE:HA	1:A:192:TYR:OH	2.17	0.44
2:B:2329:GLN:HE21	2:B:2329:GLN:C	2.25	0.44
1:A:61:ASN:ND2	1:A:165:GLN:CG	2.76	0.44
2:B:2298:ILE:HG22	2:B:2302:MET:CE	2.47	0.44
2:B:2454:ASP:OD2	2:B:2460:GLY:O	2.36	0.44
2:B:2432:ARG:HG2	2:B:2437:ASP:OD2	2.17	0.44
1:A:79:GLU:HG2	1:A:266:CYS:SG	2.58	0.44
1:A:106:GLN:NE2	1:A:150:VAL:O	2.49	0.44
1:A:209:GLN:HG3	1:A:291:LYS:HZ1	1.83	0.44
1:A:236:SER:HB3	1:A:237:LYS:CE	2.48	0.44
2:B:2236:CYS:CB	2:B:2281:ILE:HD13	2.47	0.44
2:B:2236:CYS:O	2:B:2238:ILE:HG13	2.18	0.44
1:A:118:ILE:HG21	1:A:122:HIS:C	2.43	0.44
2:B:2245:ALA:O	2:B:2249:GLU:HG3	2.17	0.44
1:A:118:ILE:C	1:A:120:LYS:H	2.25	0.43
1:A:74:GLN:O	1:A:77:GLN:CG	2.66	0.43
1:A:99:GLU:CG	1:A:100:HIS:H	2.10	0.43
1:A:175:GLY:O	1:A:176:ASN:CB	2.66	0.43
1:A:24:GLN:O	1:A:24:GLN:HG2	2.19	0.43
1:A:130:ILE:O	1:A:131:GLU:C	2.61	0.43
2:B:2248:ARG:HE	2:B:2248:ARG:HB2	1.55	0.43
2:B:2254:LEU:HD12	2:B:2254:LEU:N	2.33	0.43
2:B:2296:LEU:HD22	2:B:2340:PHE:CZ	2.53	0.43
2:B:2316:SER:OG	2:B:2317:HIS:N	2.48	0.43
1:A:122:HIS:NE2	1:A:125:THR:HG21	2.33	0.43
2:B:2233:ARG:NH2	2:B:2477:PRO:O	2.48	0.43
1:A:51:GLY:HA3	1:A:172:ASN:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2308:ASP:O	2:B:2309:CYS:HB2	2.19	0.43
1:A:17:ARG:HG3	1:A:199:TYR:CD1	2.48	0.43
1:A:297:THR:O	1:A:299:LYS:N	2.52	0.43
2:B:2241:ASN:HB3	2:B:2244:PHE:HE1	1.84	0.43
1:A:140:LYS:HE2	1:A:290:ASN:O	2.19	0.43
1:A:137:CYS:C	1:A:139:PRO:HD2	2.43	0.43
2:B:2458:ASN:O	2:B:2459:MET:C	2.62	0.43
1:A:102:SER:HB3	1:A:120:LYS:HZ2	1.82	0.42
1:A:135:LYS:HD3	1:A:136:TYR:CZ	2.53	0.42
1:A:184:HIS:N	1:A:290:ASN:OD1	2.45	0.42
2:B:2306:ASN:C	2:B:2307:MET:HE2	2.44	0.42
2:B:2401:LEU:HD11	2:B:2403:MET:CE	2.49	0.42
1:A:225:ASN:ND2	1:A:225:ASN:N	2.60	0.42
2:B:2243:ASN:HA	2:B:2259:ASP:OD2	2.19	0.42
2:B:2304:HIS:H	2:B:2347:SER:CB	2.28	0.42
2:B:2340:PHE:O	2:B:2353:LYS:HD2	2.18	0.42
2:B:2366:GLN:HB3	2:B:2461:LYS:O	2.19	0.42
2:B:2420:TRP:CD1	2:B:2420:TRP:N	2.83	0.42
1:A:210:PHE:O	1:A:214:VAL:HG23	2.19	0.42
2:B:2276:GLU:OE2	2:B:2479:ASP:O	2.37	0.42
2:B:2398:ASP:HA	2:B:2470:LEU:HA	2.02	0.42
1:A:60:ASN:ND2	1:A:62:ASN:ND2	2.47	0.42
1:A:191:LEU:HA	1:A:191:LEU:HD12	1.74	0.42
1:A:1:ACE:O	1:A:87:ASP:O	2.38	0.42
2:B:2238:ILE:HD11	2:B:2281:ILE:HD12	2.02	0.42
1:A:175:GLY:O	1:A:176:ASN:HB2	2.19	0.42
1:A:254:TRP:HB2	1:A:255:GLY:H	1.58	0.42
1:A:297:THR:O	1:A:298:ILE:C	2.63	0.42
2:B:2228:MET:CE	2:B:2233:ARG:HD2	2.45	0.42
2:B:2458:ASN:O	2:B:2458:ASN:OD1	2.38	0.42
1:A:127:LYS:HB3	1:A:131:GLU:OE1	2.19	0.42
1:A:192:TYR:CD1	1:A:290:ASN:HB2	2.55	0.41
1:A:177:LYS:NZ	1:A:296:ASN:OD1	2.44	0.41
2:B:2458:ASN:O	2:B:2460:GLY:N	2.54	0.41
1:A:50:SER:HA	1:A:179:ILE:HD13	2.02	0.41
2:B:2360:CYS:O	2:B:2361:GLN:HG2	2.20	0.41
1:A:53:ILE:HG22	1:A:55:SER:H	1.86	0.41
2:B:2442:ILE:O	2:B:2446:VAL:HG23	2.21	0.41
1:A:209:GLN:HG3	1:A:291:LYS:NZ	2.35	0.41
2:B:2279:PHE:HZ	2:B:2309:CYS:HG	1.64	0.41
2:B:2440:LEU:HD21	2:B:2468:PHE:CE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:GLU:OE2	1:A:291:LYS:NZ	2.54	0.41
2:B:2275:GLU:OE2	2:B:2281:ILE:HG12	2.21	0.41
2:B:2330:GLU:H	2:B:2330:GLU:HG2	1.59	0.41
1:A:6:PRO:O	1:A:7:VAL:C	2.64	0.41
1:A:77:GLN:HE22	1:A:239:LYS:HZ1	1.61	0.41
1:A:22:ASP:OD1	1:A:24:GLN:N	2.55	0.40
1:A:61:ASN:C	1:A:63:LEU:H	2.29	0.40
1:A:118:ILE:CG1	1:A:122:HIS:HB3	2.41	0.40
2:B:2260:ARG:CD	2:B:2317:HIS:HD2	2.32	0.40
2:B:2281:ILE:HG22	2:B:2283:PRO:CD	2.49	0.40
1:A:6:PRO:HB2	1:A:7:VAL:H	1.68	0.40
2:B:2288:THR:CG2	2:B:2326:THR:HB	2.47	0.40
2:B:2289:VAL:HG21	2:B:2329:GLN:O	2.22	0.40
1:A:237:LYS:N	1:A:237:LYS:CD	2.84	0.40
2:B:2292:ILE:HA	2:B:2295:ILE:HD12	2.02	0.40
1:A:118:ILE:HD12	1:A:118:ILE:HA	1.66	0.40
2:B:2260:ARG:HD3	2:B:2317:HIS:CD2	2.51	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	290/299 (97%)	213 (73%)	54 (19%)	23 (8%)	1	3
2	B	239/258 (93%)	191 (80%)	37 (16%)	11 (5%)	2	11
All	All	529/557 (95%)	404 (76%)	91 (17%)	34 (6%)	1	6

