



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:38 PM UTC

PDB ID : 5XPJ / pdb_00005xpj
Title : Crystal Structure of Periplasmic glucose binding protein ppGBP deletion mutant- Del-ppGBP
Authors : Pandey, S.; Phale, P.S.; Bhaumik, P.
Deposited on : 2017-06-02
Resolution : 2.50 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

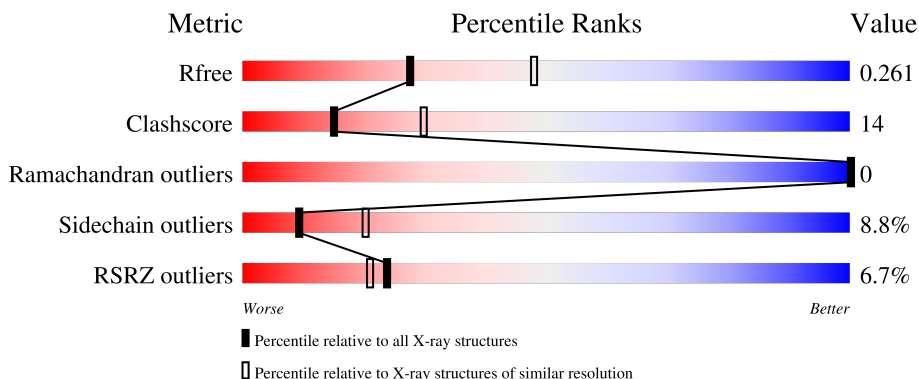
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

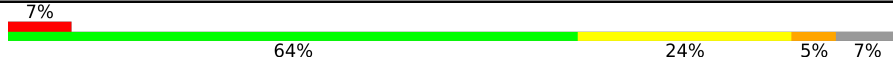
The reported resolution of this entry is 2.50 Å.

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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	417	
1	B	417	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5952 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 Binding protein component of ABC sugar transporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	389	Total	C	N	O	S	0	0	0
			2926	1859	497	558	12			
1	B	387	Total	C	N	O	S	0	0	0
			2938	1867	499	559	13			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP H7BRJ8
A	2	GLY	-	expression tag	UNP H7BRJ8
A	3	SER	-	expression tag	UNP H7BRJ8
A	4	SER	-	expression tag	UNP H7BRJ8
A	5	HIS	-	expression tag	UNP H7BRJ8
A	6	HIS	-	expression tag	UNP H7BRJ8
A	7	HIS	-	expression tag	UNP H7BRJ8
A	8	HIS	-	expression tag	UNP H7BRJ8
A	9	HIS	-	expression tag	UNP H7BRJ8
A	10	HIS	-	expression tag	UNP H7BRJ8
A	11	SER	-	expression tag	UNP H7BRJ8
A	12	SER	-	expression tag	UNP H7BRJ8
A	13	GLY	-	expression tag	UNP H7BRJ8
A	14	LEU	-	expression tag	UNP H7BRJ8
A	15	VAL	-	expression tag	UNP H7BRJ8
A	16	PRO	-	expression tag	UNP H7BRJ8
A	17	ARG	-	expression tag	UNP H7BRJ8
A	18	GLY	-	expression tag	UNP H7BRJ8
A	19	SER	-	expression tag	UNP H7BRJ8
A	20	HIS	-	expression tag	UNP H7BRJ8
A	21	MET	-	expression tag	UNP H7BRJ8
A	376	GLY	ALA	engineered mutation	UNP H7BRJ8
A	?	-	HIS	deletion	UNP H7BRJ8
A	?	-	ASN	deletion	UNP H7BRJ8
B	1	MET	-	expression tag	UNP H7BRJ8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	2	GLY	-	expression tag	UNP H7BRJ8
B	3	SER	-	expression tag	UNP H7BRJ8
B	4	SER	-	expression tag	UNP H7BRJ8
B	5	HIS	-	expression tag	UNP H7BRJ8
B	6	HIS	-	expression tag	UNP H7BRJ8
B	7	HIS	-	expression tag	UNP H7BRJ8
B	8	HIS	-	expression tag	UNP H7BRJ8
B	9	HIS	-	expression tag	UNP H7BRJ8
B	10	HIS	-	expression tag	UNP H7BRJ8
B	11	SER	-	expression tag	UNP H7BRJ8
B	12	SER	-	expression tag	UNP H7BRJ8
B	13	GLY	-	expression tag	UNP H7BRJ8
B	14	LEU	-	expression tag	UNP H7BRJ8
B	15	VAL	-	expression tag	UNP H7BRJ8
B	16	PRO	-	expression tag	UNP H7BRJ8
B	17	ARG	-	expression tag	UNP H7BRJ8
B	18	GLY	-	expression tag	UNP H7BRJ8
B	19	SER	-	expression tag	UNP H7BRJ8
B	20	HIS	-	expression tag	UNP H7BRJ8
B	21	MET	-	expression tag	UNP H7BRJ8
B	376	GLY	ALA	engineered mutation	UNP H7BRJ8
B	?	-	HIS	deletion	UNP H7BRJ8
B	?	-	ASN	deletion	UNP H7BRJ8

