



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 9, 2024 – 10:22 PM EST

PDB ID : 1CSJ
Title : CRYSTAL STRUCTURE OF THE RNA-DEPENDENT RNA POLYMERASE OF HEPATITIS C VIRUS
Authors : Bressanelli, S.; Tomei, L.; Roussel, A.; Incitti, I.; Vitale, R.L.; Mathieu, M.; De Francesco, R.; Rey, F.A.
Deposited on : 1999-08-18
Resolution : 2.80 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 : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 1.20.1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

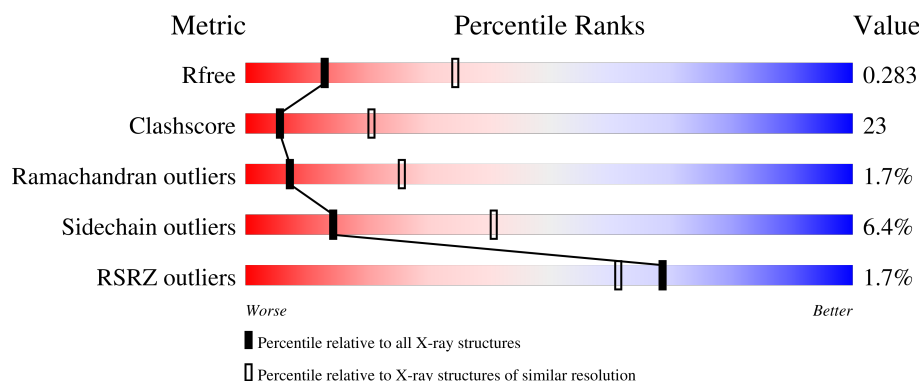
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	3657 (2.80-2.80)
Clashscore	180529	4123 (2.80-2.80)
Ramachandran outliers	177936	4071 (2.80-2.80)
Sidechain outliers	177891	4073 (2.80-2.80)
RSRZ outliers	164620	3659 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	531	
1	B	531	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8428 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 HEPATITIS C VIRUS RNA POLYMERASE (NS5B).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	531	Total 4122	C 2595	N 727	O 769	S 19	Se 12	1	0	0
1	B	531	Total 4122	C 2595	N 727	O 769	S 19	Se 12	1	0	0

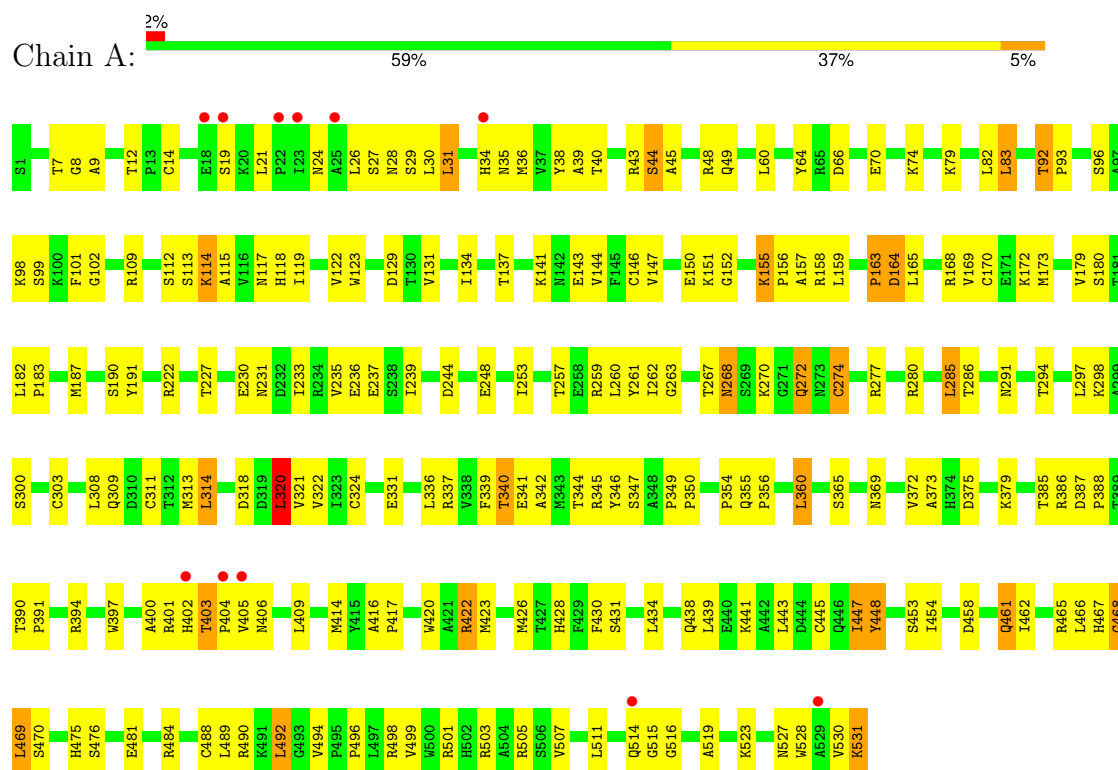
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	94	Total 94	O 94	0	0
2	B	90	Total 90	O 90	0	0

