



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:42 PM GMT

PDB ID : 1YCS
Title : P53-53BP2 COMPLEX
Authors : Gorina, S.; Pavletich, N.P.
Deposited on : 1996-09-30
Resolution : 2.20 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 ⓘ symbol.

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

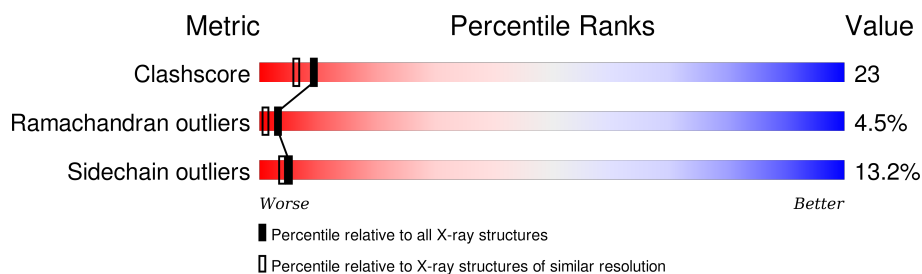
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.


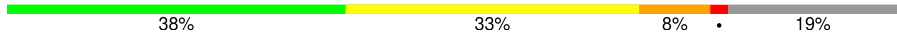
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)

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 $\leq 5\%$. 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	199	 62% 28% 5% . .
2	B	239	 38% 33% 8% . 19%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3291 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 P 53.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	191	Total	C	N	O	S	0	0	0
			1501	926	277	282	16			

- Molecule 2 is a protein called 53BP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	193	Total	C	N	O	S	0	0	0
			1514	955	243	302	14			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	325	PRO	-	INSERTION	UNP Q13625
B	326	LEU	-	INSERTION	UNP Q13625

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is water.

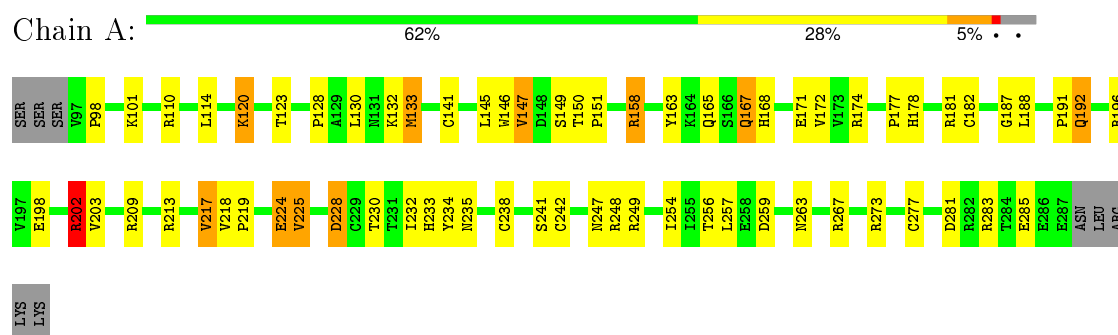
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	215	Total	O	0	0
			215	215		
4	B	60	Total	O	0	0
			60	60		

3 Residue-property plots

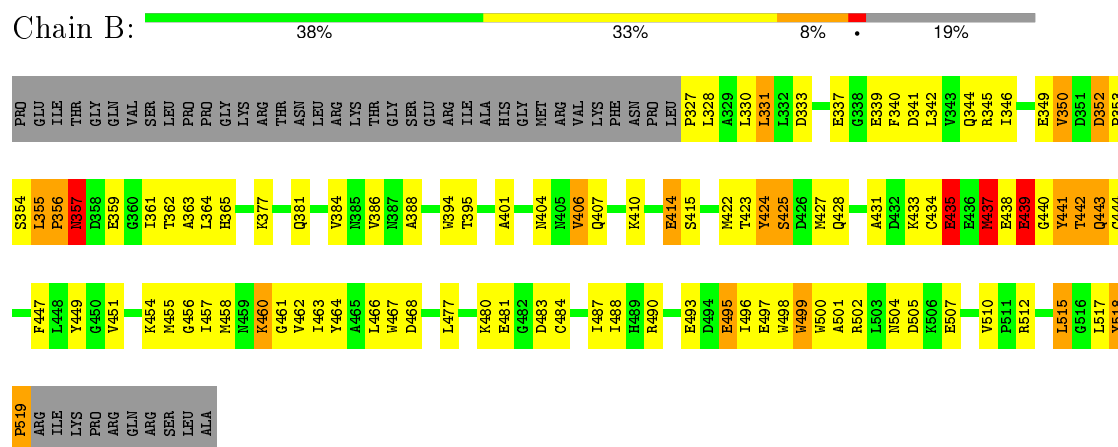
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: P53



