



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:00 AM UTC

PDB ID : 6R2S / pdb_00006r2s
Title : The structure of Plasmodium vivax Duffy binding protein (PvDBP) bound to human antibody DB9
Authors : Barber, N.M.; Higgins, M.K.
Deposited on : 2019-03-18
Resolution : 3.04 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 : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

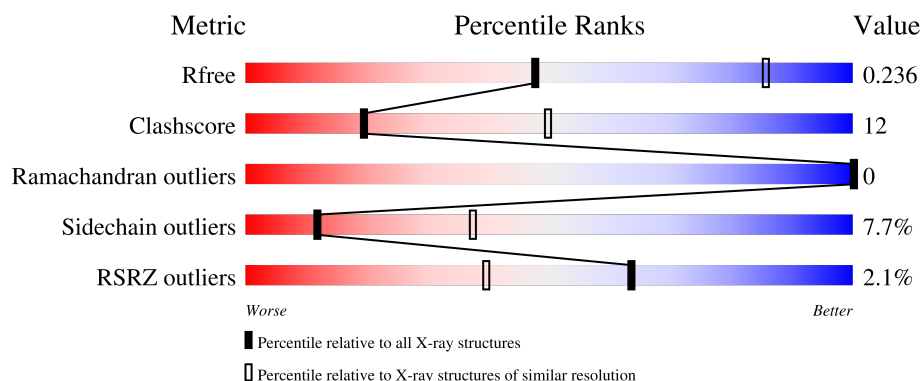
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.04 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}	180053	3685 (3.08-3.00)
Clashscore	190562	4007 (3.08-3.00)
Ramachandran outliers	187476	3834 (3.08-3.00)
Sidechain outliers	187428	3836 (3.08-3.00)
RSRZ outliers	180081	3684 (3.08-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	233	
2	B	278	
3	C	300	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5752 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 Antibody DB9 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	213	Total	C	N	O	S	0	0	0
			1645	1032	280	328	5			

- Molecule 2 is a protein called Antibody DB9 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	218	Total	C	N	O	S	0	0	0
			1612	1018	265	325	4			

- Molecule 3 is a protein called Duffy receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	299	Total	C	N	O	S	0	0	0
			2495	1578	443	456	18			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	209	SER	-	expression tag	UNP P22290
C	210	GLY	-	expression tag	UNP P22290

4 Data and refinement statistics

Property	Value	Source
Space group	P 62 2 2	Depositor
Cell constants a, b, c, α , β , γ	173.56Å 173.56Å 169.73Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.04 – 3.04 42.04 – 3.04	Depositor EDS
% Data completeness (in resolution range)	99.9 (42.04-3.04) 99.8 (42.04-3.04)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 3.01Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.202 , 0.238 0.198 , 0.236	Depositor DCC
R_{free} test set	1550 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	94.6	Xtriage
Anisotropy	0.451	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 91.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5752	wwPDB-VP
Average B, all atoms (Å ²)	115.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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	0.87	0/1684	1.26	4/2290 (0.2%)
2	B	0.82	0/1652	1.34	14/2260 (0.6%)
3	C	0.86	1/2544 (0.0%)	1.47	22/3423 (0.6%)
All	All	0.85	1/5880 (0.0%)	1.37	40/7973 (0.5%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	261	PHE	CA-C	6.04	1.61	1.52