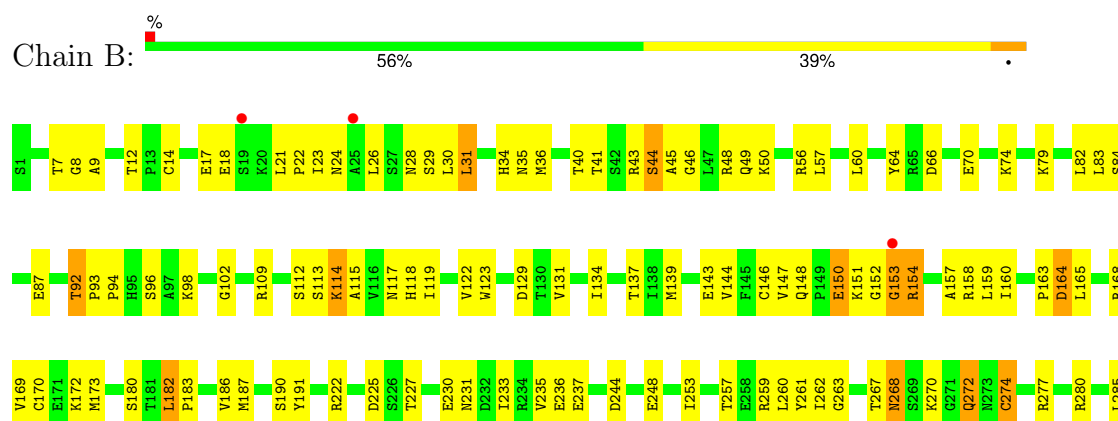
3 Residue-property plots

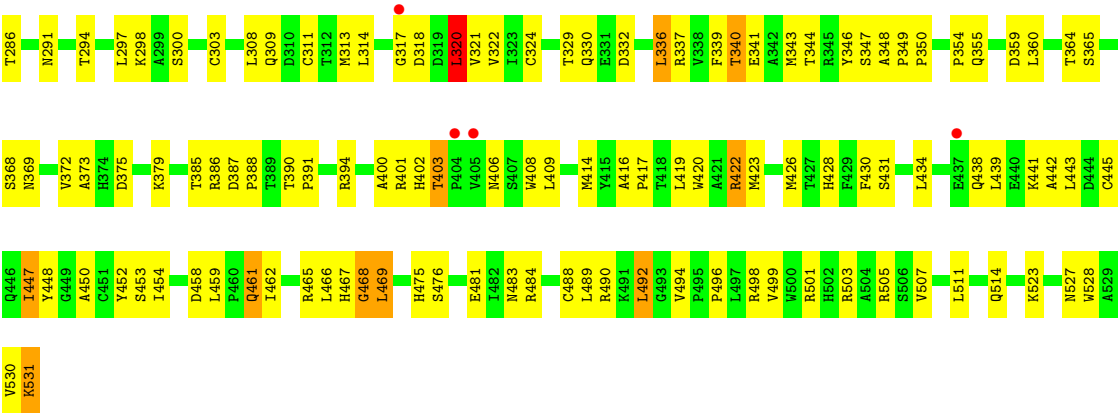
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: HEPATITIS C VIRUS RNA POLYMERASE (NS5B)



• Molecule 1: HEPATITIS C VIRUS RNA POLYMERASE (NS5B)





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	67.06Å 96.89Å 194.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.00 – 2.80 19.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	92.5 (19.00-2.80) 92.1 (19.00-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.46 (at 2.79Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.237 , 0.286 0.236 , 0.283	Depositor DCC
R_{free} test set	1985 reflections (6.74%)	wwPDB-VP
Wilson B-factor (Å ²)	30.2	Xtrriage
Anisotropy	0.695	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 52.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8428	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 58.96 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.8951e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.50	0/4198	0.68	3/5676 (0.1%)
1	B	0.49	0/4198	0.69	2/5676 (0.0%)
All	All	0.49	0/8396	0.68	5/11352 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	320	LEU	CA-CB-CG	5.35	127.61	115.30
1	A	468	GLY	N-CA-C	5.30	126.35	113.10
1	A	320	LEU	CA-CB-CG	5.29	127.46	115.30
1	B	468	GLY	N-CA-C	5.28	126.29	113.10
1	A	163	PRO	N-CA-C	5.14	125.46	112.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	4122	0	4140	184	0
1	B	4122	0	4140	203	0
2	A	94	0	0	8	0
2	B	90	0	0	11	0
All	All	8428	0	8280	380	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 23.