• Molecule 2: 53BP2



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	68.80 Å 72.80 Å 119.00 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) (7.00-2.20)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT, X-PLOR 3.1	Depositor
R, R_{free}	0.205 , 0.286	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3291	wwPDB-VP
Average B, all atoms (Å ²)	53.0	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: ZN

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	0.56	0/1536	0.86	3/2083 (0.1%)
2	B	0.50	0/1547	0.78	2/2103 (0.1%)
All	All	0.53	0/3083	0.82	5/4186 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	202	ARG	NE-CZ-NH1	6.49	123.54	120.30
2	B	327	PRO	N-CA-CB	6.11	110.63	103.30
1	A	202	ARG	NE-CZ-NH2	-5.49	117.55	120.30
1	A	158	ARG	NE-CZ-NH2	-5.34	117.63	120.30
2	B	519	PRO	N-CA-CB	5.13	109.45	103.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	163	TYR	Sidechain

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	1501	0	1458	48	0
2	B	1514	0	1413	90	0
3	A	1	0	0	0	0
4	A	215	0	0	12	0
4	B	60	0	0	6	0
All	All	3291	0	2871	134	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 (134) 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:202:ARG:HB3	1:A:202:ARG:HH11	1.25	0.98
2:B:331:LEU:HD13	2:B:355:LEU:HD21	1.53	0.89
2:B:330:LEU:HD23	2:B:346:ILE:HG21	1.56	0.85
2:B:512:ARG:HA	2:B:515:LEU:HD22	1.57	0.85
2:B:480:LYS:HD3	2:B:481:GLU:N	1.96	0.81
2:B:423:THR:O	2:B:427:MET:HA	1.82	0.79
1:A:178:HIS:HB3	2:B:427:MET:SD	2.22	0.79
1:A:202:ARG:HD3	1:A:219:PRO:HG3	1.67	0.77
1:A:232:ILE:HD12	4:A:491:HOH:O	1.86	0.76
2:B:480:LYS:NZ	2:B:481:GLU:HB3	2.01	0.74
1:A:256:THR:HG22	1:A:267:ARG:HG3	1.71	0.72
1:A:224:GLU:HG2	1:A:225:VAL:N	2.07	0.69
1:A:202:ARG:HB3	1:A:202:ARG:NH1	2.05	0.68
2:B:458:MET:HE3	2:B:517:LEU:HD11	1.75	0.68
1:A:158:ARG:HB2	1:A:217:VAL:HG13	1.75	0.67
2:B:355:LEU:HD22	2:B:363:ALA:HB2	1.77	0.67
2:B:350:VAL:C	2:B:352:ASP:H	1.98	0.65
2:B:377:LYS:O	2:B:381:GLN:HB2	1.97	0.65
2:B:456:GLY:O	2:B:461:GLY:HA2	1.97	0.65
2:B:480:LYS:HZ2	2:B:481:GLU:HB3	1.60	0.64
1:A:133:MET:HE1	1:A:141:CYS:HB3	1.79	0.63
1:A:224:GLU:HB2	4:A:488:HOH:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:350:VAL:HG13	2:B:352:ASP:OD1	1.99	0.62
2:B:487:ILE:HD13	2:B:501:ALA:HB2	1.81	0.62
2:B:454:LYS:HE3	2:B:458:MET:HE1	1.82	0.62
2:B:362:THR:OG1	2:B:365:HIS:HD2	1.82	0.61
2:B:435:GLU:CD	2:B:438:GLU:H	2.03	0.61