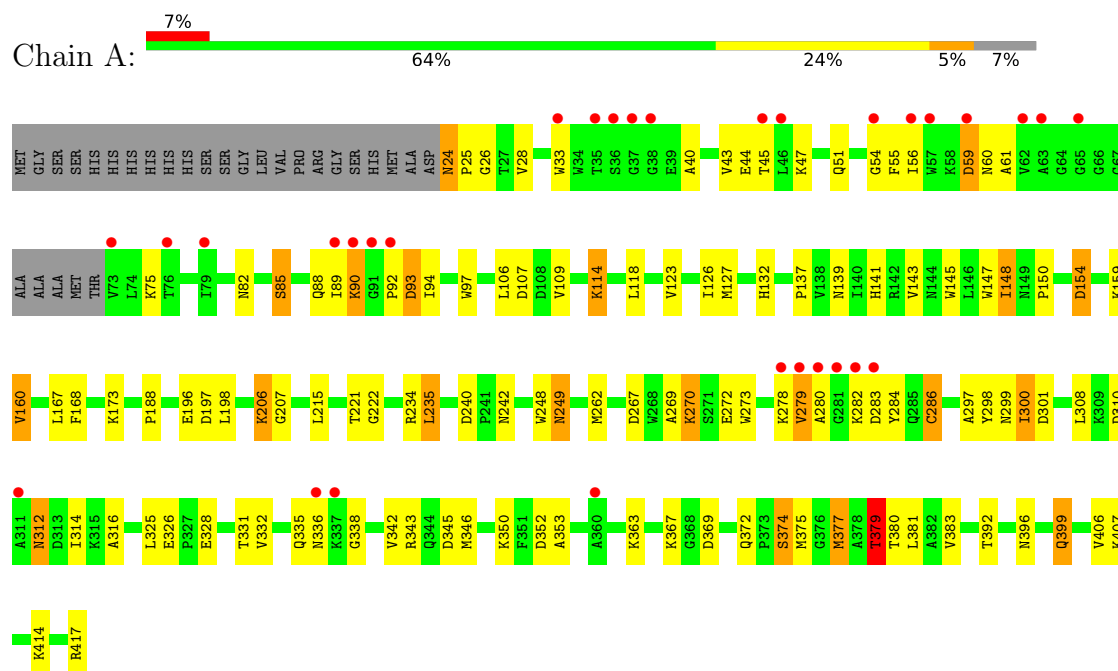
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	45	Total O 45 45	0	0
2	B	43	Total O 43 43	0	0

