Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 08:24 am BST

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

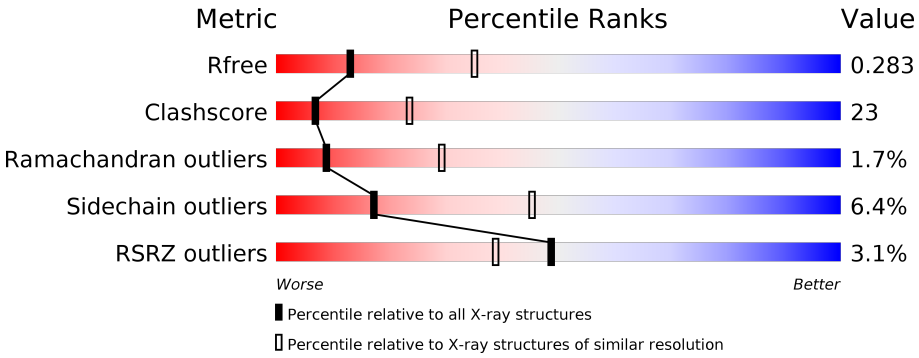
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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 on 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 <=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	3% 59% 37% 5%
1	B	531	3% 56% 39% .

2 Entry composition (i)

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	C	N	O	S	Se	1	0	0
			4122	2595	727	769	19	12			
1	B	531	Total	C	N	O	S	Se	1	0	0
			4122	2595	727	769	19	12			

- Molecule 2 is water.

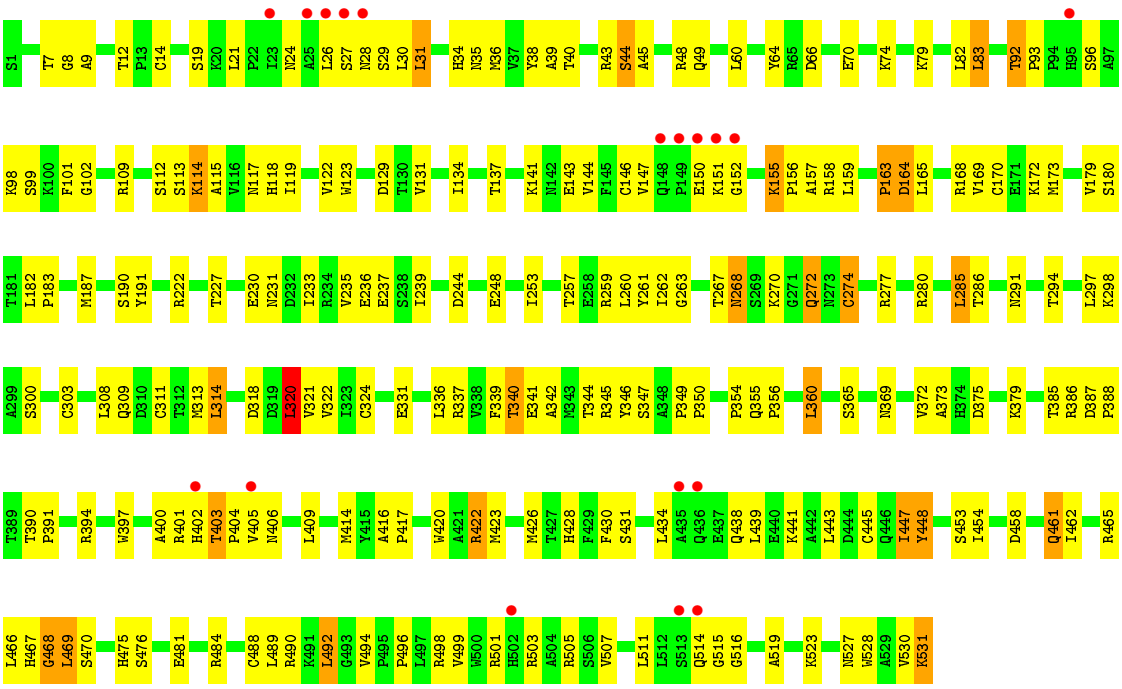
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	94	Total	O	0	0
			94	94		
2	B	90	Total	O	0	0
			90	90		

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 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.