2:B:442:THR:O	2:B:443:GLN:HG2	2.00	0.60
1:A:241:SER:HA	1:A:248:ARG:HG2	1.84	0.59
2:B:502:ARG:HG3	2:B:507:GLU:HG2	1.84	0.59
2:B:466:LEU:HB2	2:B:467:TRP:CE3	2.38	0.58
2:B:357:ASN:OD1	2:B:361:ILE:HG12	2.02	0.58
2:B:355:LEU:HD12	4:B:150:HOH:O	2.02	0.58
1:A:177:PRO:O	1:A:181:ARG:HG2	2.04	0.58
1:A:187:GLY:O	1:A:188:LEU:HD23	2.04	0.58
1:A:192:GLN:HB3	4:A:328:HOH:O	2.02	0.58
2:B:355:LEU:O	2:B:362:THR:HG22	2.04	0.58
2:B:442:THR:C	2:B:444:CYS:H	2.07	0.57
2:B:414:GLU:HA	2:B:519:PRO:O	2.05	0.57
1:A:224:GLU:HB3	4:A:380:HOH:O	2.05	0.56
1:A:182:CYS:HA	2:B:425:SER:HA	1.87	0.56
2:B:454:LYS:O	2:B:457:ILE:HG12	2.05	0.56
1:A:168:HIS:CE1	1:A:249:ARG:HD2	2.40	0.56
2:B:357:ASN:HB3	2:B:361:ILE:O	2.06	0.55
2:B:455:MET:HG2	2:B:463:ILE:CD1	2.36	0.55
2:B:350:VAL:HG12	2:B:350:VAL:O	2.06	0.55
1:A:172:VAL:HG22	1:A:213:ARG:HG2	1.89	0.55
1:A:147:VAL:HG11	1:A:151:PRO:HD3	1.89	0.55
2:B:499:TRP:HB2	2:B:510:VAL:HG23	1.89	0.55
2:B:365:HIS:HE1	2:B:394:TRP:O	1.89	0.55
2:B:442:THR:O	2:B:444:CYS:N	2.40	0.54
2:B:349:GLU:O	2:B:350:VAL:HG23	2.06	0.54
1:A:167:GLN:H	1:A:167:GLN:HE21	1.54	0.54
2:B:356:PRO:HD2	2:B:357:ASN:H	1.73	0.53
2:B:455:MET:HG2	2:B:463:ILE:HD11	1.90	0.53
2:B:328:LEU:HD11	2:B:355:LEU:HA	1.90	0.53
1:A:150:THR:HG23	4:A:389:HOH:O	2.07	0.53
1:A:168:HIS:ND1	1:A:249:ARG:HD2	2.23	0.53
2:B:345:ARG:HH11	2:B:345:ARG:HG3	1.74	0.53
2:B:410:LYS:O	2:B:414:GLU:HB2	2.09	0.52
2:B:488:ILE:HB	2:B:500:TRP:HD1	1.73	0.52
2:B:480:LYS:HZ3	2:B:481:GLU:HB3	1.73	0.52
2:B:328:LEU:CD2	2:B:355:LEU:HD23	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:333:ASP:O	2:B:337:GLU:HB2	2.09	0.51
2:B:353:PRO:HB2	4:B:150:HOH:O	2.10	0.51
2:B:328:LEU:HD21	2:B:355:LEU:HB3	1.91	0.51
2:B:463:ILE:HG21	2:B:487:ILE:HD11	1.93	0.51
2:B:401:ALA:O	2:B:434:CYS:HA	2.10	0.51
2:B:454:LYS:HB2	2:B:458:MET:CE	2.42	0.50
2:B:404:ASN:HD21	2:B:435:GLU:HA	1.76	0.50
1:A:128:PRO:HD2	4:A:306:HOH:O	2.11	0.50
1:A:191:PRO:HG2	1:A:192:GLN:HE21	1.76	0.50
2:B:356:PRO:CD	2:B:357:ASN:H	2.24	0.50
1:A:259:ASP:OD1	1:A:263:ASN:N	2.44	0.50
2:B:422:MET:HA	2:B:428:GLN:O	2.12	0.50
2:B:497:GLU:HB2	2:B:498:TRP:CD1	2.46	0.50
2:B:460:LYS:NZ	2:B:460:LYS:HA	2.26	0.49
2:B:330:LEU:HG	2:B:346:ILE:HG12	1.94	0.49
2:B:350:VAL:HB	4:B:105:HOH:O	2.12	0.49
1:A:254:ILE:HD12	4:A:417:HOH:O	2.11	0.49
2:B:355:LEU:HD13	4:B:62:HOH:O	2.12	0.49
1:A:196:ARG:NH1	4:A:506:HOH:O	2.29	0.49
2:B:447:PHE:O	2:B:451:VAL:HG23	2.13	0.49
