



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:58 PM GMT

PDB ID : 1I4E  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

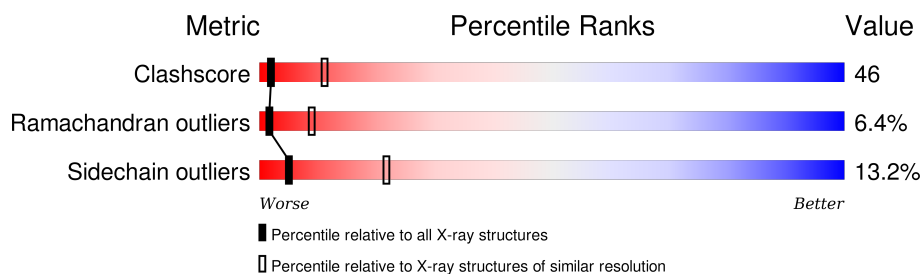
# 1 Overall quality at a glance ⓘ

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	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	299	 34% 51% 13% ••
2	B	258	 32% 51% 10% • 6%

## 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:

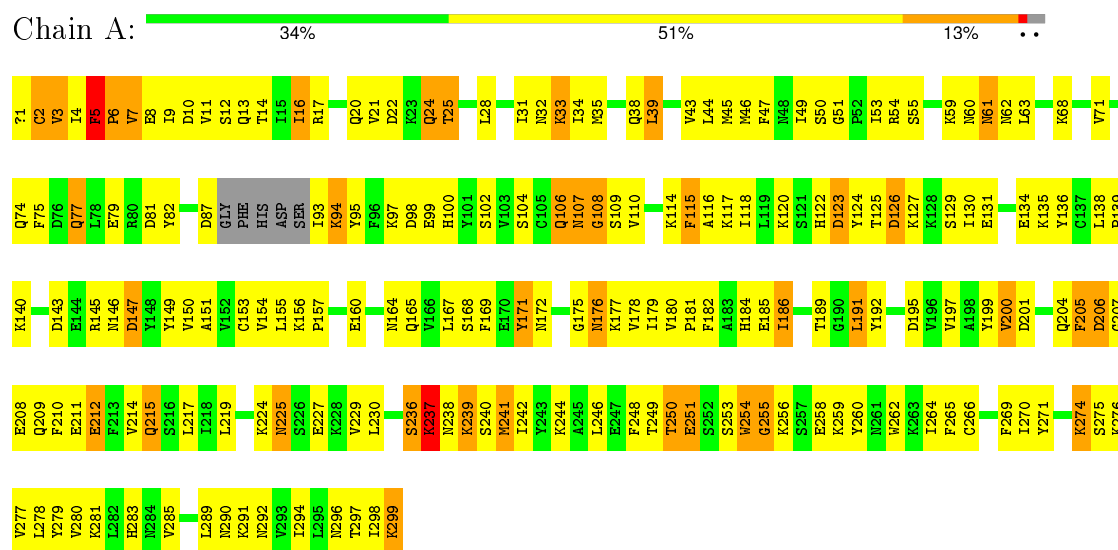
Chain	Residue	Modelled	Actual	Comment	Reference
B	2285	HIS	ASP	SEE REMARK 999	UNP Q14790