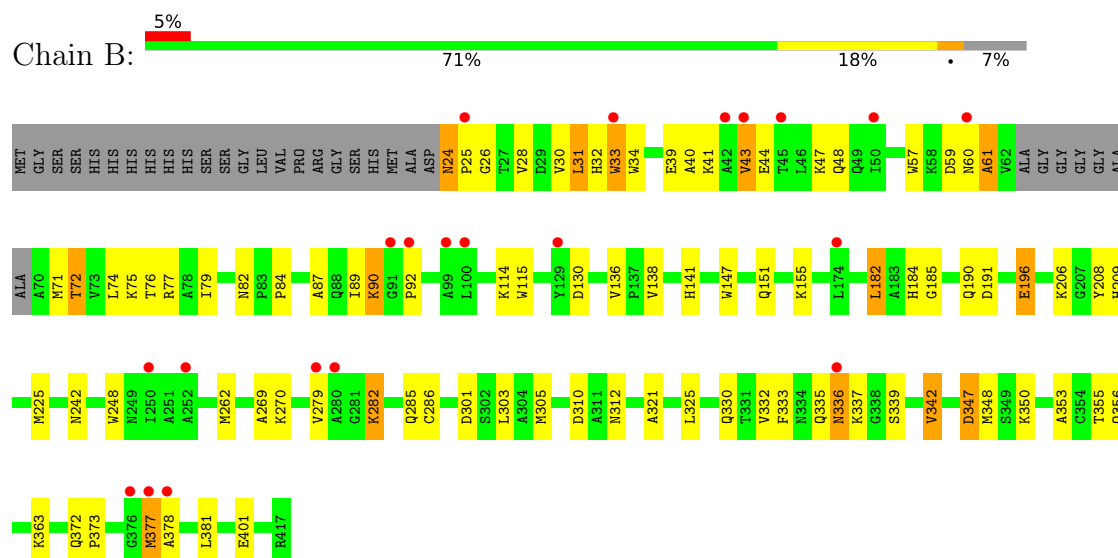
3 Residue-property plots

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: Binding protein component of ABC sugar transporter



- Molecule 1: Binding protein component of ABC sugar transporter



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	54.20Å 137.60Å 54.20Å 90.00° 109.50° 90.00°	Depositor
Resolution (Å)	37.22 – 2.50 37.22 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.4 (37.22-2.50) 99.9 (37.22-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.59 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.213 , 0.266 (Not available) , 0.261	Depositor DCC
R_{free} test set	1307 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	31.6	Xtriage
Anisotropy	0.191	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 35.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.116 for l,-k,h	Xtriage
Reported twinning fraction	0.542 for H, K, L 0.458 for L, -K, H	Depositor
Outliers	0 of 25872 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	5952	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.90% 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	0.95	2/2992 (0.1%)	1.12	9/4066 (0.2%)
1	B	0.94	1/3004 (0.0%)	1.14	10/4082 (0.2%)
All	All	0.94	3/5996 (0.1%)	1.13	19/8148 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	338	GLY	C-O	-5.59	1.16	1.24
1	A	197	ASP	C-O	-5.29	1.18	1.24
1	B	336	ASN	CA-CB	5.21	1.61	1.53

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	337	LYS	N-CA-C	-13.58	99.14	114.62
1	A	338	GLY	N-CA-C	9.09	125.83	114.37
1	A	26	GLY	N-CA-C	-7.11	102.40	111.72
1	A	326	GLU	CA-CB-CG	6.64	127.39	114.10
1	B	335	GLN	N-CA-C	-6.61	101.37	110.35
1	A	377	MET	CG-SD-CE	6.51	115.23	100.90
1	A	379	THR	N-CA-C	6.45	118.75	109.14
1	B	61	ALA	N-CA-C	6.24	119.29	110.50
1	B	90	LYS	N-CA-C	6.15	119.05	109.52
1	B	401	GLU	CB-CA-C	6.11	116.83	109.31
1	B	60	ASN	N-CA-CB	-5.89	104.72	111.79
1	B	336	ASN	N-CA-C	5.76	119.89	112.86
1	B	225	MET	N-CA-C	-5.53	105.27	112.23
1	B	82	ASN	CA-C-N	-5.37	114.85	120.38
1	B	82	ASN	C-N-CA	-5.37	114.85	120.38
1	A	300	ILE	N-CA-C	5.32	115.51	107.80
1	A	222	GLY	CA-C-N	5.28	125.09	119.28
1	A	222	GLY	C-N-CA	5.28	125.09	119.28
1	A	61	ALA	N-CA-C	5.21	116.96	108.63

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	2926	0	2837	97	0
1	B	2938	0	2871	61	0
2	A	45	0	0	3	0
2	B	43	0	0	5	1
All	All	5952	0	5708	158	1

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 14.

