Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 08:03 PM GMT

PDB ID	:	1IHM
Title	:	CRYSTAL STRUCTURE ANALYSIS OF NORWALK VIRUS CAPSID
Authors	:	Prasad, B.V.; Hardy, M.E.; Dokland, T.; Bella, J.; Rossmann, M.G.; Estes, M.K.
Deposited on	:	2001-04-19
Resolution	:	3.40 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

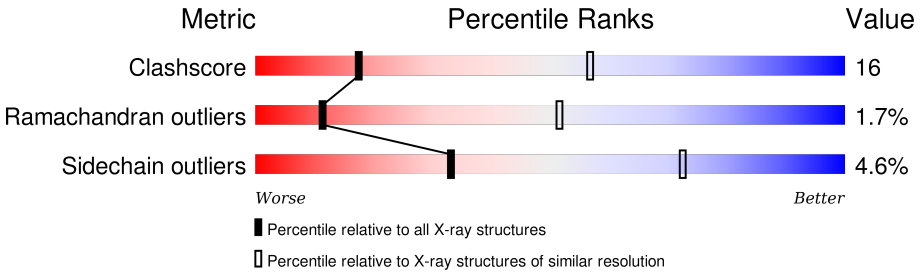
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1611 (3.50-3.30)
Ramachandran outliers	100387	1571 (3.50-3.30)
Sidechain outliers	100360	1571 (3.50-3.30)

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 >=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 <=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	530	61% 29% • 7%
1	B	530	66% 28% • •
1	C	530	62% 28% • 7%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 11284 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 capsid protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	492	Total	C	N	O	S	0	0	0
			3721	2378	628	697	18			
1	B	511	Total	C	N	O	S	0	0	0
			3842	2449	649	726	18			
1	C	492	Total	C	N	O	S	0	0	0
			3721	2378	628	697	18			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1253	MET	ILE	SEE REMARK 999	UNP Q83884
B	2253	MET	ILE	SEE REMARK 999	UNP Q83884
C	3253	MET	ILE	SEE REMARK 999	UNP Q83884

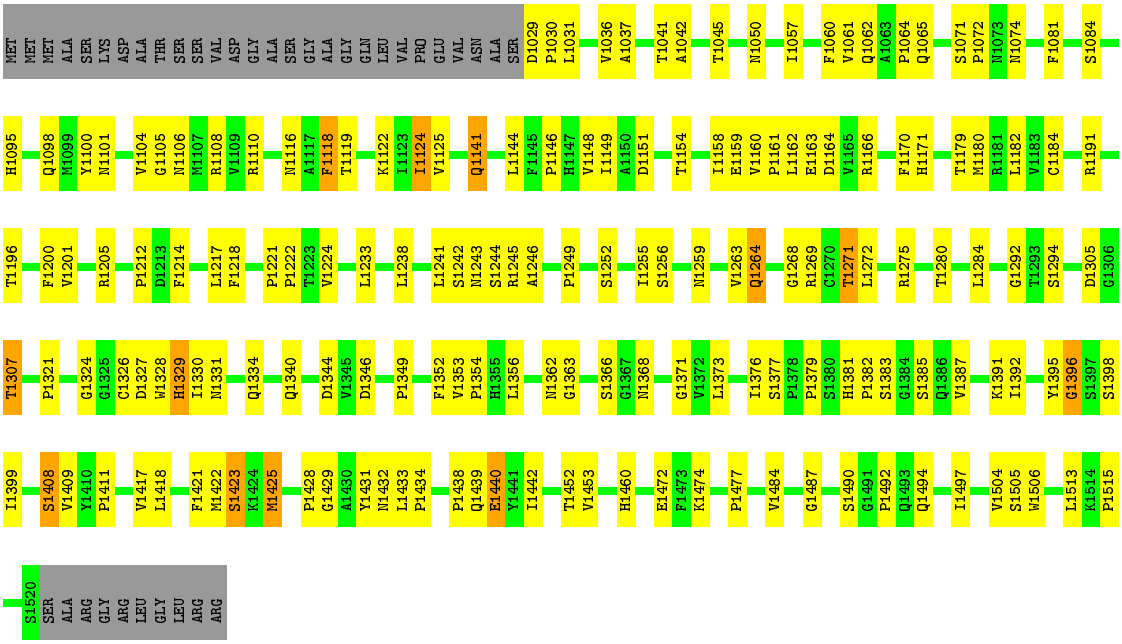
3 Residue-property plots (i)

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.

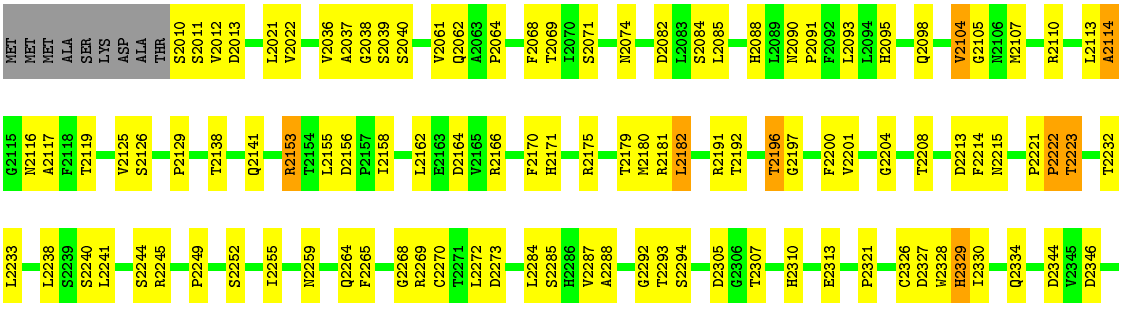
- Molecule 1: capsid protein

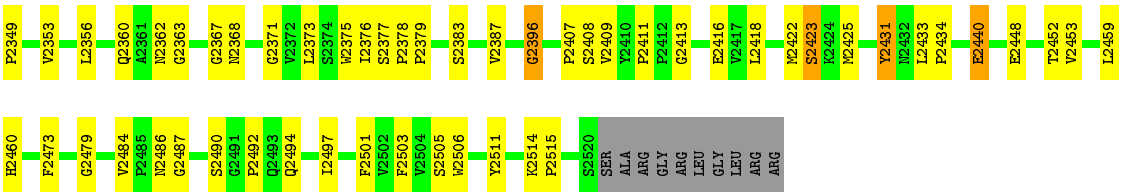
Chain A:



- Molecule 1: capsid protein

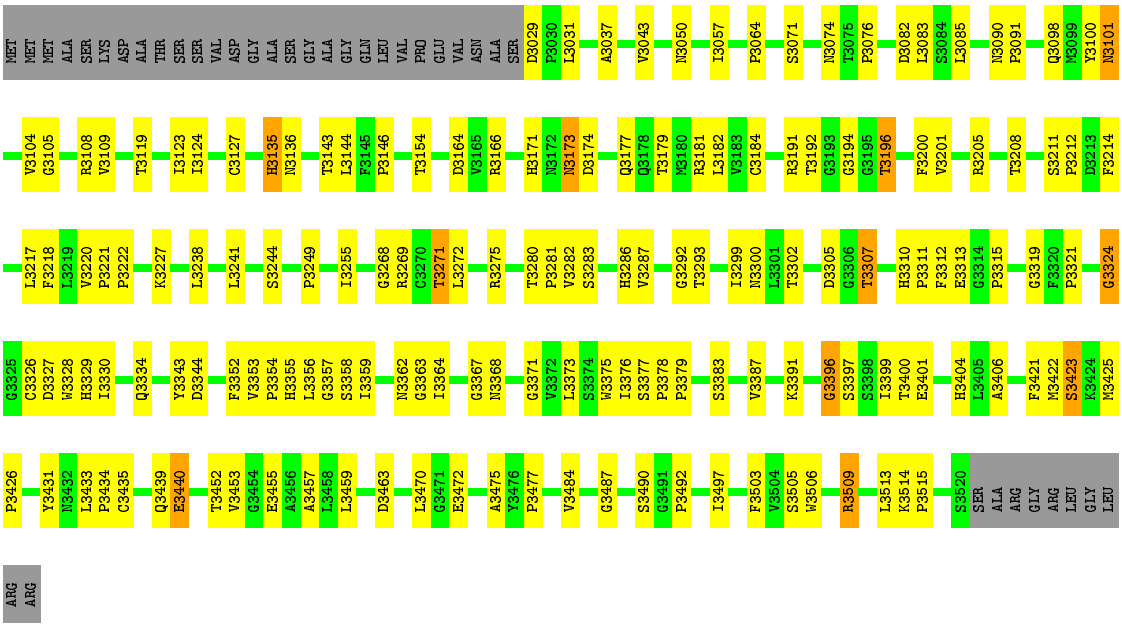
Chain B:





- Molecule 1: capsid protein

Chain C:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α, β, γ	605.74Å 605.74Å 466.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.00 – 3.40	Depositor
% Data completeness (in resolution range)	(Not available) (35.00-3.40)	Depositor
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.260 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11284	wwPDB-VP
Average B, all atoms (Å^2)	26.0	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	0.42	0/3835	0.68	0/5261
1	B	0.41	0/3957	0.68	1/5428 (0.0%)
1	C	0.41	0/3835	0.69	0/5261
All	All	0.41	0/11627	0.68	1/15950 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	2197	GLY	N-CA-C	-5.31	99.81	113.10

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	3721	0	3624	134	0
1	B	3842	0	3737	122	0
1	C	3721	0	3624	124	0
All	All	11284	0	10985	357	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 16.