### 3 Residue-property plots

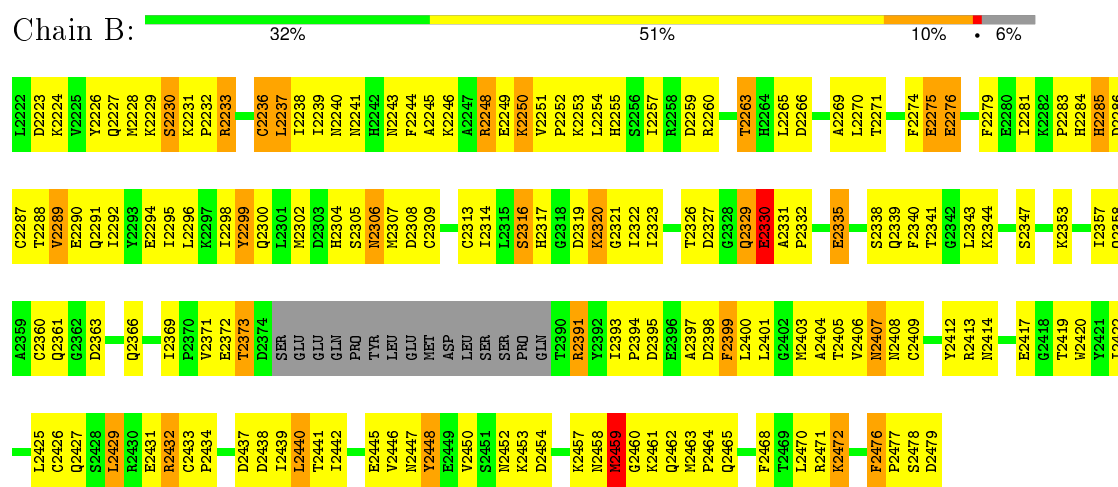
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS was not executed.

- Molecule 1: Early 35 kDa protein



- Molecule 2: Caspase-8



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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 <sup>2</sup> )	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	0.42	0/2455	0.68	0/3309
2	B	0.37	0/1987	0.62	0/2682
All	All	0.40	0/4442	0.65	0/5991

There are no bond length outliers.

There are no bond angle outliers.

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	229	0
2	B	1945	0	1914	176	0
All	All	4354	0	4308	402	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 46.