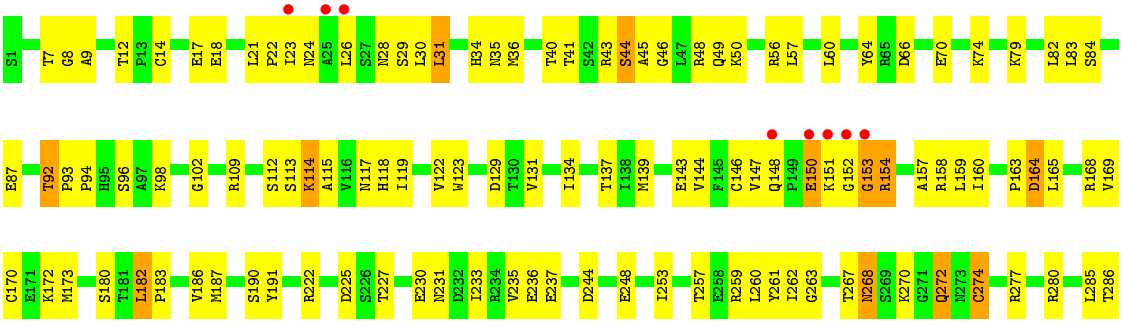
- Molecule 1: HEPATITIS C VIRUS RNA POLYMERASE (NS5B)

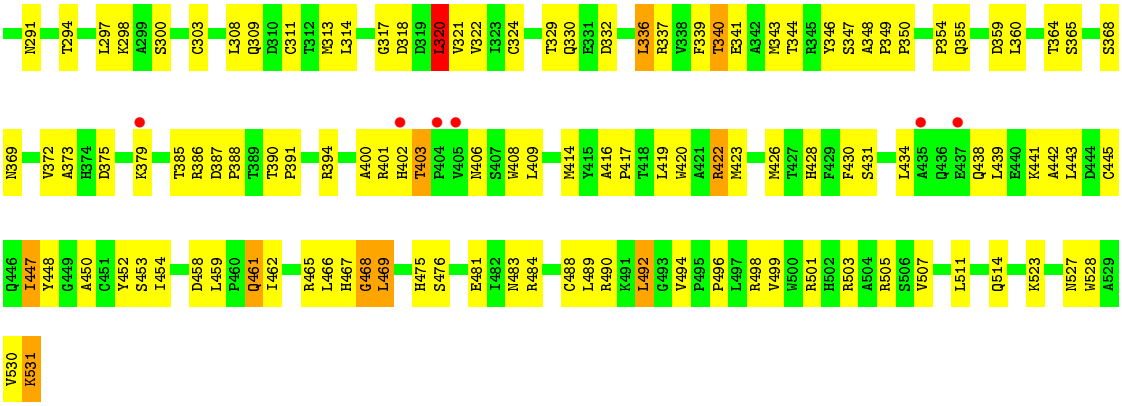
Chain A:



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

Chain B:




N291 T294 L297 K298 A299 S300 C303 L308 Q309 D310 C311 T312 M313 L314 G317 D318 D319 L320 V321 V322 I323 C324 T329 Q330 E331 D332 L336 R337 V338 F339 T340 E341 A342 M343 T344 R345 Y346 S347 A348 P349 P350 P354 Q355 D359 L360 T364 S365 S368
N369 V372 A373 H374 D375 K379 T385 R386 D387 P388 T389 T390 P391 R394 A400 R401 H402 T403 P404 V405 N406 S407 W408 L409 M414 Y415 A416 P417 T418 L419 W420 A421 R422 M423 M426 T427 H428 F429 F430 S431 L434 A435 Q436 E437 Q438 L439 E440 K441 A442 L443 D444 C445
Q446 I447 Y448 G449 A450 C451 Y452 S453 I454 D458 L459 P460 Q461 I462 R465 L466 H467 G468 L469 H475 S476 E481 I482 N483 R484 C488 L489 R490 K491 L492 G493 V494 P495 P496 L497 R498 V499 W500 R501 H502 R503 A504 R505 S506 V507 L511 Q514 K523 N527 W528 A529
V530 K531