All (380) 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:7:THR:O	1:B:9:ALA:N	1.89	1.04
1:A:170:CYS:HA	1:A:173:MSE:HE3	1.43	1.00
1:B:170:CYS:HA	1:B:173:MSE:HE3	1.44	0.99
1:B:344:THR:HG22	1:B:349:PRO:HA	1.43	0.98
1:A:344:THR:HG22	1:A:349:PRO:HA	1.46	0.97
1:A:7:THR:O	1:A:9:ALA:N	2.04	0.90
1:A:385:THR:HG22	1:A:386:ARG:H	1.37	0.89
1:A:48:ARG:HG2	1:A:159:LEU:HG	1.54	0.88
1:B:48:ARG:HG2	1:B:159:LEU:HG	1.53	0.88
1:B:148:GLN:HB3	1:B:150:GLU:HG2	1.56	0.87
1:A:96:SER:HB3	1:A:168:ARG:HH12	1.41	0.86
1:B:385:THR:HG22	1:B:386:ARG:H	1.40	0.85
1:B:7:THR:O	1:B:7:THR:HG23	1.76	0.84
1:B:96:SER:HB3	1:B:168:ARG:HH12	1.42	0.84
1:A:369:ASN:HD21	1:A:484:ARG:HH22	1.26	0.81
1:A:24:ASN:HD21	1:A:26:LEU:HB3	1.44	0.81
1:B:280:ARG:HE	1:B:291:ASN:HD21	1.25	0.81
1:B:385:THR:HG21	1:B:481:GLU:OE2	1.81	0.81
1:A:280:ARG:HE	1:A:291:ASN:HD21	1.29	0.80
1:B:369:ASN:HD21	1:B:484:ARG:HH22	1.29	0.80
1:A:79:LYS:HE2	1:B:79:LYS:HE2	1.63	0.79
1:B:253:ILE:O	1:B:257:THR:HG23	1.83	0.78
1:B:147:VAL:O	1:B:148:GLN:HG3	1.85	0.77
1:B:31:LEU:HD21	1:B:492:LEU:HD12	1.65	0.77
1:B:98:LYS:HD3	2:B:541:HOH:O	1.84	0.76
1:B:115:ALA:O	1:B:119:ILE:HG12	1.85	0.76
1:A:163:PRO:O	1:A:164:ASP:HB3	1.85	0.76
1:A:98:LYS:HD3	2:A:565:HOH:O	1.87	0.75
1:A:385:THR:HG21	1:A:481:GLU:OE2	1.87	0.75
1:A:31:LEU:HD21	1:A:492:LEU:HD12	1.68	0.74
1:A:498:ARG:HA	1:A:501:ARG:NH1	2.02	0.74
1:A:268:ASN:HB3	1:A:270:LYS:H	1.53	0.74
1:B:375:ASP:OD1	1:B:379:LYS:HG2	1.88	0.74
1:A:498:ARG:HA	1:A:501:ARG:HH12	1.53	0.73
1:B:163:PRO:O	1:B:164:ASP:HB3	1.89	0.73
1:A:309:GLN:O	1:A:324:CYS:HB2	1.90	0.72
1:A:222:ARG:HD3	2:A:602:HOH:O	1.87	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:268:ASN:HB3	1:B:270:LYS:H	1.55	0.72
1:B:498:ARG:HA	1:B:501:ARG:HH12	1.55	0.72
1:A:428:HIS:O	1:A:431:SER:HB3	1.90	0.71
1:B:23:ILE:HG22	1:B:24:ASN:N	2.05	0.71
1:B:498:ARG:HA	1:B:501:ARG:NH1	2.06	0.71
1:A:253:ILE:O	1:A:257:THR:HG23	1.91	0.71
1:A:375:ASP:OD1	1:A:379:LYS:HG2	1.90	0.71
1:A:280:ARG:HE	1:A:291:ASN:ND2	1.89	0.71
1:B:280:ARG:HE	1:B:291:ASN:ND2	1.87	0.70
1:A:26:LEU:O	1:A:29:SER:HB3	1.91	0.70
1:A:530:VAL:HG12	1:A:531:LYS:HZ2	1.57	0.70
1:A:414:MSE:HG2	1:A:448:TYR:OH	1.91	0.70
1:B:468:GLY:O	1:B:469:LEU:HB2	1.92	0.69
1:B:336:LEU:O	1:B:340:THR:HG22	1.91	0.69
1:A:163:PRO:O	1:A:164:ASP:CB	2.41	0.69
1:A:24:ASN:ND2	1:A:26:LEU:HB3	2.08	0.69
1:A:313:MSE:HG2	1:A:322:VAL:HG22	1.74	0.69
1:B:490:ARG:HH11	1:B:490:ARG:HG2	1.58	0.69
1:B:309:GLN:O	1:B:324:CYS:HB2	1.93	0.68
1:B:163:PRO:O	1:B:164:ASP:CB	2.41	0.68
1:A:340:THR:O	1:A:344:THR:HG23	1.94	0.68
1:B:14:CYS:HB2	1:B:139:MSE:HE1	1.76	0.68
1:B:313:MSE:HG2	1:B:322:VAL:HG22	1.76	0.68
1:A:385:THR:HG22	1:A:386:ARG:N	2.09	0.67
1:B:428:HIS:O	1:B:431:SER:HB3	1.94	0.67
1:B:439:LEU:HD23	1:B:439:LEU:O	1.95	0.67
1:B:530:VAL:HG12	1:B:531:LYS:HZ2	1.59	0.66
1:A:115:ALA:O	1:A:119:ILE:HG12	1.95	0.66
1:A:237:GLU:HG3	1:A:257:THR:HG21	1.78	0.66
1:B:151:LYS:HG2	1:B:152:GLY:H	1.60	0.66
1:A:19:SER:HB2	2:A:580:HOH:O	1.95	0.66
1:B:7:THR:O	1:B:7:THR:CG2	2.44	0.66
1:B:523:LYS:O	1:B:527:ASN:HB2	1.96	0.66
1:A:490:ARG:HG2	1:A:490:ARG:HH11	1.60	0.65
1:B:237:GLU:HG3	1:B:257:THR:HG21	1.77	0.65
1:B:26:LEU:O	1:B:29:SER:HB3	1.96	0.65
1:B:231:ASN:O	1:B:235:VAL:HG23	1.97	0.65
1:B:468:GLY:O	1:B:469:LEU:CB	2.45	0.65
1:A:523:LYS:O	1:A:527:ASN:HB2	1.97	0.65
1:A:439:LEU:O	1:A:439:LEU:HD23	1.96	0.64