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	429	VAL	N-CA-C	11.40	118.83	107.55
2	B	125	ASP	CA-CB-CG	9.02	121.62	112.60
3	C	373	PHE	N-CA-C	8.41	122.61	108.90
3	C	372	ASN	N-CA-C	-8.28	101.46	112.72
2	B	135	VAL	N-CA-CB	7.75	119.84	111.00
3	C	261	PHE	N-CA-C	-7.71	101.88	111.75
2	B	170	PHE	C-N-CD	7.01	136.03	120.60
3	C	430	PRO	N-CA-C	6.80	119.00	110.70
3	C	260	ASN	CA-C-N	6.44	129.78	120.38
3	C	260	ASN	C-N-CA	6.44	129.78	120.38
3	C	373	PHE	CA-CB-CG	6.25	120.05	113.80
3	C	262	HIS	N-CA-C	6.13	117.64	110.41
2	B	111	THR	N-CA-C	-6.12	100.59	109.59
2	B	87	ARG	N-CA-CB	-6.11	101.85	111.39
3	C	415	CYS	N-CA-C	5.93	121.96	114.31
2	B	56	GLY	N-CA-C	5.84	119.72	111.42
3	C	451	ASP	CA-CB-CG	5.79	118.39	112.60
1	A	227	SER	N-CA-C	5.76	118.17	109.41
3	C	492	ASN	CA-CB-CG	5.74	118.34	112.60
3	C	459	SER	CA-C-N	5.70	127.74	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	459	SER	C-N-CA	5.70	127.74	120.56
3	C	263	ARG	N-CA-C	5.66	117.57	109.14
2	B	172	GLU	N-CA-C	5.64	122.27	109.81
2	B	87	ARG	N-CA-C	5.63	119.81	111.87
3	C	418	LYS	N-CA-C	5.59	119.17	110.17
3	C	211	ASN	N-CA-C	-5.50	106.42	113.02
3	C	233	LYS	N-CA-C	-5.35	99.80	108.52
3	C	271	TYR	N-CA-C	-5.32	105.38	111.07
2	B	48	VAL	N-CA-C	-5.31	105.24	113.16
2	B	125	ASP	N-CA-C	5.27	119.56	113.18
2	B	94	THR	CA-C-N	5.22	127.23	120.44
2	B	94	THR	C-N-CA	5.22	127.23	120.44
3	C	372	ASN	CB-CA-C	5.22	117.64	111.22
1	A	225	THR	N-CA-C	5.18	117.17	107.99
1	A	28	SER	N-CA-C	-5.10	106.21	112.90
1	A	104	THR	CB-CA-C	5.10	118.54	109.72
2	B	167	LYS	CA-C-N	5.03	130.53	122.93
2	B	167	LYS	C-N-CA	5.03	130.53	122.93
3	C	216	ASN	N-CA-C	5.00	117.69	110.28
3	C	419	ILE	N-CA-CB	5.00	119.48	111.23

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	1645	0	1595	25	0
2	B	1612	0	1586	57	0
3	C	2495	0	2486	54	0
All	All	5752	0	5667	132	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 12.