All (402) 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:HD2	1:A:33:LYS:H	1.23	1.02
1:A:99:GLU:HG3	1:A:100:HIS:H	1.23	0.97
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:H	1:A:39:LEU:HD22	1.38	0.87
2:B:2439:ILE:HD11	2:B:2476:PHE:CE2	2.09	0.86
2:B:2339:GLN:HE21	2:B:2344:LYS:NZ	1.74	0.86
1:A:60:ASN:HD21	1:A:62:ASN:ND2	1.72	0.86
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
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
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: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
2:B:2339:GLN:HE21	2:B:2344:LYS:HZ2	1.32	0.77
1:A:106:GLN:NE2	1:A:106:GLN:H	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:O	1:A:118:ILE:HG23	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:225:ASN:ND2	1:A:225:ASN:H	1.86	0.74
1:A:181:PRO:HA	1:A:292:ASN:OD1	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:145:ARG:O	1:A:147:ASP:N	2.24	0.71
1:A:77:GLN:HE22	1:A:239:LYS:NZ	1.89	0.71
1:A:60:ASN:HA	1:A:164:ASN:ND2	2.05	0.71
2:B:2400:LEU:HD21	2:B:2439:ILE:HG21	1.73	0.71
1:A:35:MET:CE	1:A:167:LEU:HD12	2.20	0.71
1:A:97:LYS:NZ	1:A:97:LYS:HB2	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:CD	1:A:33:LYS:H	1.96	0.69
2:B:2304:HIS:H	2:B:2347:SER:HB3	1.56	0.69
2:B:2251:VAL:CG2	2:B:2254:LEU:HD13	2.23	0.69
1:A:179:ILE:N	1:A:179:ILE:HD12	2.07	0.69
1:A:211:GLU:O	1:A:215:GLN:HB2	1.93	0.69
1:A:34:ILE:H	1:A:34:ILE:HD12	1.56	0.69
1:A:217:LEU:HB3	1:A:285:VAL:HG21	1.73	0.69
2:B:2447:ASN:HB3	2:B:2463:MET:HE1	1.74	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
2:B:2270:LEU:HD11	2:B:2422:ILE:HD12	1.76	0.68
1:A:98:ASP:OD1	1:A:99:GLU:N	2.27	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:35:MET:HE2	1:A:167:LEU:HD12	1.76	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:THR:O	1:A:129:SER:HB3	1.96	0.66
1:A:93:ILE:O	1:A:93:ILE:HG13	1.95	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:2357:ILE:HB	2:B:2403:MET:HE1	1.77	0.65
2:B:2338:SER:O	2:B:2341:THR:HG23	1.97	0.65
1:A:108:GLY:HA2	1:A:150:VAL:HG23	1.79	0.65
2:B:2241:ASN:HD22	2:B:2316:SER:CB	2.09	0.65
2:B:2323:ILE:HD11	2:B:2357:ILE:CG2	2.27	0.64
2:B:2227:GLN:O	2:B:2308:ASP:HB3	1.96	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
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
2:B:2288:THR:HG22	2:B:2326:THR:HB	1.79	0.63
1:A:118:ILE:HG13	1:A:122:HIS:H	1.63	0.63
1:A:33:LYS:HD2	1:A:33:LYS:N	2.05	0.62
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
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:249:THR:HG21	1:A:259:LYS:HE2	1.81	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
2:B:2439:ILE:HD11	2:B:2476:PHE:HE2	1.60	0.61
2:B:2323:ILE:HD11	2:B:2357:ILE:HD13	1.80	0.61
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: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:114:LYS:O	1:A:117:LYS:HD3	2.02	0.60
2:B:2281:ILE:HG22	2:B:2283:PRO:HD3	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:145:ARG:C	1:A:147:ASP:H	2.05	0.60
2:B:2260:ARG:HH21	2:B:2263:THR:HG23	1.67	0.60
2:B:2432:ARG:HH11	2:B:2432:ARG:HG3	1.65	0.60
2:B:2246:LYS:HD3	2:B:2250:LYS:HE3	1.84	0.60