1:A:468:GLY:O	1:A:469:LEU:HB2	1.96	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:ILE:HG13	1:A:259:ARG:HB3	1.77	0.64
1:B:340:THR:O	1:B:344:THR:HG23	1.98	0.64
1:B:414:MSE:HG2	1:B:448:TYR:OH	1.98	0.64
1:A:336:LEU:O	1:A:340:THR:HG22	1.98	0.63
1:B:336:LEU:HD12	1:B:354:PRO:HG2	1.79	0.63
1:A:336:LEU:HD12	1:A:354:PRO:HG2	1.79	0.63
1:B:409:LEU:HD23	1:B:445:CYS:HB2	1.80	0.63
1:A:93:PRO:HG2	1:A:96:SER:OG	1.98	0.63
1:A:400:ALA:O	1:A:401:ARG:HG2	1.99	0.63
1:B:530:VAL:HG12	1:B:531:LYS:NZ	2.14	0.63
1:A:308:LEU:HB2	1:A:311:CYS:SG	2.38	0.62
1:B:66:ASP:O	1:B:70:GLU:HG3	1.99	0.62
1:B:400:ALA:O	1:B:401:ARG:HG2	2.00	0.62
1:A:530:VAL:HG12	1:A:531:LYS:NZ	2.14	0.62
1:A:60:LEU:HD13	1:A:64:TYR:CE2	2.34	0.61
2:A:574:HOH:O	1:B:112:SER:HB2	2.00	0.61
1:B:23:ILE:HG22	1:B:24:ASN:H	1.64	0.61
1:B:423:MSE:HG2	1:B:528:TRP:CZ3	2.35	0.61
1:B:119:ILE:HG22	1:B:173:MSE:HE1	1.82	0.61
1:B:143:GLU:OE2	1:B:158:ARG:HD3	1.99	0.61
1:B:346:TYR:O	1:B:347:SER:HB3	1.98	0.61
1:B:496:PRO:HG2	1:B:499:VAL:HG23	1.83	0.61
1:B:423:MSE:HG2	1:B:528:TRP:CH2	2.36	0.61
1:A:66:ASP:O	1:A:70:GLU:HG3	2.00	0.61
1:B:330:GLN:HB2	2:B:538:HOH:O	2.01	0.61
1:A:496:PRO:HG2	1:A:499:VAL:HG23	1.84	0.60
1:A:468:GLY:O	1:A:469:LEU:CB	2.48	0.60
1:B:294:THR:CG2	1:B:298:LYS:HE3	2.31	0.60
1:B:23:ILE:N	1:B:23:ILE:HD12	2.16	0.60
1:B:92:THR:HG21	1:B:169:VAL:HG22	1.83	0.60
1:A:180:SER:O	1:A:183:PRO:HD2	2.01	0.59
1:A:423:MSE:HG2	1:A:528:TRP:CH2	2.37	0.59
1:B:40:THR:HB	1:B:157:ALA:HB2	1.84	0.59
1:A:531:LYS:HD3	1:A:531:LYS:N	2.17	0.59
1:B:123:TRP:HZ2	1:B:248:GLU:HG2	1.67	0.59
1:B:308:LEU:HB2	1:B:311:CYS:SG	2.43	0.59
1:B:257:THR:HA	1:B:261:TYR:HB2	1.85	0.59
1:B:332:ASP:HA	2:B:604:HOH:O	2.03	0.59
1:A:346:TYR:O	1:A:347:SER:HB3	2.03	0.58
1:A:465:ARG:NH1	1:B:117:ASN:OD1	2.36	0.58
1:A:505:ARG:HG2	1:A:530:VAL:HG22	1.84	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:ILE:HG13	1:B:259:ARG:HB3	1.85	0.58
1:A:409:LEU:HD23	1:A:445:CYS:HB2	1.84	0.58
1:B:9:ALA:HB3	1:B:274:CYS:HA	1.85	0.58
1:B:257:THR:O	1:B:262:ILE:HB	2.03	0.58
1:B:31:LEU:HD21	1:B:492:LEU:CD1	2.31	0.58
1:A:423:MSE:HG2	1:A:528:TRP:CZ3	2.38	0.58
1:B:531:LYS:HD3	1:B:531:LYS:N	2.18	0.58
1:A:321:VAL:CG2	1:A:365:SER:HB2	2.34	0.58
1:A:489:LEU:HD22	1:A:494:VAL:CG2	2.33	0.57
1:A:141:LYS:HD3	1:A:158:ARG:NH2	2.18	0.57
1:A:321:VAL:HG21	1:A:365:SER:CB	2.34	0.57
1:A:237:GLU:CG	1:A:257:THR:HG21	2.35	0.57
1:A:406:ASN:ND2	1:A:443:LEU:HB3	2.19	0.57
1:A:294:THR:CG2	1:A:298:LYS:HE3	2.35	0.57
1:A:257:THR:HA	1:A:261:TYR:HB2	1.86	0.57
1:B:385:THR:HG22	1:B:386:ARG:N	2.15	0.57
1:A:123:TRP:HZ2	1:A:248:GLU:HG2	1.70	0.57
1:B:329:THR:HG23	2:B:580:HOH:O	2.04	0.57
1:B:505:ARG:HG2	1:B:530:VAL:HG22	1.86	0.57
1:A:40:THR:HB	1:A:157:ALA:HB2	1.87	0.56
1:B:180:SER:O	1:B:183:PRO:HD2	2.05	0.56
1:B:43:ARG:HG3	1:B:43:ARG:HH11	1.70	0.56
1:B:93:PRO:HG2	1:B:96:SER:OG	2.04	0.56
1:B:237:GLU:CG	1:B:257:THR:HG21	2.35	0.56
1:B:369:ASN:HD21	1:B:484:ARG:NH2	2.00	0.56
1:A:369:ASN:HD21	1:A:484:ARG:NH2	2.00	0.56
1:A:401:ARG:HG3	1:A:401:ARG:HH11	1.70	0.56
1:B:7:THR:HG22	1:B:274:CYS:C	2.26	0.56
1:B:43:ARG:HG3	1:B:43:ARG:NH1	2.21	0.56
1:B:83:LEU:HB2	1:B:173:MSE:HA	1.88	0.56
1:A:117:ASN:OD1	1:B:465:ARG:NH1	2.39	0.55
1:B:300:SER:OG	1:B:313:MSE:HE1	2.06	0.55
1:A:385:THR:CG2	1:A:420:TRP:HE1	2.20	0.55
1:A:388:PRO:HG2	1:A:488:CYS:SG	2.47	0.55