All (132) 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)
3:C:230:CYS:SG	3:C:237:CYS:SG	1.37	1.36
1:A:48:ILE:HG23	1:A:111:ASN:HB2	1.53	0.89
3:C:379:LEU:O	3:C:383:VAL:HG12	1.76	0.85
3:C:429:VAL:HG12	3:C:431:PRO:HD2	1.58	0.84
3:C:233:LYS:HD2	3:C:320:GLU:O	1.80	0.81
3:C:263:ARG:HD2	3:C:267:PHE:CD2	2.15	0.79
2:B:173:PRO:HG2	2:B:226:PRO:CG	2.15	0.76
3:C:264:ASP:O	3:C:268:ARG:HG3	1.85	0.76
3:C:214:MET:HE2	3:C:216:ASN:OD1	1.86	0.75
2:B:169:TYR:CZ	2:B:174:VAL:HG11	2.21	0.75
2:B:171:PRO:HG2	2:B:173:PRO:HD2	1.70	0.73
2:B:173:PRO:HG2	2:B:226:PRO:HG2	1.69	0.73
1:A:164:LYS:HB3	1:A:216:THR:HG22	1.71	0.72
3:C:263:ARG:HD2	3:C:267:PHE:CE2	2.25	0.71
1:A:127:ARG:HH12	1:A:130:ALA:HB2	1.57	0.70
2:B:168:ASP:HB3	2:B:199:LEU:HD13	1.74	0.69
1:A:39:THR:HG22	1:A:93:THR:HG23	1.74	0.68
1:A:132:PRO:HD2	1:A:220:LEU:HD13	1.75	0.68
1:A:164:LYS:HB3	1:A:216:THR:CG2	2.24	0.67
3:C:425:LYS:O	3:C:429:VAL:HB	1.94	0.67
3:C:251:THR:O	3:C:254:VAL:HG23	1.94	0.67
3:C:354:LYS:HD2	3:C:383:VAL:HG22	1.77	0.66
2:B:169:TYR:CZ	2:B:174:VAL:CG1	2.78	0.65
3:C:312:ASP:OD2	3:C:388:GLN:HG3	1.95	0.65
2:B:171:PRO:C	2:B:173:PRO:HD2	2.23	0.64
2:B:172:GLU:O	2:B:172:GLU:HG2	1.95	0.64
2:B:40:THR:HG22	2:B:100:SER:HB3	1.79	0.64
2:B:169:TYR:HE1	2:B:172:GLU:HA	1.61	0.64
2:B:174:VAL:HG13	2:B:202:LEU:HD21	1.80	0.63
3:C:429:VAL:CG1	3:C:431:PRO:HD2	2.29	0.63
2:B:111:THR:HG23	2:B:134:THR:HA	1.79	0.63
3:C:418:LYS:HB2	3:C:421:TYR:HA	1.81	0.62
2:B:121:THR:O	2:B:121:THR:HG22	1.99	0.61
1:A:131:ALA:HB1	1:A:220:LEU:CD1	2.31	0.59
2:B:103:LEU:HD13	2:B:106:VAL:HG12	1.84	0.59
1:A:40:ILE:HG12	1:A:121:THR:HG21	1.84	0.58
2:B:166:VAL:HG11	2:B:174:VAL:HG21	1.85	0.58
2:B:80:TYR:HB2	2:B:85:LYS:HG3	1.85	0.58
2:B:169:TYR:CE1	2:B:172:GLU:HA	2.37	0.58
2:B:183:LEU:HD21	2:B:206:VAL:HG21	1.86	0.58
2:B:154:SER:O	2:B:155:THR:HG23	2.05	0.57
1:A:208:HIS:O	1:A:230:ARG:HD3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:37:LEU:HD11	2:B:133:VAL:HG11	1.86	0.57
1:A:23:MET:HE3	1:A:42:CYS:SG	2.45	0.56
3:C:319:MET:HE2	3:C:388:GLN:HB3	1.85	0.56
3:C:447:LYS:HD3	3:C:494:ILE:HD12	1.86	0.56
2:B:88:VAL:CG2	2:B:103:LEU:HD23	2.36	0.56
2:B:88:VAL:HG23	2:B:103:LEU:HD23	1.88	0.56
2:B:155:THR:HG21	2:B:210:SER:OG	2.07	0.55
2:B:171:PRO:HG2	2:B:173:PRO:CD	2.37	0.54
2:B:150:PRO:HG2	2:B:237:PRO:HG3	1.88	0.54
2:B:72:ILE:HG12	2:B:90:ILE:HG22	1.90	0.54
3:C:265:ILE:O	3:C:268:ARG:N	2.40	0.54
3:C:369:LEU:O	3:C:373:PHE:HB2	2.07	0.54
3:C:354:LYS:HD2	3:C:383:VAL:CG2	2.38	0.53
3:C:429:VAL:O	3:C:433:GLN:HG3	2.09	0.53
1:A:127:ARG:HG2	1:A:128:THR:N	2.24	0.53
2:B:171:PRO:HD2	2:B:226:PRO:CB	2.39	0.52
3:C:217:CYS:SG	3:C:248:LYS:HB2	2.49	0.52
2:B:59:ARG:HB2	2:B:69:ILE:HD11	1.89	0.52
2:B:170:PHE:HA	2:B:171:PRO:C	2.34	0.52
3:C:216:ASN:ND2	3:C:248:LYS:NZ	2.58	0.52
2:B:59:ARG:CG	2:B:112:ALA:CB	2.89	0.51
2:B:37:LEU:CD1	2:B:133:VAL:HG11	2.39	0.51
2:B:169:TYR:CE2	2:B:174:VAL:HG11	2.45	0.51
2:B:27:GLY:HA3	2:B:39:LEU:HD23	1.93	0.50
2:B:169:TYR:OH	2:B:174:VAL:CG1	2.59	0.50
1:A:32:ALA:HB3	1:A:97:LEU:HD22	1.94	0.50
2:B:173:PRO:CG	2:B:226:PRO:CG	2.88	0.50
1:A:127:ARG:HG2	1:A:128:THR:H	1.76	0.50