2:B:2231:LYS:HB2	2:B:2232:PRO:CD	2.22	0.59
1:A:87:ASP:HB3	2:B:2317:HIS:HA	1.84	0.59
2:B:2406:VAL:HG13	2:B:2463:MET:O	2.02	0.59
2:B:2228:MET:HE3	2:B:2233:ARG:HD2	1.83	0.59
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
2:B:2339:GLN:NE2	2:B:2344:LYS:NZ	2.50	0.58
1:A:102:SER:HB3	1:A:120:LYS:HZ1	1.69	0.58
1:A:179:ILE:HG22	1:A:179:ILE:O	2.03	0.58
1:A:43:VAL:HG12	1:A:155:LEU:O	2.02	0.58
1:A:107:ASN:HB3	1:A:110:VAL:HG23	1.86	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
2:B:2226:TYR:CE1	2:B:2472:LYS:HG3	2.40	0.57
2:B:2228:MET:HE1	2:B:2476:PHE:HD1	1.70	0.57
1:A:24:GLN:H	1:A:24:GLN:NE2	2.03	0.57
2:B:2270:LEU:HD13	2:B:2313:CYS:SG	2.44	0.57
2:B:2248:ARG:HD3	2:B:2257:ILE:O	2.05	0.57
1:A:115:PHE:HE1	1:A:138:LEU:HD13	1.68	0.57
2:B:2298:ILE:C	2:B:2300:GLN:H	2.08	0.57
2:B:2343:LEU:HG	2:B:2395:ASP:OD1	2.04	0.56
2:B:2251:VAL:HG11	2:B:2254:LEU:HD22	1.87	0.56
2:B:2237:LEU:HD21	2:B:2299:TYR:CD2	2.40	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
2:B:2241:ASN:HD22	2:B:2316:SER:HB2	1.71	0.56
1:A:102:SER:HB3	1:A:120:LYS:NZ	2.21	0.56
1:A:185:GLU:O	1:A:186:ILE:C	2.43	0.55
2:B:2260:ARG:HH21	2:B:2263:THR:CG2	2.19	0.55
1:A:237:LYS:N	1:A:237:LYS:HD2	2.21	0.55
1:A:21:VAL:HB	1:A:25:THR:HG22	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:2248:ARG:NH2	2:B:2259:ASP:OD1	2.39	0.55
1:A:134:GLU:O	1:A:139:PRO:HD3	2.06	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:164:ASN:N	1:A:164:ASN:HD22	2.04	0.55
1:A:77:GLN:HE22	1:A:239:LYS:HZ3	1.55	0.55
1:A:43:VAL:CG1	1:A:155:LEU:HB2	2.36	0.55
1:A:178:VAL:C	1:A:179:ILE:HD12	2.27	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:77:GLN:HE22	1:A:239:LYS:HZ1	1.55	0.54
1:A:107:ASN:O	1:A:110:VAL:HG23	2.07	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
2:B:2339:GLN:HE21	2:B:2344:LYS:HZ3	1.54	0.54
2:B:2248:ARG:HA	2:B:2254:LEU:O	2.08	0.54
2:B:2357:ILE:HD12	2:B:2403:MET:HE1	1.89	0.54
1:A:12:SER:HB3	1:A:33:LYS:HA	1.89	0.53
2:B:2224:LYS:CG	2:B:2472:LYS:HD3	2.34	0.53
1:A:5:PHE:N	1:A:6:PRO:CD	2.72	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:60:ASN:ND2	1:A:62:ASN:H	2.06	0.53
1:A:50:SER:OG	1:A:178:VAL:HA	2.08	0.53
1:A:250:THR:HG22	1:A:260:TYR:HD1	1.73	0.53
1:A:118:ILE:CG2	1:A:118:ILE:O	2.53	0.53
2:B:2450:VAL:HG11	2:B:2464:PRO:HD3	1.90	0.53
1:A:100:HIS:O	1:A:156:LYS:HB2	2.09	0.53
1:A:50:SER:CB	1:A:177:LYS:O	2.56	0.53
2:B:2322:ILE:HD12	2:B:2322:ILE:C	2.29	0.53
2:B:2339:GLN:NE2	2:B:2344:LYS:HZ3	2.07	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:35:MET:HE1	1:A:167:LEU:HD12	1.90	0.53
2:B:2236:CYS:HB3	2:B:2281:ILE:HD13	1.91	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:2229:LYS:O	2:B:2230:SER:C	2.49	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
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
1:A:264:ILE:HG13	1:A:265:PHE:CD2	2.46	0.51
2:B:2251:VAL:HG22	2:B:2254:LEU:HD13	1.93	0.51
1:A:71:VAL:HG11	1:A:197:VAL:CG1	2.41	0.51
1:A:47:PHE:CE1	1:A:151:ALA:HB3	2.45	0.51
1:A:4:ILE:O	1:A:4:ILE:HG22	2.11	0.50
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:115:PHE:CD1	1:A:138:LEU:HD22	2.47	0.50
1:A:75:PHE:CD2	1:A:270:ILE:HD11	2.47	0.50
2:B:2393:ILE:HB	2:B:2394:PRO:HD2	1.94	0.49