2:B:488:ILE:HB	2:B:500:TRP:CD1	2.48	0.48
2:B:424:TYR:O	2:B:425:SER:HB3	2.14	0.48
1:A:110:ARG:HG3	1:A:146:TRP:HB2	1.96	0.48
1:A:165:GLN:HB3	1:A:167:GLN:NE2	2.28	0.48
2:B:457:ILE:HG13	2:B:458:MET:N	2.29	0.47
2:B:477:LEU:HD11	2:B:501:ALA:O	2.15	0.47
1:A:259:ASP:OD2	1:A:263:ASN:HB2	2.14	0.47
1:A:120:LYS:HE2	1:A:120:LYS:HA	1.96	0.47
2:B:342:LEU:HA	2:B:345:ARG:HD2	1.96	0.47
1:A:146:TRP:CZ3	1:A:228:ASP:HB3	2.50	0.47
1:A:120:LYS:NZ	1:A:277:CYS:HA	2.30	0.46
2:B:406:VAL:HG22	2:B:444:CYS:HA	1.98	0.46
2:B:480:LYS:HD3	2:B:481:GLU:H	1.78	0.46
2:B:464:TYR:HA	2:B:483:ASP:O	2.17	0.45
2:B:388:ALA:O	2:B:395:THR:HA	2.15	0.45
1:A:120:LYS:HZ1	1:A:277:CYS:HA	1.82	0.45
2:B:437:MET:C	2:B:439:GLU:H	2.19	0.45
1:A:281:ASP:O	1:A:285:GLU:HG3	2.15	0.45
1:A:234:TYR:O	1:A:235:ASN:ND2	2.49	0.45
2:B:455:MET:HG3	2:B:517:LEU:HG	1.99	0.45
2:B:502:ARG:NH1	2:B:505:ASP:HA	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:ARG:NH2	4:A:407:HOH:O	2.50	0.44
2:B:357:ASN:CG	2:B:361:ILE:HG12	2.38	0.44
1:A:191:PRO:HD2	1:A:192:GLN:NE2	2.33	0.44
1:A:168:HIS:CE1	1:A:249:ARG:CD	3.00	0.44
1:A:171:GLU:HA	4:A:354:HOH:O	2.18	0.44
2:B:328:LEU:HD23	2:B:355:LEU:HD23	2.00	0.43
1:A:233:HIS:HD2	4:A:308:HOH:O	2.00	0.43
2:B:431:ALA:HB1	2:B:449:TYR:CE1	2.53	0.43
1:A:132:LYS:HE2	1:A:273:ARG:HB2	2.01	0.43
2:B:496:ILE:HG23	2:B:497:GLU:N	2.34	0.43
2:B:364:LEU:HB2	2:B:384:VAL:HG11	2.00	0.43
2:B:341:ASP:HB2	4:B:59:HOH:O	2.19	0.42
2:B:352:ASP:N	2:B:353:PRO:HD3	2.34	0.42
2:B:451:VAL:O	2:B:455:MET:HB2	2.18	0.42
1:A:248:ARG:HH11	2:B:495:GLU:CG	2.33	0.42
2:B:340:PHE:O	2:B:344:GLN:HG3	2.19	0.42
2:B:462:VAL:CG1	2:B:484:CYS:SG	3.08	0.42
1:A:174:ARG:NH1	4:A:328:HOH:O	2.53	0.41
2:B:433:LYS:HA	2:B:433:LYS:HD3	1.87	0.41
2:B:454:LYS:HB2	2:B:458:MET:HE1	2.03	0.41
1:A:120:LYS:HZ1	1:A:277:CYS:CA	2.33	0.41
2:B:364:LEU:O	2:B:364:LEU:HD12	2.20	0.41
1:A:203:VAL:HA	1:A:218:VAL:HG12	2.03	0.41
1:A:98:PRO:HD3	1:A:213:ARG:NH1	2.36	0.40
2:B:328:LEU:HD21	2:B:355:LEU:CB	2.51	0.40
2:B:434:CYS:HB3	2:B:442:THR:HG23	2.04	0.40
2:B:442:THR:C	2:B:444:CYS:N	2.74	0.40
2:B:354:SER:N	4:B:150:HOH:O	2.54	0.40
2:B:350:VAL:C	2:B:352:ASP:N	2.72	0.40
1:A:248:ARG:HH11	2:B:495:GLU:CD	2.25	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	189/199 (95%)	183 (97%)	4 (2%)	2 (1%)	17	14
2	B	191/239 (80%)	158 (83%)	18 (9%)	15 (8%)	1	0
All	All	380/438 (87%)	341 (90%)	22 (6%)	17 (4%)	3	1