All (357) 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:2330:ILE:CG2	1:B:2373:LEU:HD23	1.44	1.44
1:A:1330:ILE:CG2	1:A:1373:LEU:HD23	1.47	1.44
1:B:2321:PRO:CB	1:B:2373:LEU:HD11	1.60	1.30
1:C:3321:PRO:CB	1:C:3373:LEU:HD11	1.72	1.20
1:B:2321:PRO:HB3	1:B:2373:LEU:CD1	1.72	1.19
1:B:2330:ILE:HG22	1:B:2373:LEU:CD2	1.72	1.17
1:C:3330:ILE:CG2	1:C:3373:LEU:HD23	1.77	1.13
1:C:3330:ILE:HG22	1:C:3373:LEU:HD23	1.21	1.11
1:A:1330:ILE:HG22	1:A:1373:LEU:CD2	1.78	1.11
1:B:2321:PRO:HB3	1:B:2373:LEU:HD11	1.20	1.08
1:A:1321:PRO:CB	1:A:1373:LEU:HD11	1.84	1.06
1:C:3321:PRO:HB3	1:C:3373:LEU:CD1	1.86	1.04
1:A:1330:ILE:CG2	1:A:1373:LEU:CD2	2.35	1.03
1:A:1321:PRO:HB3	1:A:1373:LEU:HD11	1.41	1.00
1:B:2330:ILE:CG2	1:B:2373:LEU:CD2	2.33	0.99
1:C:3123:ILE:HD11	1:C:3184:CYS:SG	2.02	0.98
1:C:3321:PRO:HB3	1:C:3373:LEU:HD11	1.45	0.97
1:A:1321:PRO:HB3	1:A:1373:LEU:CD1	1.94	0.97
1:B:2329:HIS:HB3	1:B:2344:ASP:HA	1.50	0.93
1:C:3330:ILE:HD12	1:C:3371:GLY:HA3	1.51	0.92
1:A:1329:HIS:HB3	1:A:1344:ASP:HA	1.50	0.92
1:C:3321:PRO:CB	1:C:3373:LEU:CD1	2.46	0.91
1:C:3387:VAL:HG21	1:C:3431:TYR:HE2	1.35	0.90
1:A:1326:CYS:SG	1:A:1376:ILE:HB	2.15	0.86
1:B:2138:THR:H	1:B:2141:GLN:HG3	1.39	0.86
1:C:3487:GLY:H	1:C:3490:SER:HB3	1.42	0.85
1:C:3329:HIS:HB3	1:C:3344:ASP:HA	1.58	0.83
1:C:3321:PRO:HB3	1:C:3373:LEU:HD12	1.60	0.83
1:B:2321:PRO:HB3	1:B:2373:LEU:HD12	1.60	0.83
1:B:2129:PRO:HA	1:B:2180:MET:HE2	1.61	0.82
1:A:1330:ILE:HG22	1:A:1373:LEU:HD23	0.82	0.80
1:B:2326:CYS:SG	1:B:2376:ILE:HB	2.22	0.80
1:A:1327:ASP:HB2	1:A:1379:PRO:HA	1.64	0.80
1:B:2038:GLY:HA3	1:B:2213:ASP:HB3	1.64	0.80
1:B:2119:THR:HG22	1:B:2192:THR:HG22	1.64	0.79
1:B:2272:LEU:HB2	1:B:2452:THR:HG21	1.64	0.79
1:B:2321:PRO:CB	1:B:2373:LEU:CD1	2.41	0.77
1:C:3321:PRO:CG	1:C:3373:LEU:HD11	2.14	0.77
1:B:2321:PRO:HB2	1:B:2373:LEU:HD11	1.67	0.77
1:C:3174:ASP:HB2	1:C:3177:GLN:HG2	1.68	0.75
1:B:2321:PRO:CG	1:B:2373:LEU:HD11	2.16	0.75
1:C:3387:VAL:HG21	1:C:3431:TYR:CE2	2.21	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3328:TRP:HB3	1:C:3376:ILE:HG22	1.67	0.75
1:B:2330:ILE:HG22	1:B:2373:LEU:HD23	0.76	0.74
1:C:3326:CYS:SG	1:C:3376:ILE:HB	2.26	0.74
1:A:1272:LEU:HB2	1:A:1452:THR:HG21	1.68	0.74
1:A:1249:PRO:O	1:A:1423:SER:HB3	1.87	0.73
1:B:2249:PRO:O	1:B:2423:SER:HB3	1.89	0.72
1:B:2061:VAL:HG11	1:C:3144:LEU:HD23	1.70	0.72
1:C:3127:CYS:HB2	1:C:3146:PRO:HG2	1.72	0.71
1:B:2327:ASP:HB2	1:B:2379:PRO:HA	1.71	0.71
1:C:3064:PRO:HB2	1:C:3505:SER:HB3	1.72	0.71
1:C:3472:GLU:OE2	1:C:3514:LYS:HG3	1.91	0.69
1:A:1141:GLN:HA	1:A:1144:LEU:HD12	1.74	0.69
1:A:1399:ILE:HB	1:C:3399:ILE:HG21	1.75	0.69
1:C:3329:HIS:CB	1:C:3344:ASP:HA	2.24	0.68
1:B:2255:ILE:HD11	1:B:2492:PRO:HD2	1.76	0.68
1:C:3421:PHE:O	1:C:3435:CYS:HB3	1.94	0.68
1:C:3315:PRO:HA	1:C:3355:HIS:HD2	1.58	0.68
1:C:3321:PRO:HB2	1:C:3373:LEU:HD11	1.70	0.67
1:B:2119:THR:HG21	1:B:2200:PHE:CE2	2.30	0.66
1:A:1353:VAL:HG13	1:A:1396:GLY:HA3	1.77	0.66
1:C:3310:HIS:O	1:C:3313:GLU:HG2	1.96	0.66
1:C:3330:ILE:HG22	1:C:3373:LEU:CD2	2.14	0.65
1:C:3241:LEU:HD22	1:C:3440:GLU:HG3	1.78	0.65
1:C:3311:PRO:HB2	1:C:3401:GLU:HG3	1.76	0.65
1:A:1116:ASN:ND2	1:A:1200:PHE:CE1	2.65	0.65
1:B:2129:PRO:HA	1:B:2180:MET:CE	2.27	0.65
1:B:2328:TRP:HB3	1:B:2376:ILE:HG22	1.78	0.65
1:C:3287:VAL:HG21	1:C:3439:GLN:OE1	1.95	0.65
1:C:3433:LEU:HD12	1:C:3434:PRO:HD2	1.79	0.65