4 Data and refinement statistics (i)

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 19.96 – 2.80	Depositor EDS
% Data completeness (in resolution range)	92.5 (19.00-2.80) 92.5 (19.96-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.46 (at 2.79Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.237 , 0.286 0.236 , 0.283	Depositor DCC
R_{free} test set	1989 reflections (6.74%)	wwPDB-VP
Wilson B-factor (Å^2)	30.2	Xtriage
Anisotropy	0.695	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 44.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
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

Xtriage'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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	0.50	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(^{o})	Ideal(^{o})
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

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

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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:HG2	1:B:490:ARG:HH11	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:O	1:B:439:LEU:HD23	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:HH11	1:A:490:ARG:HG2	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:HD23	1:A:439:LEU:O	1.96	0.64
1:A:468:GLY:O	1:A:469:LEU:HB2	1.96	0.64

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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:400:ALA:O	1:A:401:ARG:HG2	1.99	0.63
1:A:93:PRO:HG2	1:A:96:SER:OG	1.98	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:HD12	1:B:23:ILE:N	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:505:ARG:HG2	1:A:530:VAL:HG22	1.84	0.58
1:A:465:ARG:NH1	1:B:117:ASN:OD1	2.36	0.58

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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:HH11	1:B:43:ARG:HG3	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:HH11	1:A:401:ARG:HG3	1.70	0.56
1:B:7:THR:HG22	1:B:274:CYS:C	2.26	0.56
1:B:43:ARG:NH1	1:B:43:ARG:HG3	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

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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:HH11	1:A:43:ARG:HG3	1.72	0.54
1:A:475:HIS:O	1:A:476:SER:HB2	2.08	0.54
1:A:31:LEU:HD21	1:A:492:LEU:CD1	2.37	0.54
1:A:43:ARG:NH1	1:A:43:ARG:HG3	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: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:A:83:LEU:HB2	1:A:173:MSE:HA	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:489:LEU:HD22	1:B:494:VAL:CG2	2.39	0.53
1:B:82:LEU:HD11	1:B:248:GLU:HB3	1.91	0.53
1:A:92:THR:HG21	1:A:169:VAL:HG22	1.90	0.53
1:A:257:THR:O	1:A:262:ILE:HB	2.08	0.52
1:A:30:LEU:O	1:A:494:VAL:HB	2.10	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:163:PRO:HG2	1:B:168:ARG:HG3	1.92	0.52
1:B:23:ILE:CG2	1:B:24:ASN:H	2.23	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

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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:402:HIS:O	1:A:403:THR:C	2.49	0.51
1:A:7:THR:HG22	1:A:274:CYS:C	2.31	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:280:ARG:NE	1:B:291:ASN:ND2	2.60	0.48
1:B:36:MSE:O	1:B:146:CYS:HA	2.13	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