1:A:321:VAL:CG2	1:A:365:SER:CB	2.83	0.55
1:B:321:VAL:CG2	1:B:365:SER:HB2	2.37	0.55
1:B:321:VAL:HG21	1:B:365:SER:CB	2.37	0.55
1:A:489:LEU:HD22	1:A:494:VAL:HG21	1.87	0.55
1:B:402:HIS:CG	1:B:403:THR:N	2.75	0.55
1:A:109:ARG:HG3	1:A:109:ARG:HH11	1.72	0.54
1:A:9:ALA:HB3	1:A:274:CYS:HA	1.87	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:LEU:HD13	1:B:64:TYR:CE2	2.42	0.54
1:A:43:ARG:HG3	1:A:43:ARG:HH11	1.72	0.54
1:A:31:LEU:HD21	1:A:492:LEU:CD1	2.37	0.54
1:A:475:HIS:O	1:A:476:SER:HB2	2.08	0.54
1:A:43:ARG:HG3	1:A:43:ARG:NH1	2.22	0.54
1:B:257:THR:HG22	1:B:261:TYR:HD2	1.72	0.54
1:B:385:THR:CG2	1:B:420:TRP:HE1	2.20	0.54
1:A:119:ILE:HG22	1:A:173:MSE:HE1	1.88	0.54
1:B:337:ARG:HA	1:B:340:THR:HG23	1.90	0.54
1:A:336:LEU:HD12	1:A:354:PRO:CG	2.38	0.54
1:A:82:LEU:HD11	1:A:248:GLU:HB3	1.90	0.53
1:B:263:GLY:HA2	1:B:277:ARG:NH1	2.23	0.53
1:A:83:LEU:HB2	1:A:173:MSE:HA	1.90	0.53
1:A:257:THR:HG22	1:A:261:TYR:HD2	1.72	0.53
1:A:337:ARG:HA	1:A:340:THR:HG23	1.90	0.53
1:B:321:VAL:CG2	1:B:365:SER:CB	2.85	0.53
1:B:503:ARG:O	1:B:507:VAL:HG23	2.08	0.53
1:B:336:LEU:HD12	1:B:354:PRO:CG	2.39	0.53
1:B:23:ILE:CG2	1:B:24:ASN:N	2.71	0.53
1:B:82:LEU:HD11	1:B:248:GLU:HB3	1.91	0.53
1:B:489:LEU:HD22	1:B:494:VAL:CG2	2.39	0.53
1:A:92:THR:HG21	1:A:169:VAL:HG22	1.90	0.53
1:A:30:LEU:O	1:A:494:VAL:HB	2.10	0.52
1:A:257:THR:O	1:A:262:ILE:HB	2.08	0.52
1:A:12:THR:OG1	1:A:270:LYS:HG2	2.09	0.52
1:A:187:MSE:HB2	1:A:190:SER:HB2	1.91	0.52
1:A:336:LEU:O	1:A:339:PHE:HB3	2.09	0.52
1:B:12:THR:OG1	1:B:270:LYS:HG2	2.08	0.52
1:B:475:HIS:O	1:B:476:SER:HB2	2.09	0.52
1:B:483:ASN:HB2	2:B:596:HOH:O	2.08	0.52
1:A:96:SER:HB3	1:A:168:ARG:NH1	2.19	0.52
1:B:337:ARG:O	1:B:341:GLU:HG3	2.09	0.52
1:B:14:CYS:CB	1:B:139:MSE:HE1	2.40	0.52
1:B:434:LEU:HD11	1:B:511:LEU:HG	1.92	0.52
1:A:233:ILE:HD13	1:A:261:TYR:O	2.10	0.52
1:A:503:ARG:O	1:A:507:VAL:HG23	2.10	0.52
1:B:23:ILE:CG2	1:B:24:ASN:H	2.23	0.52
1:B:163:PRO:HG2	1:B:168:ARG:HG3	1.92	0.52
1:A:434:LEU:HD11	1:A:511:LEU:HG	1.92	0.52
1:A:231:ASN:O	1:A:235:VAL:HG23	2.10	0.52
1:B:187:MSE:HB2	1:B:190:SER:HB2	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:385:THR:CG2	1:B:386:ARG:H	2.20	0.51
1:B:233:ILE:HD13	1:B:261:TYR:O	2.11	0.51
1:A:507:VAL:HG12	1:A:511:LEU:HD12	1.92	0.51
1:B:30:LEU:O	1:B:494:VAL:HB	2.10	0.51
1:B:484:ARG:NE	2:B:568:HOH:O	2.38	0.51
1:A:7:THR:HG22	1:A:274:CYS:C	2.31	0.51
1:A:402:HIS:O	1:A:403:THR:C	2.49	0.51
1:B:430:PHE:HD2	1:B:511:LEU:HD11	1.76	0.51
1:A:385:THR:HG23	1:A:420:TRP:HE1	1.75	0.50
1:B:22:PRO:HG2	1:B:400:ALA:HB3	1.92	0.50
1:A:430:PHE:HD2	1:A:511:LEU:HD11	1.77	0.50
1:A:30:LEU:HB2	1:A:428:HIS:CD2	2.47	0.50
1:A:422:ARG:HA	1:A:426:MSE:HE3	1.94	0.50
1:B:109:ARG:HG3	1:B:109:ARG:HH11	1.77	0.50
1:B:406:ASN:O	1:B:409:LEU:N	2.44	0.50
1:A:118:HIS:O	1:A:122:VAL:HG23	2.13	0.49
1:A:300:SER:OG	1:A:313:MSE:HE1	2.12	0.49
1:B:489:LEU:HD22	1:B:494:VAL:HG21	1.94	0.49
1:A:230:GLU:HG2	1:A:262:ILE:HG13	1.94	0.49
1:B:317:GLY:HA3	2:B:539:HOH:O	2.13	0.49
1:B:507:VAL:HG12	1:B:511:LEU:HD12	1.93	0.49
1:A:514:GLN:O	1:A:514:GLN:HG2	2.13	0.49
1:B:36:MSE:O	1:B:146:CYS:HA	2.13	0.48
1:B:280:ARG:NE	1:B:291:ASN:ND2	2.60	0.48
1:A:21:LEU:HD23	1:A:34:HIS:HA	1.94	0.48
1:A:320:LEU:HD22	1:A:321:VAL:N	2.28	0.48
1:B:164:ASP:HA	2:B:590:HOH:O	2.13	0.48
1:B:170:CYS:CA	1:B:173:MSE:HE3	2.31	0.48
1:B:442:ALA:O	1:B:443:LEU:HD23	2.12	0.48