All (158) 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:336:ASN:CG	2:B:501:HOH:O	1.73	1.24
1:B:336:ASN:OD1	2:B:501:HOH:O	1.53	1.19
1:B:336:ASN:HB2	2:B:516:HOH:O	1.39	1.18
1:A:279:VAL:O	1:A:284:TYR:CE1	1.96	1.18
1:A:90:LYS:CG	1:A:300:ILE:O	2.00	1.09
1:A:90:LYS:HG3	1:A:300:ILE:O	1.53	1.08
1:B:25:PRO:O	1:B:312:ASN:HB3	1.57	1.04
1:A:25:PRO:HB2	1:A:54:GLY:O	1.61	1.01
1:A:215:LEU:HD13	1:A:417:ARG:HD3	1.50	0.93
1:A:279:VAL:O	1:A:284:TYR:HE1	1.48	0.91
1:A:336:ASN:HB2	2:A:501:HOH:O	1.71	0.90
1:B:336:ASN:ND2	2:B:501:HOH:O	1.87	0.90
1:B:348:MET:HE3	1:B:348:MET:HA	1.54	0.87
1:B:77:ARG:HH12	1:B:84:PRO:HB3	1.40	0.86
1:A:280:ALA:HB1	1:A:353:ALA:HB3	1.58	0.85
1:A:240:ASP:OD1	1:A:242:ASN:OD1	1.97	0.83
1:B:44:GLU:O	1:B:48:GLN:HG3	1.78	0.82
1:A:150:PRO:O	1:A:154:ASP:OD1	1.97	0.82
1:A:215:LEU:CD1	1:A:417:ARG:HD3	2.10	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:ASP:O	1:A:97:TRP:HD1	1.64	0.80
1:A:143:VAL:HG21	1:A:374:SER:HB2	1.64	0.80
1:A:346:MET:HA	1:A:346:MET:HE2	1.63	0.79
1:A:90:LYS:HE3	1:A:301:ASP:OD1	1.83	0.78
1:A:249:ASN:ND2	1:A:249:ASN:H	1.80	0.77
1:A:90:LYS:HG3	1:A:301:ASP:HA	1.67	0.77
1:B:196:GLU:OE1	1:B:208:TYR:OH	2.01	0.77
1:A:143:VAL:HG11	1:A:196:GLU:OE2	1.85	0.76
1:B:24:ASN:HD22	1:B:24:ASN:N	1.84	0.75
1:A:168:PHE:CE1	1:A:234:ARG:HG2	2.22	0.74
1:A:89:ILE:HG23	1:A:93:ASP:HB3	1.68	0.74
1:A:280:ALA:CB	1:A:353:ALA:HB3	2.17	0.73
1:B:279:VAL:HB	1:B:282:LYS:HD3	1.70	0.73
1:A:24:ASN:N	1:A:312:ASN:OD1	2.21	0.73
1:A:335:GLN:NE2	1:A:350:LYS:O	2.21	0.72
1:B:348:MET:HA	1:B:348:MET:CE	2.22	0.70
1:B:74:LEU:HD21	1:B:89:ILE:HD11	1.75	0.69
1:B:25:PRO:O	1:B:312:ASN:CB	2.39	0.69
1:B:353:ALA:HA	1:B:356:GLN:OE1	1.93	0.68
1:A:25:PRO:CB	1:A:54:GLY:O	2.40	0.68
1:A:47:LYS:HE3	1:A:51:GLN:HE22	1.60	0.67
1:A:143:VAL:HG21	1:A:374:SER:CB	2.25	0.67
1:A:90:LYS:HG2	1:A:300:ILE:O	1.93	0.66
1:A:328:GLU:O	1:A:332:VAL:HG22	1.96	0.66
1:A:28:VAL:HG23	1:A:316:ALA:HB1	1.79	0.65
1:A:215:LEU:CD1	1:A:417:ARG:CD	2.73	0.65
1:B:57:TRP:HE1	1:B:59:ASP:HB2	1.60	0.64
1:A:310:ASP:O	1:A:314:ILE:HG12	1.96	0.64
1:A:123:VAL:HG11	1:A:342:VAL:HG21	1.79	0.64
1:A:379:THR:HG21	1:A:383:VAL:HG11	1.80	0.62
1:A:248:TRP:CZ3	1:A:269:ALA:HA	2.34	0.62
1:B:90:LYS:HE2	1:B:377:MET:HG2	1.82	0.62
1:A:240:ASP:CG	1:A:242:ASN:OD1	2.42	0.62
1:A:33:TRP:NE1	1:A:88:GLN:HE22	1.98	0.62