1:A:1255:ILE:HG23	1:A:1417:VAL:HG11	1.78	0.65
1:A:1387:VAL:HG21	1:A:1431:TYR:HE2	1.60	0.64
1:B:2330:ILE:HD12	1:B:2371:GLY:HA3	1.78	0.64
1:C:3173:ASN:O	1:C:3227:LYS:HD3	1.97	0.64
1:C:3249:PRO:O	1:C:3423:SER:HB3	1.97	0.64
1:A:1321:PRO:HB3	1:A:1373:LEU:HD12	1.79	0.64
1:B:2330:ILE:HG21	1:B:2373:LEU:HD23	1.70	0.64
1:C:3101:ASN:HB3	1:C:3220:VAL:HG21	1.81	0.63
1:B:2116:ASN:HD22	1:B:2200:PHE:HE1	1.45	0.62
1:C:3330:ILE:CG2	1:C:3373:LEU:CD2	2.67	0.62
1:C:3272:LEU:HB2	1:C:3452:THR:HG21	1.82	0.61
1:A:1330:ILE:HD12	1:A:1371:GLY:HA3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3330:ILE:HG23	1:C:3373:LEU:HD23	1.77	0.61
1:C:3327:ASP:HB2	1:C:3379:PRO:HA	1.83	0.60
1:B:2269:ARG:HH22	1:B:2409:VAL:HG13	1.66	0.60
1:B:2484:VAL:O	1:B:2515:PRO:HA	2.02	0.60
1:C:3100:TYR:HA	1:C:3218:PHE:O	2.01	0.60
1:A:1241:LEU:HD22	1:A:1440:GLU:HG3	1.84	0.60
1:C:3071:SER:H	1:C:3074:ASN:ND2	2.00	0.60
1:B:2071:SER:H	1:B:2074:ASN:HD22	1.51	0.59
1:B:2353:VAL:HG13	1:B:2396:GLY:HA3	1.84	0.59
1:A:1148:VAL:HG21	1:A:1160:VAL:HG22	1.84	0.59
1:A:1245:ARG:HB2	1:A:1433:LEU:HD21	1.84	0.59
1:B:2387:VAL:HG21	1:B:2431:TYR:CE2	2.38	0.59
1:B:2192:THR:OG1	1:B:2196:THR:HG23	2.03	0.59
1:A:1119:THR:HG21	1:A:1200:PHE:HE2	1.67	0.59
1:B:2245:ARG:HB2	1:B:2433:LEU:HD21	1.83	0.59
1:C:3343:TYR:CD1	1:C:3364:ILE:HD11	2.38	0.58
1:B:2105:GLY:HA3	1:B:2214:PHE:HA	1.85	0.58
1:B:2200:PHE:CE1	1:C:3191:ARG:HB3	2.39	0.58
1:C:3105:GLY:O	1:C:3164:ASP:HB2	2.04	0.58
1:B:2162:LEU:HD13	1:B:2182:LEU:HG	1.86	0.57
1:A:1057:ILE:HD12	1:A:1212:PRO:HA	1.85	0.57
1:A:1379:PRO:HB2	1:A:1382:PRO:HG3	1.86	0.57
1:C:3321:PRO:HG3	1:C:3373:LEU:HD11	1.85	0.57
1:A:1411:PRO:HD3	1:A:1418:LEU:HG	1.86	0.57
1:A:1125:VAL:HG12	1:A:1182:LEU:HD22	1.87	0.57
1:B:2514:LYS:HZ2	1:C:3076:PRO:HD2	1.70	0.56
1:C:3425:MET:HG3	1:C:3426:PRO:HD2	1.87	0.56
1:A:1037:ALA:O	1:A:1166:ARG:NH2	2.38	0.56
1:A:1060:PHE:HZ	1:A:1108:ARG:HD3	1.70	0.56
1:A:1328:TRP:HB3	1:A:1376:ILE:HG22	1.87	0.56
1:A:1098:GLN:O	1:A:1222:PRO:HA	2.05	0.56
1:A:1071:SER:HB3	1:A:1201:VAL:HG12	1.87	0.56
1:C:3459:LEU:HD11	1:C:3475:ALA:HB2	1.88	0.56
1:C:3353:VAL:HG11	1:C:3356:LEU:HD12	1.88	0.56
1:B:2265:PHE:O	1:B:2269:ARG:HD2	2.04	0.56
1:C:3354:PRO:HD2	1:C:3396:GLY:H	1.68	0.56
1:A:1326:CYS:HG	1:A:1376:ILE:HB	1.69	0.56
1:A:1122:LYS:NZ	1:A:1151:ASP:HB2	2.20	0.56
1:C:3272:LEU:HB2	1:C:3452:THR:CG2	2.36	0.55
1:A:1164:ASP:OD1	1:A:1171:HIS:HE1	1.89	0.55
1:B:2334:GLN:HG3	1:B:2368:ASN:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2113:LEU:O	1:B:2114:ALA:HB2	2.07	0.55
1:A:1242:SER:HB3	1:B:2285:SER:HB3	1.87	0.55
1:C:3271:THR:OG1	1:C:3275:ARG:HB2	2.06	0.55
1:A:1122:LYS:HD2	1:A:1151:ASP:HA	1.89	0.55
1:B:2098:GLN:O	1:B:2222:PRO:HA	2.06	0.55
1:B:2061:VAL:HG11	1:C:3144:LEU:CD2	2.36	0.55
1:A:1255:ILE:HD11	1:A:1492:PRO:HD2	1.87	0.55
1:B:2411:PRO:HD3	1:B:2418:LEU:HG	1.88	0.55
1:A:1321:PRO:CG	1:A:1373:LEU:HD11	2.37	0.54
1:A:1071:SER:H	1:A:1074:ASN:HD22	1.55	0.54
1:C:3292:GLY:O	1:C:3368:ASN:HA	2.08	0.54
1:A:1321:PRO:HB2	1:A:1373:LEU:HD11	1.85	0.54
1:B:2269:ARG:NH2	1:B:2409:VAL:HG13	2.22	0.54
1:A:1104:VAL:HG22	1:A:1170:PHE:HB2	1.90	0.54
1:A:1105:GLY:HA3	1:A:1214:PHE:HA	1.90	0.54
1:C:3334:GLN:HG3	1:C:3368:ASN:O	2.08	0.54
1:C:3085:LEU:HB3	1:C:3179:THR:HB	1.90	0.54
1:A:1065:GLN:HG2	1:A:1506:TRP:HB2	1.90	0.53
1:B:2232:THR:OG1	1:B:2448:GLU:OE1	2.27	0.53