1:B:30:LEU:HB2	1:B:428:HIS:CD2	2.48	0.48
1:A:308:LEU:CB	1:A:311:CYS:SG	3.01	0.48
1:B:172:LYS:HE3	2:B:536:HOH:O	2.14	0.48
1:A:113:SER:OG	1:B:454:ILE:HA	2.14	0.48
1:A:36:MSE:O	1:A:146:CYS:HA	2.13	0.47
1:A:403:THR:O	1:A:405:VAL:N	2.46	0.47
1:A:164:ASP:HA	2:A:545:HOH:O	2.13	0.47
1:A:453:SER:O	1:B:112:SER:HA	2.14	0.47
1:A:227:THR:HB	1:A:347:SER:O	2.15	0.47
1:A:416:ALA:HB3	1:A:417:PRO:HD3	1.96	0.47
1:B:385:THR:HG23	1:B:420:TRP:HE1	1.79	0.47
1:B:152:GLY:O	1:B:153:GLY:O	2.32	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:422:ARG:HA	1:B:426:MSE:HE3	1.96	0.47
1:B:462:ILE:HA	1:B:465:ARG:HH12	1.79	0.47
1:A:179:VAL:HG21	1:A:285:LEU:HD22	1.96	0.47
1:B:461:GLN:H	1:B:461:GLN:NE2	2.12	0.47
1:B:372:VAL:HG12	1:B:373:ALA:N	2.30	0.47
1:A:263:GLY:HA2	1:A:277:ARG:NH1	2.30	0.47
1:B:46:GLY:O	1:B:50:LYS:HG3	2.15	0.47
1:B:364:THR:HA	1:B:368:SER:O	2.15	0.47
1:B:102:GLY:O	1:B:114:LYS:HD2	2.15	0.47
1:B:514:GLN:O	1:B:514:GLN:HG2	2.15	0.47
1:A:163:PRO:HG2	1:A:168:ARG:HG3	1.97	0.46
1:B:160:ILE:O	1:B:160:ILE:HG13	2.15	0.46
1:B:336:LEU:O	1:B:339:PHE:HB3	2.13	0.46
1:B:96:SER:HB3	1:B:168:ARG:NH1	2.21	0.46
1:B:466:LEU:HB3	1:B:467:HIS:CD2	2.50	0.46
1:A:102:GLY:O	1:A:114:LYS:HD2	2.15	0.46
1:A:129:ASP:O	1:A:259:ARG:NH1	2.48	0.46
1:A:385:THR:CG2	1:A:386:ARG:H	2.17	0.46
1:A:466:LEU:HB3	1:A:467:HIS:CD2	2.51	0.46
1:B:402:HIS:CG	1:B:403:THR:H	2.33	0.46
1:A:45:ALA:O	1:A:49:GLN:HG3	2.16	0.46
1:B:268:ASN:HB2	1:B:272:GLN:H	1.81	0.46
1:A:355:GLN:HA	1:A:355:GLN:NE2	2.31	0.46
1:B:490:ARG:HG2	1:B:490:ARG:NH1	2.27	0.46
1:A:268:ASN:HB2	1:A:272:GLN:H	1.80	0.46
1:A:321:VAL:HG21	1:A:365:SER:HB3	1.97	0.46
1:B:45:ALA:O	1:B:49:GLN:HG3	2.16	0.46
1:A:28:ASN:HA	1:A:31:LEU:O	2.15	0.46
1:A:151:LYS:HB3	1:A:152:GLY:H	1.60	0.46
1:A:515:GLY:O	1:A:519:ALA:HB2	2.15	0.46
1:B:79:LYS:HG2	1:B:244:ASP:HB3	1.98	0.46
1:B:40:THR:HB	1:B:157:ALA:CB	2.45	0.45
1:A:112:SER:HA	1:B:453:SER:O	2.16	0.45
1:B:26:LEU:N	1:B:26:LEU:HD22	2.32	0.45
1:A:143:GLU:CD	1:A:158:ARG:HH21	2.20	0.45
1:A:390:THR:HB	1:A:391:PRO:HD3	1.98	0.45
1:B:187:MSE:HG3	1:B:191:TYR:HB2	1.99	0.45
1:B:447:ILE:O	1:B:448:TYR:C	2.54	0.45
1:A:280:ARG:NE	1:A:291:ASN:ND2	2.62	0.45
1:A:490:ARG:HG2	1:A:490:ARG:NH1	2.29	0.45
1:B:344:THR:HG22	1:B:350:PRO:HD3	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:GLU:OE1	1:A:150:GLU:N	2.48	0.45
1:A:360:LEU:HD23	1:A:360:LEU:O	2.17	0.45
1:A:401:ARG:HB3	1:A:403:THR:HG23	1.98	0.45
1:A:79:LYS:HG2	1:A:244:ASP:HB3	1.99	0.44
1:B:466:LEU:HD23	1:B:467:HIS:NE2	2.32	0.44
1:A:454:ILE:HA	1:B:113:SER:OG	2.17	0.44
1:A:40:THR:HB	1:A:157:ALA:CB	2.47	0.44
1:A:337:ARG:O	1:A:341:GLU:HG3	2.17	0.44
1:A:447:ILE:O	1:A:448:TYR:C	2.56	0.44
1:B:34:HIS:C	1:B:36:MSE:H	2.19	0.44
1:A:24:ASN:HB3	1:A:27:SER:OG	2.18	0.44
1:A:314:LEU:HD23	1:A:314:LEU:HA	1.86	0.44
1:A:236:GLU:OE2	1:A:280:ARG:NH2	2.37	0.44
1:B:225:ASP:HB2	2:B:619:HOH:O	2.18	0.44
1:B:450:ALA:HB3	1:B:452:TYR:CE1	2.52	0.44
1:A:403:THR:C	1:A:405:VAL:H	2.22	0.44
1:A:36:MSE:O	1:A:147:VAL:HG23	2.18	0.43
1:A:38:TYR:OH	1:A:155:LYS:HG2	2.18	0.43
1:A:347:SER:O	1:A:347:SER:OG	2.36	0.43
1:A:461:GLN:H	1:A:461:GLN:NE2	2.16	0.43
1:B:227:THR:HB	1:B:347:SER:O	2.17	0.43
1:B:321:VAL:HG21	1:B:365:SER:HB3	1.99	0.43
1:A:280:ARG:HH21	1:A:291:ASN:HD22	1.65	0.43
1:A:372:VAL:HG12	1:A:373:ALA:N	2.33	0.43
1:B:21:LEU:HD12	1:B:22:PRO:HD2	2.00	0.43