1:A:131:ALA:HB1	1:A:220:LEU:HD12	1.94	0.49
2:B:72:ILE:HD13	2:B:92:VAL:HG22	1.94	0.49
3:C:386:GLU:HG2	3:C:387:PRO:HD2	1.94	0.48
3:C:365:VAL:O	3:C:369:LEU:HB2	2.13	0.47
2:B:174:VAL:HG13	2:B:174:VAL:O	2.15	0.47
2:B:171:PRO:HG2	2:B:226:PRO:HG2	1.95	0.47
2:B:171:PRO:HD2	2:B:226:PRO:HB2	1.97	0.47
3:C:289:LYS:HG2	3:C:293:TYR:CZ	2.49	0.47
1:A:200:LEU:HD11	1:A:205:TYR:HA	1.96	0.46
3:C:265:ILE:O	3:C:266:THR:C	2.57	0.46
3:C:304:ARG:HG3	3:C:382:ALA:HA	1.96	0.46
2:B:172:GLU:N	2:B:173:PRO:CD	2.79	0.46
2:B:173:PRO:HG2	2:B:226:PRO:CD	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:416:ASP:OD1	3:C:416:ASP:O	2.34	0.46
3:C:230:CYS:CB	3:C:237:CYS:SG	2.83	0.46
3:C:456:LYS:O	3:C:460:VAL:HG23	2.15	0.46
2:B:169:TYR:OH	2:B:174:VAL:HG12	2.15	0.46
2:B:172:GLU:N	2:B:173:PRO:HD2	2.30	0.46
1:A:182:VAL:HG22	1:A:194:LEU:HD12	1.98	0.45
3:C:258:ASP:C	3:C:260:ASN:H	2.24	0.45
2:B:59:ARG:NH2	2:B:67:GLU:OE1	2.49	0.45
1:A:109:HIS:ND1	1:A:109:HIS:C	2.74	0.45
3:C:310:PHE:O	3:C:314:ILE:HG12	2.16	0.45
3:C:312:ASP:CG	3:C:388:GLN:HG3	2.41	0.45
3:C:418:LYS:CB	3:C:421:TYR:HA	2.46	0.44
1:A:48:ILE:HG22	1:A:51:TRP:H	1.82	0.44
3:C:371:GLY:C	3:C:373:PHE:H	2.26	0.44
3:C:220:LYS:NZ	3:C:244:GLN:O	2.50	0.44
2:B:169:TYR:CZ	2:B:174:VAL:HG12	2.53	0.44
3:C:319:MET:HG3	3:C:388:GLN:OE1	2.18	0.44
2:B:143:PRO:HD2	2:B:229:THR:HG21	1.99	0.43
2:B:59:ARG:CG	2:B:112:ALA:HB1	2.49	0.43
3:C:354:LYS:HB2	3:C:383:VAL:HG23	2.00	0.43
1:A:81:PHE:CE1	1:A:94:ILE:HG12	2.54	0.43
3:C:262:HIS:CG	3:C:262:HIS:O	2.71	0.43
1:A:56:GLN:OE1	1:A:58:ARG:HD2	2.18	0.43
2:B:155:THR:CG2	2:B:210:SER:OG	2.66	0.43
3:C:370:LYS:C	3:C:372:ASN:H	2.27	0.43
1:A:55:TYR:CE1	1:A:108:GLN:OE1	2.71	0.43
1:A:56:GLN:HB2	1:A:66:LEU:HD11	2.01	0.42
3:C:258:ASP:C	3:C:260:ASN:N	2.77	0.42
2:B:52:THR:HG21	3:C:493:GLU:OE2	2.20	0.42
3:C:315:MET:HG2	3:C:347:LYS:HG3	2.00	0.42
3:C:414:LYS:O	3:C:432:CYS:HB2	2.19	0.42
3:C:280:ALA:HB1	3:C:361:MET:HG3	2.00	0.42
3:C:426:VAL:HG22	3:C:426:VAL:O	2.19	0.42
3:C:265:ILE:C	3:C:267:PHE:N	2.76	0.41
2:B:37:LEU:O	2:B:102:LYS:HA	2.21	0.41
2:B:177:SER:HB3	2:B:221:ASN:HB2	2.01	0.41
3:C:295:TYR:CD2	3:C:376:ILE:HD12	2.56	0.41
2:B:173:PRO:O	2:B:224:HIS:HD2	2.03	0.41
3:C:407:GLU:HG3	3:C:442:TRP:CD2	2.55	0.41
2:B:173:PRO:CG	2:B:226:PRO:HG2	2.44	0.41
3:C:329:GLU:O	3:C:333:ARG:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:LEU:HD11	2:B:205:VAL:HG11	2.03	0.40
3:C:303:ILE:HD12	3:C:361:MET:HB3	2.03	0.40
2:B:59:ARG:HG3	2:B:112:ALA:CB	2.51	0.40
1:A:110:TYR:CB	2:B:122:GLY:HA3	2.51	0.40
3:C:383:VAL:HG22	3:C:383:VAL:O	2.21	0.40
3:C:426:VAL:HG21	3:C:505:CYS:HA	2.04	0.40
1:A:232:GLU:OE1	2:B:152:SER:OG	2.38	0.40
3:C:421:TYR:O	3:C:421:TYR:CG	2.74	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	211/233 (91%)	205 (97%)	6 (3%)	0	100	100
2	B	216/278 (78%)	201 (93%)	15 (7%)	0	100	100
3	C	297/300 (99%)	281 (95%)	16 (5%)	0	100	100
All	All	724/811 (89%)	687 (95%)	37 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	187/202 (93%)	175 (94%)	12 (6%)	16	44
2	B	186/240 (78%)	173 (93%)	13 (7%)	14	41
3	C	275/276 (100%)	250 (91%)	25 (9%)	9	31
All	All	648/718 (90%)	598 (92%)	50 (8%)	12	37