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	VAL

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Mol	Chain	Res	Type
1	A	7	VAL
1	A	94	LYS
1	A	108	GLY
1	A	115	PHE
1	A	126	ASP
1	A	146	ASN
1	A	186	ILE
1	A	255	GLY
1	A	298	ILE
2	B	2250	LYS
2	B	2285	HIS
1	A	124	TYR
1	A	236	SER
1	A	256	LYS
1	A	275	SER
2	B	2320	LYS
2	B	2330	GLU
2	B	2457	LYS
2	B	2459	MET
1	A	6	PRO
1	A	147	ASP
1	A	205	PHE
2	B	2233	ARG
2	B	2237	LEU
2	B	2299	TYR
1	A	10	ASP
1	A	206	ASP
1	A	237	LYS
1	A	274	LYS
2	B	2230	SER
1	A	5	PHE
2	B	2289	VAL
1	A	9	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	276/280 (99%)	237 (86%)	39 (14%)	3	16
2	B	218/233 (94%)	190 (87%)	28 (13%)	4	19
All	All	494/513 (96%)	427 (86%)	67 (14%)	3	17

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	CYS
1	A	5	PHE
1	A	16	ILE
1	A	20	GLN
1	A	24	GLN
1	A	25	THR
1	A	27	GLU
1	A	31	ILE
1	A	33	LYS
1	A	39	LEU
1	A	46	MET
1	A	49	ILE
1	A	61	ASN
1	A	70	LYS
1	A	77	GLN
1	A	97	LYS
1	A	106	GLN
1	A	118	ILE
1	A	126	ASP
1	A	142	VAL
1	A	143	ASP
1	A	153	CYS
1	A	176	ASN
1	A	179	ILE
1	A	189	THR
1	A	191	LEU
1	A	200	VAL
1	A	208	GLU
1	A	212	GLU
1	A	225	ASN
1	A	237	LYS
1	A	239	LYS
1	A	241	MET
1	A	250	THR
1	A	251	GLU

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Mol	Chain	Res	Type
1	A	254	TRP
1	A	258	GLU
1	A	269	PHE
1	A	289	LEU
2	B	2223	ASP
2	B	2236	CYS
2	B	2246	LYS
2	B	2248	ARG
2	B	2263	THR
2	B	2275	GLU
2	B	2276	GLU
2	B	2287	CYS
2	B	2306	ASN
2	B	2316	SER
2	B	2329	GLN
2	B	2330	GLU
2	B	2335	GLU
2	B	2347	SER
2	B	2363	ASP
2	B	2373	THR
2	B	2391	ARG
2	B	2399	PHE
2	B	2405	THR
2	B	2427	GLN
2	B	2429	LEU
2	B	2432	ARG
2	B	2440	LEU
2	B	2453	LYS
2	B	2459	MET
2	B	2465	GLN
2	B	2472	LYS
2	B	2476	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	GLN
1	A	38	GLN
1	A	60	ASN
1	A	77	GLN
1	A	85	GLN
1	A	100	HIS

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Mol	Chain	Res	Type
1	A	106	GLN
1	A	164	ASN
1	A	172	ASN
1	A	176	ASN
1	A	204	GLN
1	A	209	GLN
1	A	225	ASN
1	A	283	HIS
2	B	2241	ASN
2	B	2261	ASN
2	B	2306	ASN
2	B	2329	GLN
2	B	2339	GLN
2	B	2366	GLN
2	B	2407	ASN
2	B	2414	ASN
2	B	2427	GLN
2	B	2447	ASN
2	B	2458	ASN
2	B	2465	GLN

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 [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

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.