1:B:343:MSE:HG3	1:B:348:ALA:HB3	2.00	0.43
1:B:303:CYS:SG	1:B:308:LEU:HD12	2.58	0.43
1:A:182:LEU:O	1:A:182:LEU:HD22	2.19	0.43
1:A:344:THR:HG22	1:A:350:PRO:HD3	2.00	0.43
1:B:36:MSE:O	1:B:147:VAL:HG23	2.19	0.43
1:B:74:LYS:HB3	1:B:74:LYS:HE2	1.87	0.43
1:B:320:LEU:HD22	1:B:321:VAL:N	2.34	0.43
1:A:516:GLY:O	1:A:519:ALA:HB3	2.19	0.43
1:B:182:LEU:HD22	1:B:186:VAL:HG23	1.99	0.43
1:B:236:GLU:OE2	1:B:280:ARG:NH2	2.37	0.43
1:B:308:LEU:CB	1:B:311:CYS:SG	3.06	0.43
1:B:390:THR:HB	1:B:391:PRO:HD3	2.00	0.42
1:A:321:VAL:CG2	1:A:365:SER:HB3	2.49	0.42
1:A:391:PRO:HG3	2:A:621:HOH:O	2.18	0.42
1:B:17:GLU:OE1	1:B:41:THR:HB	2.19	0.42
1:B:94:PRO:HA	1:B:109:ARG:NH1	2.34	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:347:SER:O	1:B:347:SER:OG	2.33	0.42
1:B:144:VAL:HB	1:B:394:ARG:HG2	2.00	0.42
1:B:230:GLU:HG2	1:B:262:ILE:HG13	2.02	0.42
1:A:40:THR:HB	1:A:157:ALA:CA	2.49	0.42
1:A:187:MSE:HG3	1:A:191:TYR:HB2	2.01	0.42
1:B:355:GLN:NE2	1:B:355:GLN:HA	2.35	0.42
1:A:34:HIS:C	1:A:36:MSE:H	2.22	0.42
1:A:469:LEU:O	1:A:470:SER:C	2.58	0.42
1:B:18:GLU:OE2	1:B:401:ARG:NE	2.53	0.42
1:B:21:LEU:HD12	1:B:22:PRO:CD	2.49	0.42
1:B:40:THR:HB	1:B:157:ALA:CA	2.48	0.42
1:B:388:PRO:HG2	1:B:488:CYS:SG	2.60	0.42
1:B:462:ILE:HA	1:B:465:ARG:NH1	2.35	0.42
1:A:462:ILE:HA	1:A:465:ARG:HH12	1.85	0.42
1:B:406:ASN:HB3	1:B:408:TRP:NE1	2.35	0.42
1:A:180:SER:HB3	2:A:551:HOH:O	2.20	0.42
1:B:318:ASP:OD2	1:B:318:ASP:N	2.43	0.42
1:A:44:SER:HB3	1:A:156:PRO:HA	2.02	0.42
1:A:318:ASP:OD2	1:A:318:ASP:N	2.47	0.41
1:B:416:ALA:HB3	1:B:417:PRO:HD3	2.02	0.41
1:B:118:HIS:O	1:B:122:VAL:HG23	2.20	0.41
1:B:222:ARG:HH11	1:B:222:ARG:HG2	1.85	0.41
1:B:84:SER:OG	1:B:87:GLU:HG3	2.20	0.41
1:B:154:ARG:HH11	1:B:154:ARG:HG3	1.84	0.41
1:A:99:SER:C	1:A:101:PHE:H	2.23	0.41
1:B:44:SER:O	1:B:45:ALA:C	2.59	0.41
1:B:129:ASP:O	1:B:259:ARG:NH1	2.54	0.41
1:B:344:THR:CG2	1:B:350:PRO:HD3	2.51	0.41
1:B:459:LEU:HD23	1:B:459:LEU:HA	1.88	0.41
1:A:39:ALA:HB2	1:A:397:TRP:CH2	2.56	0.41
1:A:144:VAL:HB	1:A:394:ARG:HG2	2.02	0.41
1:B:490:ARG:NH1	1:B:490:ARG:CG	2.82	0.41
1:A:303:CYS:SG	1:A:308:LEU:HD12	2.61	0.41
1:B:406:ASN:HD22	1:B:408:TRP:HE1	1.68	0.41
1:A:74:LYS:HE2	1:A:74:LYS:HB3	1.88	0.41
1:A:342:ALA:HA	1:A:345:ARG:CZ	2.50	0.41
1:A:466:LEU:HD23	1:A:467:HIS:NE2	2.36	0.41
1:B:28:ASN:HA	1:B:31:LEU:O	2.21	0.41
1:B:419:LEU:C	1:B:419:LEU:HD23	2.41	0.41
1:A:331:GLU:OE1	1:A:331:GLU:N	2.53	0.41
1:B:119:ILE:HG22	1:B:173:MSE:CE	2.51	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:THR:HG22	1:B:274:CYS:O	2.21	0.40
1:B:147:VAL:HG12	1:B:148:GLN:N	2.36	0.40
1:B:280:ARG:HH21	1:B:291:ASN:HD22	1.70	0.40
1:A:355:GLN:HA	1:A:356:PRO:HD3	1.96	0.40
1:A:7:THR:HG22	1:A:274:CYS:O	2.21	0.40
1:A:172:LYS:HE3	2:A:563:HOH:O	2.21	0.40
1:A:222:ARG:HH11	1:A:222:ARG:HG2	1.85	0.40
1:A:489:LEU:HD22	1:A:494:VAL:HG22	2.01	0.40
1:B:56:ARG:O	1:B:57:LEU:HD23	2.20	0.40
1:B:119:ILE:HG12	1:B:119:ILE:H	1.72	0.40
1:B:375:ASP:O	1:B:475:HIS:HE1	2.04	0.40
1:A:235:VAL:O	1:A:239:ILE:HG13	2.21	0.40
1:B:359:ASP:HA	2:B:595:HOH:O	2.22	0.40
1:A:7:THR:O	1:A:7:THR:HG23	2.21	0.40
1:A:468:GLY:O	1:A:469:LEU:HG	2.21	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	529/531 (100%)	480 (91%)	40 (8%)	9 (2%)	7	26
1	B	529/531 (100%)	476 (90%)	44 (8%)	9 (2%)	7	26
All	All	1058/1062 (100%)	956 (90%)	84 (8%)	18 (2%)	7	26