1:C:3064:PRO:HB2	1:C:3505:SER:CB	2.38	0.53
1:C:3484:VAL:O	1:C:3515:PRO:HA	2.08	0.53
1:A:1106:ASN:HD22	1:A:1163:GLU:HA	1.72	0.53
1:C:3326:CYS:HB3	1:C:3328:TRP:HD1	1.74	0.53
1:C:3037:ALA:O	1:C:3166:ARG:NH2	2.42	0.53
1:B:2012:VAL:HG12	1:C:3154:THR:HG21	1.90	0.53
1:A:1221:PRO:HB3	1:C:3144:LEU:HD12	1.89	0.52
1:A:1460:HIS:ND1	1:A:1504:VAL:HG21	2.23	0.52
1:A:1095:HIS:O	1:B:2095:HIS:HE1	1.91	0.52
1:C:3330:ILE:HG22	1:C:3373:LEU:HA	1.91	0.52
1:B:2490:SER:HA	1:B:2494:GLN:NE2	2.25	0.52
1:B:2238:LEU:HB3	1:B:2497:ILE:HG22	1.90	0.52
1:B:2433:LEU:HD12	1:B:2434:PRO:HD2	1.91	0.52
1:B:2288:ALA:HB1	1:B:2373:LEU:HD12	1.91	0.52
1:B:2129:PRO:CA	1:B:2180:MET:HE2	2.36	0.52
1:B:2164:ASP:OD2	1:B:2171:HIS:HE1	1.93	0.52
1:B:2241:LEU:HD22	1:B:2440:GLU:HG3	1.92	0.52
1:B:2514:LYS:NZ	1:C:3076:PRO:HD2	2.25	0.51
1:A:1244:SER:HB2	1:A:1268:GLY:CA	2.39	0.51
1:A:1036:VAL:HB	1:A:1106:ASN:HD21	1.75	0.51
1:C:3211:SER:HB2	1:C:3212:PRO:HD2	1.91	0.51
1:A:1119:THR:HG21	1:A:1200:PHE:CE2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1269:ARG:HH22	1:A:1409:VAL:HG13	1.76	0.51
1:B:2068:PHE:CZ	1:B:2204:GLY:HA3	2.46	0.51
1:A:1116:ASN:HB3	1:A:1118:PHE:H	1.75	0.51
1:C:3293:THR:HA	1:C:3367:GLY:O	2.11	0.51
1:B:2330:ILE:HG22	1:B:2373:LEU:HA	1.92	0.51
1:A:1330:ILE:HG22	1:A:1373:LEU:HA	1.93	0.51
1:A:1243:ASN:HB3	1:A:1246:ALA:O	2.11	0.51
1:A:1050:ASN:HD22	1:A:1100:TYR:HE2	1.58	0.51
1:B:2153:ARG:HB2	1:B:2153:ARG:HH11	1.76	0.51
1:A:1305:ASP:HB2	1:A:1307:THR:OG1	2.11	0.50
1:B:2353:VAL:HG11	1:B:2356:LEU:HD12	1.93	0.50
1:A:1399:ILE:HB	1:C:3399:ILE:CG2	2.40	0.50
1:A:1460:HIS:CD2	1:A:1472:GLU:HG3	2.46	0.50
1:A:1064:PRO:O	1:A:1505:SER:HB2	2.11	0.50
1:C:3123:ILE:CD1	1:C:3184:CYS:SG	2.90	0.50
1:B:2422:MET:HG2	1:B:2434:PRO:HA	1.94	0.50
1:C:3378:PRO:HA	1:C:3387:VAL:HG22	1.93	0.50
1:A:1242:SER:CB	1:B:2285:SER:HB3	2.42	0.49
1:A:1346:ASP:OD1	1:A:1349:PRO:HD3	2.11	0.49
1:B:2200:PHE:CD1	1:C:3191:ARG:HB3	2.47	0.49
1:C:3050:ASN:ND2	1:C:3217:LEU:O	2.46	0.49
1:B:2191:ARG:HH11	1:B:2191:ARG:HG2	1.76	0.49
1:C:3377:SER:OG	1:C:3378:PRO:HD2	2.13	0.49
1:C:3315:PRO:HD3	1:C:3404:HIS:O	2.13	0.49
1:A:1484:VAL:O	1:A:1515:PRO:HA	2.12	0.49
1:A:1029:ASP:HB3	1:A:1030:PRO:HD2	1.94	0.49
1:B:2062:GLN:H	1:C:3143:THR:HG21	1.78	0.49
1:C:3399:ILE:H	1:C:3399:ILE:HD12	1.78	0.49
1:C:3310:HIS:HB3	1:C:3312:PHE:CE2	2.48	0.49
1:C:3105:GLY:HA3	1:C:3214:PHE:HA	1.94	0.49
1:B:2125:VAL:HG12	1:B:2182:LEU:HD22	1.95	0.48
1:A:1387:VAL:HG21	1:A:1431:TYR:CE2	2.45	0.48
1:C:3123:ILE:HG12	1:C:3124:ILE:N	2.28	0.48
1:C:3119:THR:HG22	1:C:3192:THR:HG22	1.95	0.48
1:A:1118:PHE:CD1	1:A:1118:PHE:N	2.81	0.48
1:C:3457:ALA:HB3	1:C:3475:ALA:HB3	1.95	0.48
1:A:1105:GLY:O	1:A:1164:ASP:HB2	2.14	0.48
1:B:2085:LEU:HB3	1:B:2179:THR:HB	1.96	0.48
1:C:3164:ASP:OD1	1:C:3171:HIS:HE1	1.97	0.48
1:B:2125:VAL:CG1	1:B:2182:LEU:HD22	2.43	0.48
1:C:3299:ILE:HB	1:C:3359:ILE:HG13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1321:PRO:CB	1:A:1373:LEU:CD1	2.64	0.48
1:C:3352:PHE:C	1:C:3354:PRO:HD3	2.33	0.48
1:A:1124:ILE:HG12	1:A:1149:ILE:HG12	1.94	0.48
1:A:1118:PHE:N	1:A:1118:PHE:HD1	2.12	0.48
1:C:3459:LEU:HD23	1:C:3503:PHE:HA	1.94	0.48
1:A:1110:ARG:HA	1:A:1158:ILE:O	2.13	0.48
1:A:1340:GLN:HB2	1:B:2375:TRP:CE3	2.49	0.48
1:A:1329:HIS:HE1	1:A:1377:SER:HB2	1.78	0.47
1:A:1334:GLN:HG3	1:A:1368:ASN:O	2.13	0.47
1:B:2293:THR:HG22	1:B:2368:ASN:HB3	1.96	0.47