1:B:305:MET:HE3	1:B:321:ALA:HB2	1.82	0.61
1:B:151:GLN:O	1:B:155:LYS:HG3	2.00	0.61
1:A:249:ASN:ND2	1:A:249:ASN:N	2.49	0.61
1:A:118:LEU:HD22	1:A:345:ASP:OD2	2.00	0.61
1:A:89:ILE:O	1:A:89:ILE:HG22	2.00	0.60
1:A:75:LYS:HD2	1:A:75:LYS:H	1.67	0.60
1:A:59:ASP:OD1	1:A:60:ASN:N	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:ASN:HB3	1:A:272:GLU:HG3	1.84	0.60
1:A:33:TRP:CE2	1:A:88:GLN:NE2	2.71	0.59
1:B:348:MET:HE2	1:B:355:THR:HG22	1.83	0.59
1:A:33:TRP:NE1	1:A:88:GLN:NE2	2.51	0.59
1:A:154:ASP:OD1	1:A:154:ASP:N	2.35	0.59
1:B:147:TRP:CZ3	1:B:286:CYS:HB3	2.37	0.58
1:A:377:MET:HE3	2:A:510:HOH:O	2.04	0.57
1:A:89:ILE:HG22	1:A:94:ILE:HG13	1.86	0.56
1:A:123:VAL:HG11	1:A:342:VAL:CG2	2.37	0.54
1:B:32:HIS:O	1:B:61:ALA:HA	2.06	0.54
1:A:215:LEU:HD13	1:A:417:ARG:CD	2.30	0.54
1:A:278:LYS:HD2	1:A:283:ASP:CG	2.32	0.54
1:A:392:THR:HG22	1:A:396:ASN:ND2	2.23	0.54
1:B:248:TRP:CZ3	1:B:269:ALA:HA	2.43	0.54
1:B:347:ASP:O	1:B:347:ASP:OD1	2.26	0.54
1:A:25:PRO:HD2	1:A:56:ILE:HG12	1.89	0.53
1:B:76:THR:O	1:B:79:ILE:N	2.42	0.53
1:A:90:LYS:CD	1:A:300:ILE:O	2.57	0.53
1:B:336:ASN:CB	2:B:516:HOH:O	2.20	0.53
1:B:92:PRO:HD3	1:B:377:MET:O	2.09	0.52
1:A:273:TRP:HE3	1:A:278:LYS:HG3	1.74	0.52
1:B:209:HIS:HD2	1:B:372:GLN:OE1	1.93	0.52
1:B:182:LEU:HD23	1:B:262:MET:HE3	1.92	0.52
1:B:138:VAL:HG22	1:B:301:ASP:O	2.10	0.51
1:A:75:LYS:HG3	1:A:97:TRP:CH2	2.46	0.51
1:B:332:VAL:HG23	1:B:333:PHE:N	2.26	0.51
1:A:147:TRP:CZ3	1:A:286:CYS:HB3	2.46	0.50
1:A:33:TRP:CE2	1:A:88:GLN:CD	2.90	0.50
1:A:24:ASN:N	1:A:25:PRO:HA	2.27	0.49
1:B:24:ASN:HB2	1:B:26:GLY:HA2	1.94	0.48
1:A:85:SER:OG	1:A:308:LEU:HD11	2.13	0.48
1:A:270:LYS:NZ	1:A:352:ASP:OD1	2.47	0.48
1:B:136:VAL:HG12	1:B:303:LEU:HB2	1.94	0.48
1:A:118:LEU:CD2	1:A:345:ASP:OD2	2.61	0.48
1:B:92:PRO:CD	1:B:377:MET:O	2.61	0.48
1:A:221:THR:HA	1:A:406:VAL:HB	1.96	0.48
1:B:373:PRO:HB2	1:B:378:ALA:HB2	1.97	0.47
1:A:25:PRO:HG2	1:A:55:PHE:HA	1.96	0.47
1:B:348:MET:HE3	1:B:348:MET:CA	2.36	0.47
1:B:347:ASP:OD1	1:B:347:ASP:C	2.57	0.47
1:A:107:ASP:OD1	1:A:132:HIS:HD2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:GLU:OE1	1:A:375:MET:HB3	2.15	0.47
1:B:47:LYS:HG3	1:B:57:TRP:CG	2.49	0.47
1:B:77:ARG:NH1	1:B:84:PRO:HB3	2.20	0.47
1:A:92:PRO:C	1:A:94:ILE:H	2.22	0.47
1:B:115:TRP:CE2	1:B:325:LEU:HD12	2.49	0.47
1:A:148:ILE:HD12	1:A:160:VAL:HG13	1.96	0.47
1:A:379:THR:HG21	1:A:383:VAL:CG1	2.45	0.47