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	GLY
1	A	164	ASP
1	A	268	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	8	GLY
1	B	154	ARG
1	B	164	ASP
1	B	268	ASN
1	B	403	THR
1	A	404	PRO
1	A	438	GLN
1	A	469	LEU
1	B	153	GLY
1	B	438	GLN
1	B	469	LEU
1	B	35	ASN
1	A	35	ASN
1	A	403	THR
1	A	448	TYR

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	452/440 (103%)	423 (94%)	29 (6%)	14	41
1	B	452/440 (103%)	423 (94%)	29 (6%)	14	41
All	All	904/880 (103%)	846 (94%)	58 (6%)	14	41

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

Mol	Chain	Res	Type
1	A	14	CYS
1	A	31	LEU
1	A	44	SER
1	A	83	LEU
1	A	92	THR
1	A	114	LYS
1	A	131	VAL
1	A	137	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	155	LYS
1	A	165	LEU
1	A	260	LEU
1	A	267	THR
1	A	272	GLN
1	A	274	CYS
1	A	285	LEU
1	A	286	THR
1	A	297	LEU
1	A	314	LEU
1	A	320	LEU
1	A	340	THR
1	A	360	LEU
1	A	387	ASP
1	A	422	ARG
1	A	441	LYS
1	A	447	ILE
1	A	458	ASP
1	A	461	GLN
1	A	492	LEU
1	A	531	LYS
1	B	31	LEU
1	B	44	SER
1	B	92	THR
1	B	114	LYS
1	B	131	VAL
1	B	137	THR
1	B	150	GLU
1	B	165	LEU
1	B	182	LEU
1	B	260	LEU
1	B	267	THR
1	B	272	GLN
1	B	274	CYS
1	B	285	LEU
1	B	286	THR
1	B	297	LEU
1	B	314	LEU
1	B	320	LEU
1	B	336	LEU
1	B	340	THR
1	B	360	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	387	ASP
1	B	422	ARG
1	B	441	LYS
1	B	447	ILE
1	B	458	ASP
1	B	461	GLN
1	B	492	LEU
1	B	531	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	35	ASN
1	A	58	GLN
1	A	63	HIS
1	A	142	ASN
1	A	194	GLN
1	A	206	ASN
1	A	272	GLN
1	A	291	ASN
1	A	355	GLN
1	A	369	ASN
1	A	374	HIS
1	A	406	ASN
1	A	461	GLN
1	A	475	HIS
1	A	514	GLN
1	B	35	ASN
1	B	58	GLN
1	B	120	HIS
1	B	142	ASN
1	B	194	GLN
1	B	206	ASN
1	B	272	GLN
1	B	291	ASN
1	B	355	GLN
1	B	369	ASN
1	B	374	HIS
1	B	406	ASN
1	B	461	GLN
1	B	475	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	514	GLN

5.3.3 RNA [i](#)

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 oligosaccharides 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	519/531 (97%)	-0.05	11 (2%) 63 55	8, 26, 68, 89	0
1	B	519/531 (97%)	-0.02	7 (1%) 74 67	9, 26, 67, 88	0
All	All	1038/1062 (97%)	-0.04	18 (1%) 69 61	8, 26, 67, 89	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	23	ILE	4.7
1	A	405	VAL	4.0
1	A	18	GLU	3.5
1	B	19	SER	3.5
1	A	402	HIS	3.2
1	A	19	SER	3.0
1	B	153	GLY	2.8
1	B	405	VAL	2.6
1	A	22	PRO	2.5
1	A	404	PRO	2.5
1	B	25	ALA	2.4
1	A	34	HIS	2.3
1	B	317	GLY	2.2
1	A	529	ALA	2.2
1	A	25	ALA	2.1
1	A	514	GLN	2.0
1	B	404	PRO	2.0
1	B	437	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.