1:C:3238:LEU:HB3	1:C:3497:ILE:HG22	1.95	0.47
1:A:1439:GLN:HA	1:A:1442:ILE:HD12	1.96	0.47
1:A:1429:GLY:N	1:A:1431:TYR:HE1	2.13	0.47
1:C:3082:ASP:O	1:C:3083:LEU:HD23	2.15	0.47
1:A:1272:LEU:HB2	1:A:1452:THR:CG2	2.43	0.47
1:B:2321:PRO:HG3	1:B:2373:LEU:HD11	1.95	0.46
1:A:1162:LEU:HD13	1:A:1182:LEU:HG	1.97	0.46
1:A:1244:SER:HB2	1:A:1268:GLY:HA2	1.98	0.46
1:B:2090:ASN:HB3	1:B:2093:LEU:HD12	1.98	0.46
1:B:2413:GLY:HA3	1:B:2416:GLU:CD	2.36	0.46
1:A:1110:ARG:NH1	1:A:1159:GLU:OE1	2.49	0.46
1:C:3182:LEU:HA	1:C:3182:LEU:HD23	1.79	0.46
1:C:3071:SER:HA	1:C:3201:VAL:HG12	1.97	0.46
1:B:2238:LEU:HB3	1:B:2497:ILE:CG2	2.46	0.46
1:B:2252:SER:HA	1:B:2497:ILE:HD11	1.98	0.46
1:B:2293:THR:HA	1:B:2367:GLY:O	2.16	0.45
1:B:2473:PHE:CD1	1:B:2501:PHE:HE2	2.34	0.45
1:A:1238:LEU:HB3	1:A:1497:ILE:HG22	1.97	0.45
1:B:2107:MET:CE	1:B:2208:THR:HB	2.46	0.45
1:B:2191:ARG:NH1	1:B:2191:ARG:HG2	2.30	0.45
1:A:1474:LYS:HG3	1:A:1513:LEU:HD21	1.98	0.45
1:B:2330:ILE:HG21	1:B:2373:LEU:CD2	2.39	0.45
1:A:1242:SER:HB3	1:B:2285:SER:CB	2.46	0.45
1:A:1095:HIS:HE1	1:B:2095:HIS:O	1.99	0.45
1:A:1031:LEU:HD12	1:A:1161:PRO:HG2	1.98	0.45
1:A:1221:PRO:HA	1:A:1222:PRO:HD3	1.78	0.45
1:C:3422:MET:HA	1:C:3433:LEU:O	2.16	0.45
1:C:3269:ARG:HH11	1:C:3406:ALA:HB1	1.80	0.45
1:A:1071:SER:H	1:A:1074:ASN:ND2	2.14	0.45
1:A:1292:GLY:O	1:A:1368:ASN:HA	2.17	0.45
1:C:3090:ASN:HA	1:C:3091:PRO:HD2	1.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1376:ILE:CD1	1:A:1425:MET:HG2	2.47	0.45
1:C:3455:GLU:OE1	1:C:3509:ARG:HB2	2.18	0.45
1:C:3472:GLU:HG2	1:C:3513:LEU:HD22	1.99	0.44
1:A:1453:VAL:O	1:A:1506:TRP:CD2	2.71	0.44
1:C:3255:ILE:HD11	1:C:3492:PRO:HD2	1.99	0.44
1:B:2431:TYR:CD1	1:B:2431:TYR:N	2.85	0.44
1:B:2104:VAL:HG13	1:B:2170:PHE:HA	1.98	0.44
1:B:2022:VAL:HG12	1:B:2153:ARG:HD2	2.00	0.44
1:C:3282:VAL:HG23	1:C:3283:SER:N	2.33	0.44
1:A:1352:PHE:C	1:A:1354:PRO:HD3	2.38	0.44
1:C:3271:THR:HG22	1:C:3477:PRO:O	2.17	0.44
1:B:2222:PRO:O	1:B:2223:THR:CB	2.65	0.44
1:B:2487:GLY:H	1:B:2490:SER:HB3	1.82	0.44
1:C:3238:LEU:HB3	1:C:3497:ILE:CG2	2.47	0.44
1:B:2010:SER:OG	1:C:3029:ASP:HB2	2.17	0.44
1:B:2069:THR:HG23	1:B:2511:TYR:CE1	2.53	0.44
1:B:2013:ASP:HB2	1:B:2155:LEU:HD22	2.00	0.44
1:A:1071:SER:HB2	1:A:1072:PRO:HD2	1.98	0.43
1:A:1487:GLY:H	1:A:1490:SER:HB3	1.83	0.43
1:C:3280:THR:HA	1:C:3281:PRO:HD3	1.75	0.43
1:A:1255:ILE:HG22	1:A:1256:SER:O	2.18	0.43
1:A:1122:LYS:HZ2	1:A:1151:ASP:HB2	1.81	0.43
1:B:2037:ALA:O	1:B:2166:ARG:NH2	2.51	0.43
1:B:2064:PRO:HG3	1:B:2088:HIS:O	2.19	0.43
1:A:1422:MET:HA	1:A:1433:LEU:O	2.18	0.43
1:B:2082:ASP:OD1	1:B:2181:ARG:HD2	2.18	0.43
1:C:3244:SER:OG	1:C:3268:GLY:HA3	2.19	0.43
1:C:3300:ASN:HA	1:C:3357:GLY:O	2.18	0.43
1:A:1182:LEU:HA	1:A:1182:LEU:HD23	1.78	0.43
1:C:3192:THR:HG21	1:C:3200:PHE:CD2	2.53	0.43
1:A:1490:SER:HA	1:A:1494:GLN:NE2	2.33	0.43
1:B:2064:PRO:O	1:B:2505:SER:HB2	2.19	0.43
1:A:1252:SER:HA	1:A:1497:ILE:CD1	2.49	0.43
1:A:1263:VAL:HG12	1:A:1264:GLN:N	2.34	0.43
1:A:1324:GLY:HA3	1:A:1391:LYS:C	2.38	0.43
1:A:1061:VAL:HG12	1:A:1062:GLN:N	2.33	0.43
1:A:1381:HIS:N	1:A:1382:PRO:HD2	2.34	0.43
1:C:3244:SER:OG	1:C:3435:CYS:SG	2.76	0.43
1:C:3453:VAL:O	1:C:3506:TRP:CD2	2.72	0.43
1:C:3329:HIS:HB2	1:C:3343:TYR:O	2.19	0.42
1:B:2327:ASP:HB2	1:B:2379:PRO:CA	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2346:ASP:OD1	1:B:2349:PRO:HD3	2.19	0.42