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	SER
1	A	29	THR
1	A	38	VAL
1	A	77	VAL
1	A	79	SER
1	A	109	HIS
1	A	116	THR
1	A	171	ASN
1	A	182	VAL
1	A	183	THR
1	A	222	SER
1	A	232	GLU
2	B	26	SER
2	B	42	THR
2	B	72	ILE
2	B	92	VAL
2	B	95	SER
2	B	100	SER
2	B	103	LEU
2	B	135	VAL
2	B	140	THR
2	B	154	SER
2	B	155	THR
2	B	205	VAL
2	B	233	LYS
3	C	226	ARG
3	C	230	CYS
3	C	231	ASN
3	C	248	LYS
3	C	253	LEU
3	C	254	VAL
3	C	259	THR
3	C	269	LYS
3	C	294	ARG

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Mol	Chain	Res	Type
3	C	313	ILE
3	C	320	GLU
3	C	347	LYS
3	C	364	SER
3	C	366	LYS
3	C	372	ASN
3	C	374	ILE
3	C	381	VAL
3	C	388	GLN
3	C	408	VAL
3	C	456	LYS
3	C	458	ILE
3	C	480	GLN
3	C	483	ASP
3	C	503	GLU
3	C	506	VAL

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

Mol	Chain	Res	Type
1	A	46	GLN
1	A	98	GLN
1	A	156	ASN
2	B	188	HIS
2	B	223	ASN
2	B	228	ASN
3	C	292	ASN
3	C	434	ASN
3	C	495	ASN

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 [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 ⓘ

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, 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	213/233 (91%)	-0.09	2 (0%) 81 60	81, 106, 144, 184	0
2	B	218/278 (78%)	0.05	4 (1%) 67 43	86, 109, 157, 196	0
3	C	299/300 (99%)	0.00	9 (3%) 52 29	79, 108, 194, 223	0
All	All	730/811 (90%)	-0.01	15 (2%) 63 39	79, 108, 172, 223	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	172	GLU	7.4
2	B	173	PRO	5.6
3	C	419	ILE	4.5
1	A	232	GLU	3.1
2	B	154	SER	2.8
2	B	171	PRO	2.6
3	C	265	ILE	2.5
3	C	209	SER	2.5
3	C	210	GLY	2.3
3	C	374	ILE	2.3
3	C	261	PHE	2.3
1	A	231	GLY	2.2
3	C	257	THR	2.2
3	C	507	CYS	2.1
3	C	259	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.