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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:HG13	1:B:160:ILE:O	2.15	0.46
1:B:336:LEU:O	1:B:339:PHE:HB3	2.13	0.46
1:B:466:LEU:HB3	1:B:467:HIS:CD2	2.50	0.46
1:B:96:SER:HB3	1:B:168:ARG:NH1	2.21	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:NE2	1:A:355:GLN:HA	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:151:LYS:HB3	1:A:152:GLY:H	1.60	0.46
1:A:28:ASN:HA	1:A:31:LEU:O	2.15	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:B:26:LEU:N	1:B:26:LEU:HD22	2.32	0.45
1:A:112:SER:HA	1:B:453:SER:O	2.16	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:GLU:N	1:A:150:GLU:OE1	2.48	0.45
1:A:360:LEU:O	1:A:360:LEU:HD23	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:337:ARG:O	1:A:341:GLU:HG3	2.17	0.44
1:A:40:THR:HB	1:A:157:ALA:CB	2.47	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:347:SER:OG	1:A:347:SER:O	2.36	0.43
1:A:38:TYR:OH	1:A:155:LYS:HG2	2.18	0.43
1:A:461:GLN:NE2	1:A:461:GLN:H	2.16	0.43
1:B:321:VAL:HG21	1:B:365:SER:HB3	1.99	0.43
1:B:227:THR:HB	1:B:347:SER:O	2.17	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:HD22	1:A:182:LEU:O	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:320:LEU:HD22	1:B:321:VAL:N	2.34	0.43
1:B:74:LYS:HB3	1:B:74:LYS:HE2	1.87	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:347:SER:O	1:B:347:SER:OG	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:PRO:HA	1:B:109:ARG:NH1	2.34	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:HA	1:B:355:GLN:NE2	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:40:THR:HB	1:B:157:ALA:CA	2.48	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:462:ILE:HA	1:B:465:ARG:NH1	2.35	0.42
1:B:388:PRO:HG2	1:B:488:CYS:SG	2.60	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:N	1:A:318:ASP:OD2	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:HG2	1:B:222:ARG:HH11	1.85	0.41
1:B:154:ARG:HH11	1:B:154:ARG:HG3	1.84	0.41
1:B:84:SER:OG	1:B:87:GLU:HG3	2.20	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:144:VAL:HB	1:A:394:ARG:HG2	2.02	0.41
1:A:39:ALA:HB2	1:A:397:TRP:CH2	2.56	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:342:ALA:HA	1:A:345:ARG:CZ	2.50	0.41
1:B:28:ASN:HA	1:B:31:LEU:O	2.21	0.41
1:A:466:LEU:HD23	1:A:467:HIS:NE2	2.36	0.41
1:A:74:LYS:HE2	1:A:74:LYS:HB3	1.88	0.41
1:B:419:LEU:C	1:B:419:LEU:HD23	2.41	0.41
1:A:331:GLU:N	1:A:331:GLU:OE1	2.53	0.41
1:B:119:ILE:HG22	1:B:173:MSE:CE	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:VAL:HG12	1:B:148:GLN:N	2.36	0.40
1:B:7:THR:HG22	1:B:274:CYS:O	2.21	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: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:A:7:THR:HG22	1:A:274:CYS:O	2.21	0.40
1:B:119:ILE:H	1:B:119:ILE:HG12	1.72	0.40
1:B:375:ASP:O	1:B:475:HIS:HE1	2.04	0.40
1:B:56:ARG:O	1:B:57:LEU:HD23	2.20	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:468:GLY:O	1:A:469:LEU:HG	2.21	0.40
1:A:7:THR:O	1:A:7:THR:HG23	2.21	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	529/531 (100%)	480 (91%)	40 (8%)	9 (2%)	9	29
1	B	529/531 (100%)	476 (90%)	44 (8%)	9 (2%)	9	29
All	All	1058/1062 (100%)	956 (90%)	84 (8%)	18 (2%)	9	29

All (18) Ramachandran outliers are listed below:

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

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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 (i)

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%)	17 45
1	B	452/440 (103%)	423 (94%)	29 (6%)	17 45
All	All	904/880 (103%)	846 (94%)	58 (6%)	17 45

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

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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

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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

Some 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

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Mol	Chain	Res	Type
1	B	514	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

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, 95^{th} 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%)	-0.02	18 (3%)	44	34	8, 26, 68, 89	0
1	B	519/531 (97%)	0.00	14 (2%)	54	44	9, 26, 67, 88	0
All	All	1038/1062 (97%)	-0.01	32 (3%)	49	39	8, 26, 67, 89	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	25	ALA	5.2
1	A	151	LYS	3.9
1	A	27	SER	3.8
1	B	25	ALA	3.8
1	B	405	VAL	3.8
1	B	402	HIS	3.6
1	B	151	LYS	3.4
1	B	152	GLY	3.4
1	A	23	ILE	3.3
1	A	148	GLN	3.1
1	A	513	SER	3.1
1	A	26	LEU	3.0
1	B	153	GLY	2.6
1	B	26	LEU	2.6
1	B	150	GLU	2.6
1	B	23	ILE	2.4
1	A	402	HIS	2.3
1	A	405	VAL	2.3
1	A	435	ALA	2.3
1	B	148	GLN	2.3
1	A	152	GLY	2.3
1	A	514	GLN	2.3
1	A	150	GLU	2.2
1	B	435	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	149	PRO	2.2
1	A	502	HIS	2.2
1	B	379	LYS	2.1
1	A	436	GLN	2.1
1	B	437	GLU	2.1
1	B	404	PRO	2.1
1	A	95	HIS	2.0
1	A	28	ASN	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 carbohydrates 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.