2:B:2413:ARG:NH1	2:B:2413:ARG:HB3	2.27	0.49
2:B:2439:ILE:HD11	2:B:2476:PHE:CZ	2.46	0.49
1:A:224:LYS:O	1:A:227:GLU:HG2	2.12	0.49
1:A:13:GLN:HG3	1:A:14:THR:N	2.18	0.49
1:A:39:LEU:CD2	1:A:39:LEU:N	2.74	0.49
1:A:4:ILE:C	1:A:6:PRO:HD2	2.32	0.49
1:A:28:LEU:O	1:A:168:SER:HA	2.12	0.49
2:B:2306:ASN:HB2	2:B:2307:MET:HE3	1.95	0.49
2:B:2260:ARG:NH1	2:B:2413:ARG:HD3	2.27	0.49
2:B:2391:ARG:CD	2:B:2391:ARG:H	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:HA	2:B:2275:GLU:OE2	2.13	0.49
1:A:106:GLN:CD	1:A:106:GLN:N	2.66	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:2400:LEU:HD21	2:B:2439:ILE:CG2	2.43	0.48
1:A:107:ASN:HA	1:A:149:TYR:CD2	2.48	0.48
1:A:107:ASN:O	1:A:109:SER:N	2.46	0.48
1:A:32:ASN:ND2	1:A:35:MET:HG3	2.28	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
2:B:2299:TYR:CD1	2:B:2302:MET:HE1	2.49	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
2:B:2398:ASP:OD2	2:B:2471:ARG:NH1	2.47	0.47
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:2322:ILE:HG13	2.14	0.47
1:A:219:LEU:HD12	1:A:229:VAL:HG13	1.96	0.47
1:A:277:VAL:HG12	1:A:278:LEU:N	2.29	0.47
1:A:248:PHE:O	1:A:248:PHE:CD1	2.66	0.47
2:B:2228:MET:CE	2:B:2233:ARG:HD2	2.45	0.47
1:A:201:ASP:OD2	1:A:201:ASP:C	2.53	0.47
1:A:217:LEU:HB3	1:A:285:VAL:CG2	2.44	0.47
2:B:2358:GLN:HE21	2:B:2419:THR:CB	2.28	0.47
1:A:123:ASP:O	1:A:125:THR:N	2.47	0.47
1:A:35:MET:HG2	1:A:155:LEU:CD2	2.45	0.47
2:B:2241:ASN:HD22	2:B:2316:SER:HB3	1.80	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: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
1:A:44:LEU:HD23	1:A:44:LEU:C	2.35	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
1:A:107:ASN:O	1:A:108:GLY:C	2.54	0.46
2:B:2314:ILE:CG2	2:B:2323:ILE:HG21	2.45	0.46
2:B:2447:ASN:HB3	2:B:2463:MET:CE	2.44	0.46
2:B:2458:ASN:C	2:B:2459:MET:HG3	2.35	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:LYS:HD2	1:A:299:LYS:OXT	2.15	0.46
1:A:269:PHE:CD1	1:A:269:PHE:N	2.83	0.46
1:A:154:VAL:O	1:A:156:LYS:HG3	2.15	0.46
1:A:249:THR:CG2	1:A:259:LYS:HB2	2.46	0.46
2:B:2306:ASN:H	2:B:2306:ASN:ND2	2.14	0.46
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:22:ASP:OD1	1:A:22:ASP:C	2.55	0.45
1:A:240:SER:OG	1:A:271:TYR:HB3	2.16	0.45
2:B:2400:LEU:CD2	2:B:2439:ILE:HG21	2.43	0.45
1:A:97:LYS:HZ1	1:A:97:LYS:HB2	1.78	0.45
1:A:120:LYS:HB3	1:A:120:LYS:HE3	1.76	0.45
1:A:127:LYS:HA	1:A:130:ILE:CG1	2.46	0.45
1:A:123:ASP:C	1:A:125:THR:H	2.20	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
1:A:61:ASN:ND2	1:A:165:GLN:HG3	2.30	0.45
2:B:2429:LEU:HD23	2:B:2442:ILE:HD13	1.99	0.45
2:B:2398:ASP:CA	2:B:2470:LEU:HD23	2.40	0.45
2:B:2314:ILE:HG21	2:B:2323:ILE:HD13	1.98	0.45
1:A:75:PHE:CE1	1:A:281:LYS:HB2	2.52	0.45
2:B:2369:ILE:C	2:B:2369:ILE:HD12	2.38	0.45
1:A:13:GLN:NE2	1:A:68:LYS:NZ	2.65	0.44
1:A:186:ILE:HA	1:A:192:TYR:OH	2.17	0.44
1:A:135:LYS:HD3	1:A:136:TYR:CE2	2.52	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:236:SER:HB3	1:A:237:LYS:CE	2.48	0.44
1:A:106:GLN:NE2	1:A:150:VAL:O	2.49	0.44
2:B:2236:CYS:O	2:B:2238:ILE:HG13	2.18	0.44
2:B:2236:CYS:CB	2:B:2281:ILE:HD13	2.47	0.44
2:B:2319:ASP:O	2:B:2320:LYS:C	2.56	0.44
1:A:79:GLU:HG2	1:A:266:CYS:SG	2.58	0.44