1:B:2431:TYR:HD1	1:B:2431:TYR:N	2.17	0.42
1:C:3282:VAL:HG23	1:C:3283:SER:H	1.84	0.42
1:B:2021:LEU:HB3	1:B:2117:ALA:HB1	2.00	0.42
1:B:2377:SER:OG	1:B:2378:PRO:HD2	2.19	0.42
1:B:2244:SER:HB3	1:B:2268:GLY:CA	2.49	0.42
1:A:1100:TYR:HA	1:A:1218:PHE:O	2.19	0.42
1:A:1233:LEU:HA	1:A:1233:LEU:HD23	1.84	0.42
1:B:2453:VAL:O	1:B:2506:TRP:CD2	2.72	0.42
1:C:3422:MET:HG2	1:C:3434:PRO:HA	2.02	0.42
1:A:1433:LEU:HA	1:A:1434:PRO:HD3	1.73	0.42
1:B:2292:GLY:O	1:B:2368:ASN:HA	2.20	0.42
1:B:2284:LEU:HD23	1:B:2287:VAL:HG21	2.02	0.42
1:C:3324:GLY:HA3	1:C:3391:LYS:C	2.40	0.42
1:A:1376:ILE:O	1:A:1428:PRO:HD2	2.20	0.42
1:B:2221:PRO:HA	1:B:2222:PRO:HD2	1.57	0.42
1:A:1264:GLN:HG3	1:A:1408:SER:HB3	2.02	0.42
1:A:1327:ASP:HB2	1:A:1379:PRO:CA	2.41	0.42
1:A:1119:THR:CG2	1:A:1200:PHE:CE2	3.03	0.42
1:A:1392:ILE:HD11	1:A:1395:TYR:HE1	1.84	0.42
1:A:1399:ILE:CG1	1:C:3399:ILE:HG12	2.49	0.42
1:A:1224:VAL:HG12	1:C:3135:HIS:CD2	2.55	0.42
1:B:2459:LEU:HD23	1:B:2503:PHE:HA	2.01	0.42
1:B:2071:SER:HB2	1:B:2201:VAL:HG12	2.02	0.42
1:C:3109:VAL:HG22	1:C:3208:THR:HG22	2.02	0.42
1:C:3375:TRP:CD1	1:C:3375:TRP:C	2.92	0.42
1:A:1060:PHE:CZ	1:A:1108:ARG:HD3	2.54	0.41
1:A:1271:THR:OG1	1:A:1275:ARG:HB2	2.20	0.41
1:A:1042:ALA:HB2	1:A:1170:PHE:HB3	2.02	0.41
1:B:2252:SER:HA	1:B:2497:ILE:CD1	2.50	0.41
1:A:1031:LEU:HD22	1:A:1146:PRO:HB2	2.01	0.41
1:A:1271:THR:HG22	1:A:1477:PRO:O	2.20	0.41
1:A:1294:SER:O	1:A:1366:SER:HA	2.20	0.41
1:B:2039:SER:OG	1:B:2215:ASN:HB2	2.19	0.41
1:A:1399:ILE:HB	1:C:3399:ILE:HG12	2.03	0.41
1:A:1356:LEU:HG	1:A:1398:SER:OG	2.21	0.41
1:B:2269:ARG:NH2	1:B:2407:PRO:O	2.53	0.41
1:A:1243:ASN:OD1	1:A:1244:SER:N	2.53	0.41
1:C:3083:LEU:O	1:C:3181:ARG:HA	2.20	0.41
1:B:2310:HIS:O	1:B:2313:GLU:HB3	2.21	0.41
1:B:2071:SER:N	1:B:2074:ASN:HD22	2.16	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2036:VAL:HG11	1:B:2164:ASP:O	2.21	0.41
1:A:1217:LEU:HA	1:A:1217:LEU:HD23	1.87	0.41
1:C:3221:PRO:HA	1:C:3222:PRO:HD2	1.80	0.41
1:B:2175:ARG:HG2	1:B:2175:ARG:O	2.20	0.41
1:A:1268:GLY:H	1:A:1280:THR:HG23	1.85	0.41
1:A:1340:GLN:HB2	1:B:2375:TRP:HE3	1.85	0.41
1:C:3269:ARG:NH1	1:C:3406:ALA:HB1	2.36	0.41
1:C:3302:THR:HB	1:C:3307:THR:O	2.21	0.41
1:B:2270:CYS:O	1:B:2479:GLY:HA3	2.21	0.41
1:A:1346:ASP:OD1	1:A:1381:HIS:HB2	2.20	0.41
1:A:1399:ILE:HG13	1:C:3399:ILE:HG12	2.03	0.41
1:B:2090:ASN:HA	1:B:2091:PRO:HD2	1.90	0.41
1:C:3098:GLN:O	1:C:3222:PRO:HA	2.21	0.41
1:B:2233:LEU:HD23	1:B:2233:LEU:HA	1.87	0.41
1:A:1421:PHE:CE1	1:A:1438:PRO:HD3	2.56	0.41
1:C:3286:HIS:O	1:C:3319:GLY:HA3	2.20	0.41
1:A:1331:ASN:OD1	1:A:1340:GLN:HG3	2.21	0.40
1:B:2110:ARG:HA	1:B:2158:ILE:O	2.22	0.40
1:A:1353:VAL:HG12	1:A:1356:LEU:HB2	2.03	0.40
1:B:2294:SER:N	1:B:2367:GLY:O	2.54	0.40
1:C:3194:GLY:C	1:C:3196:THR:H	2.25	0.40
1:C:3268:GLY:H	1:C:3280:THR:HG23	1.86	0.40
1:A:1116:ASN:ND2	1:A:1200:PHE:CZ	2.90	0.40
1:C:3497:ILE:HG22	1:C:3497:ILE:O	2.21	0.40
1:A:1252:SER:HA	1:A:1497:ILE:HD11	2.03	0.40
1:C:3463:ASP:HB2	1:C:3470:LEU:HD11	2.04	0.40
1:A:1081:PHE:CZ	1:A:1184:CYS:HB2	2.57	0.40
1:B:2264:GLN:CG	1:B:2408:SER:HB3	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	490/530 (92%)	444 (91%)	41 (8%)	5 (1%)	19 63
1	B	509/530 (96%)	460 (90%)	39 (8%)	10 (2%)	9 48
1	C	490/530 (92%)	445 (91%)	35 (7%)	10 (2%)	9 48
All	All	1489/1590 (94%)	1349 (91%)	115 (8%)	25 (2%)	11 51