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	350	VAL
2	B	356	PRO
2	B	441	TYR
2	B	442	THR
2	B	443	GLN
2	B	518	TYR
2	B	425	SER
2	B	437	MET
2	B	439	GLU
2	B	440	GLY
1	A	242	CYS
2	B	357	ASN
2	B	435	GLU
1	A	225	VAL
2	B	493	GLU
2	B	495	GLU
2	B	504	ASN

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	171/179 (96%)	149 (87%)	22 (13%)	5	4
2	B	162/205 (79%)	140 (86%)	22 (14%)	5	3
All	All	333/384 (87%)	289 (87%)	44 (13%)	5	4

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	101	LYS
1	A	114	LEU
1	A	120	LYS
1	A	123	THR
1	A	130	LEU
1	A	133	MET
1	A	145	LEU
1	A	147	VAL
1	A	149	SER
1	A	167	GLN
1	A	192	GLN
1	A	198	GLU
1	A	202	ARG
1	A	209	ARG
1	A	217	VAL
1	A	224	GLU
1	A	228	ASP
1	A	230	THR
1	A	238	CYS
1	A	247	ASN
1	A	257	LEU
1	A	283	ARG
2	B	331	LEU
2	B	339	GLU
2	B	352	ASP
2	B	355	LEU
2	B	357	ASN
2	B	359	GLU
2	B	386	VAL
2	B	406	VAL
2	B	407	GLN
2	B	414	GLU
2	B	415	SER
2	B	424	TYR
2	B	435	GLU
2	B	437	MET
2	B	439	GLU
2	B	441	TYR
2	B	460	LYS
2	B	468	ASP
2	B	490	ARG
2	B	499	TRP

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Mol	Chain	Res	Type
2	B	515	LEU
2	B	518	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	ASN
1	A	167	GLN
1	A	192	GLN
2	B	365	HIS
2	B	366	ASN
2	B	385	ASN
2	B	407	GLN
2	B	459	ASN
2	B	513	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.