1:A:209:GLN:HG3	1:A:291:LYS:HZ1	1.83	0.44
2:B:2245:ALA:O	2:B:2249:GLU:HG3	2.17	0.44
1:A:299:LYS:C	1:A:299:LYS:HD2	2.38	0.44
2:B:2401:LEU:HD11	2:B:2403:MET:HE3	1.99	0.43
1:A:99:GLU:CG	1:A:100:HIS:H	2.10	0.43
1:A:74:GLN:O	1:A:77:GLN:CG	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:GLY:O	1:A:176:ASN:CB	2.66	0.43
1:A:24:GLN:HG2	1:A:24:GLN:O	2.19	0.43
2:B:2316:SER:OG	2:B:2317:HIS:N	2.48	0.43
2:B:2248:ARG:HB2	2:B:2248:ARG:HE	1.55	0.43
2:B:2254:LEU:N	2:B:2254:LEU:HD12	2.33	0.43
2:B:2296:LEU:HD22	2:B:2340:PHE:CZ	2.53	0.43
2:B:2233:ARG:NH2	2:B:2477:PRO:O	2.48	0.43
1:A:122:HIS:NE2	1:A:125:THR:HG21	2.33	0.43
2:B:2308:ASP:O	2:B:2309:CYS:HB2	2.19	0.43
1:A:51:GLY:HA3	1:A:172:ASN:O	2.19	0.43
1:A:17:ARG:HG3	1:A:199:TYR:CD1	2.48	0.43
2:B:2241:ASN:HB3	2:B:2244:PHE:HE1	1.84	0.43
1:A:297:THR:O	1:A:299:LYS:N	2.52	0.43
1:A:61:ASN:C	1:A:63:LEU:N	2.71	0.43
1:A:140:LYS:HE2	1:A:290:ASN:O	2.19	0.43
1:A:250:THR:CG2	1:A:251:GLU:N	2.82	0.43
2:B:2401:LEU:HD11	2:B:2403:MET:CE	2.49	0.42
1:A:184:HIS:N	1:A:290:ASN:OD1	2.45	0.42
1:A:135:LYS:HD3	1:A:136:TYR:CZ	2.53	0.42
1:A:11:VAL:O	1:A:12:SER:OG	2.33	0.42
2:B:2243:ASN:HA	2:B:2259:ASP:OD2	2.19	0.42
1:A:118:ILE:C	1:A:120:LYS:N	2.73	0.42
1:A:225:ASN:ND2	1:A:225:ASN:N	2.60	0.42
2:B:2304:HIS:H	2:B:2347:SER:CB	2.28	0.42
2:B:2366:GLN:HB3	2:B:2461:LYS:O	2.19	0.42
2:B:2340:PHE:O	2:B:2353:LYS:HD2	2.18	0.42
1:A:81:ASP:C	1:A:81:ASP:OD1	2.57	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:2398:ASP:HA	2:B:2470:LEU:HA	2.02	0.42
2:B:2276:GLU:OE2	2:B:2479:ASP:O	2.37	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
2:B:2458:ASN:OD1	2:B:2458:ASN:O	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
2:B:2431:GLU:CD	2:B:2431:GLU:C	2.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:2288:THR:O	2:B:2289:VAL:C	2.59	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
2:B:2305:SER:C	2:B:2307:MET:H	2.22	0.41
2:B:2442:ILE:O	2:B:2446:VAL:HG23	2.21	0.41
1:A:53:ILE:HG22	1:A:55:SER:H	1.86	0.41
2:B:2452:ASN:O	2:B:2453:LYS:C	2.59	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
1:A:209:GLN:HG3	1:A:291:LYS:NZ	2.35	0.41
1:A:246:LEU:HD23	1:A:246:LEU:C	2.41	0.41
2:B:2330:GLU:H	2:B:2330:GLU:HG2	1.59	0.41
2:B:2275:GLU:OE2	2:B:2281:ILE:HG12	2.21	0.41
1:A:212:GLU:OE2	1:A:291:LYS:NZ	2.54	0.41
2:B:2438:ASP:OD1	2:B:2441:THR:OG1	2.31	0.41
2:B:2260:ARG:CD	2:B:2317:HIS:HD2	2.32	0.40
1:A:118:ILE:CG1	1:A:122:HIS:HB3	2.41	0.40
1:A:114:LYS:O	1:A:115:PHE:C	2.58	0.40
2:B:2281:ILE:HG22	2:B:2283:PRO:CD	2.49	0.40
1:A:22:ASP:OD1	1:A:24:GLN:N	2.55	0.40
2:B:2289:VAL:HG21	2:B:2329:GLN:O	2.22	0.40
2:B:2288:THR:CG2	2:B:2326:THR:HB	2.47	0.40
1:A:106:GLN:CD	1:A:106:GLN:H	2.25	0.40
2:B:2298:ILE:C	2:B:2300:GLN:N	2.74	0.40
1:A:6:PRO:HB2	1:A:7:VAL:H	1.68	0.40
1:A:206:ASP:O	1:A:206:ASP:CG	2.60	0.40
2:B:2292:ILE:HA	2:B:2295:ILE:HD12	2.02	0.40
1:A:237:LYS:CD	1:A:237:LYS:N	2.84	0.40
2:B:2260:ARG:HD3	2:B:2317:HIS:CD2	2.51	0.40
1:A:118:ILE:HA	1:A:118:ILE:HD12	1.66	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	5
2	B	239/258 (93%)	191 (80%)	37 (16%)	11 (5%)	3	18
All	All	529/557 (95%)	404 (76%)	91 (17%)	34 (6%)	2	9