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1383	SER
1	B	2114	ALA
1	C	3383	SER
1	A	1196	THR
1	A	1362	ASN
1	B	2223	THR
1	B	2486	ASN
1	C	3173	ASN
1	C	3196	THR
1	C	3362	ASN
1	C	3396	GLY
1	B	2040	SER
1	B	2196	THR
1	B	2222	PRO
1	B	2362	ASN
1	B	2363	GLY
1	B	2383	SER
1	C	3043	VAL
1	C	3363	GLY
1	C	3324	GLY
1	C	3397	SER
1	B	2396	GLY
1	C	3057	ILE
1	A	1363	GLY
1	A	1396	GLY

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	418/445 (94%)	394 (94%)	24 (6%)	25 65
1	B	431/445 (97%)	412 (96%)	19 (4%)	35 73
1	C	418/445 (94%)	403 (96%)	15 (4%)	42 78
All	All	1267/1335 (95%)	1209 (95%)	58 (5%)	33 72

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1041	THR
1	A	1045	THR
1	A	1084	SER
1	A	1101	ASN
1	A	1118	PHE
1	A	1124	ILE
1	A	1141	GLN
1	A	1154	THR
1	A	1179	THR
1	A	1180	MET
1	A	1191	ARG
1	A	1205	ARG
1	A	1259	ASN
1	A	1264	GLN
1	A	1271	THR
1	A	1284	LEU
1	A	1307	THR
1	A	1329	HIS
1	A	1385	SER
1	A	1408	SER
1	A	1423	SER
1	A	1425	MET
1	A	1432	ASN
1	A	1440	GLU
1	B	2011	SER
1	B	2084	SER
1	B	2104	VAL
1	B	2126	SER
1	B	2153	ARG
1	B	2156	ASP
1	B	2182	LEU
1	B	2240	SER
1	B	2259	ASN
1	B	2273	ASP

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Mol	Chain	Res	Type
1	B	2305	ASP
1	B	2307	THR
1	B	2329	HIS
1	B	2360	GLN
1	B	2423	SER
1	B	2425	MET
1	B	2431	TYR
1	B	2440	GLU
1	B	2460	HIS
1	C	3031	LEU
1	C	3101	ASN
1	C	3104	VAL
1	C	3108	ARG
1	C	3135	HIS
1	C	3136	ASN
1	C	3205	ARG
1	C	3271	THR
1	C	3305	ASP
1	C	3307	THR
1	C	3358	SER
1	C	3400	THR
1	C	3423	SER
1	C	3440	GLU
1	C	3509	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1074	ASN
1	A	1095	HIS
1	A	1106	ASN
1	A	1116	ASN
1	A	1171	HIS
1	A	1342	GLN
1	B	2074	ASN
1	B	2095	HIS
1	B	2171	HIS
1	B	2342	GLN
1	B	2444	HIS
1	C	3050	ASN
1	C	3059	ASN
1	C	3074	ASN

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Mol	Chain	Res	Type
1	C	3135	HIS
1	C	3171	HIS
1	C	3177	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 carbohydrates 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 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.