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	VAL
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

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Mol	Chain	Res	Type
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%)	239 (87%)	37 (13%)	5	21
2	B	218/233 (94%)	190 (87%)	28 (13%)	5	23
All	All	494/513 (96%)	429 (87%)	65 (13%)	5	22

All (65) 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	31	ILE
1	A	33	LYS
1	A	39	LEU
1	A	46	MET
1	A	49	ILE
1	A	61	ASN
1	A	77	GLN
1	A	106	GLN
1	A	107	ASN
1	A	123	ASP
1	A	126	ASP
1	A	143	ASP
1	A	153	CYS
1	A	171	TYR

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Mol	Chain	Res	Type
1	A	176	ASN
1	A	189	THR
1	A	191	LEU
1	A	200	VAL
1	A	208	GLU
1	A	212	GLU
1	A	215	GLN
1	A	225	ASN
1	A	237	LYS
1	A	239	LYS
1	A	241	MET
1	A	250	THR
1	A	251	GLU
1	A	254	TRP
1	A	258	GLU
1	A	289	LEU
1	A	299	LYS
2	B	2223	ASP
2	B	2236	CYS
2	B	2248	ARG
2	B	2263	THR
2	B	2275	GLU
2	B	2276	GLU
2	B	2286	ASP
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	2363	ASP
2	B	2373	THR
2	B	2391	ARG
2	B	2399	PHE
2	B	2405	THR
2	B	2407	ASN
2	B	2427	GLN
2	B	2429	LEU
2	B	2432	ARG
2	B	2440	LEU
2	B	2448	TYR
2	B	2459	MET

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Mol	Chain	Res	Type
2	B	2465	GLN
2	B	2472	LYS
2	B	2476	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	GLN
1	A	20	GLN
1	A	60	ASN
1	A	77	GLN
1	A	85	GLN
1	A	106	GLN
1	A	107	ASN
1	A	122	HIS
1	A	164	ASN
1	A	172	ASN
1	A	176	ASN
1	A	204	GLN
1	A	225	ASN
1	A	283	HIS
2	B	2241	ASN
2	B	2300	GLN
2	B	2306	ASN
2	B	2317	HIS
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 [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates 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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.