1:A:379:THR:HG22	1:A:380:THR:H	1.78	0.47
1:B:141:HIS:CE1	1:B:339:SER:HB3	2.50	0.47
1:B:40:ALA:O	1:B:43:VAL:HG12	2.15	0.47
1:A:47:LYS:CE	1:A:51:GLN:HE22	2.26	0.46
1:A:336:ASN:CB	2:A:501:HOH:O	2.47	0.46
1:A:325:LEU:O	1:A:343:ARG:HD2	2.15	0.46
1:A:331:THR:O	1:A:335:GLN:HB2	2.15	0.46
1:B:347:ASP:OD1	1:B:350:LYS:N	2.45	0.46
1:A:206:LYS:HG2	1:A:207:GLY:N	2.30	0.46
1:B:114:LYS:HB2	1:B:114:LYS:HE3	1.71	0.46
1:B:32:HIS:O	1:B:61:ALA:CA	2.64	0.46
1:A:198:LEU:HD11	1:A:235:LEU:CD2	2.46	0.46
1:A:215:LEU:HD12	1:A:417:ARG:CD	2.44	0.46
1:B:34:TRP:HB3	1:B:39:GLU:HB3	1.97	0.46
1:A:40:ALA:HA	1:A:43:VAL:HG12	1.98	0.45
1:A:141:HIS:HB2	1:A:299:ASN:HB3	1.98	0.45
1:A:92:PRO:C	1:A:94:ILE:N	2.74	0.45
1:B:147:TRP:O	1:B:262:MET:HA	2.17	0.45
1:B:330:GLN:NE2	1:B:342:VAL:H	2.14	0.45
1:B:185:GLY:HA3	1:B:190:GLN:HE22	1.82	0.44
1:B:71:MET:O	1:B:75:LYS:HG3	2.17	0.44
1:A:399:GLN:HE21	1:A:399:GLN:HB2	1.67	0.44
1:A:273:TRP:CE3	1:A:278:LYS:HG3	2.52	0.44
1:A:167:LEU:HD12	1:A:262:MET:HE1	2.00	0.44
1:A:137:PRO:HG2	1:A:342:VAL:HG11	2.00	0.43
1:B:32:HIS:CE1	1:B:61:ALA:HB2	2.54	0.43
1:A:346:MET:HA	1:A:346:MET:CE	2.43	0.43
1:A:297:ALA:HA	1:A:372:GLN:O	2.18	0.42
1:A:90:LYS:HG3	1:A:300:ILE:C	2.36	0.42
1:B:184:HIS:HE1	1:B:191:ASP:OD1	2.03	0.42
1:A:126:ILE:HG22	1:A:127:MET:HE2	2.01	0.42
1:A:139:ASN:OD1	1:A:139:ASN:C	2.63	0.42
1:B:377:MET:HE3	1:B:377:MET:HB3	1.64	0.42
1:A:145:TRP:CD1	1:A:267:ASP:HB3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:LYS:HB2	1:A:114:LYS:HE3	1.68	0.42
1:B:24:ASN:HB2	1:B:26:GLY:CA	2.50	0.42
1:B:330:GLN:HE22	1:B:342:VAL:HG12	1.84	0.42
1:A:196:GLU:OE1	1:A:375:MET:CB	2.69	0.41
1:A:363:LYS:O	1:A:367:LYS:HG2	2.19	0.41
1:B:31:LEU:O	1:B:87:ALA:HA	2.20	0.41
1:A:367:LYS:HG2	1:A:367:LYS:H	1.76	0.41
1:B:33:TRP:CD1	1:B:33:TRP:O	2.73	0.41
1:B:141:HIS:ND1	1:B:339:SER:HB3	2.35	0.41
1:B:28:VAL:HG12	1:B:30:VAL:HG23	2.02	0.41
1:B:72:THR:HA	1:B:75:LYS:HD2	2.02	0.41
1:A:106:LEU:HB3	1:A:109:VAL:CG1	2.51	0.40
1:A:106:LEU:HB3	1:A:109:VAL:HG12	2.03	0.40
1:B:32:HIS:CE1	1:B:34:TRP:HB2	2.56	0.40
1:A:150:PRO:HD3	1:A:284:TYR:HA	2.03	0.40
1:A:126:ILE:HD11	1:A:298:TYR:OH	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:522:HOH:O	2:B:530:HOH:O[1_556]	2.12	0.08

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	385/417 (92%)	372 (97%)	13 (3%)	0	100	100
1	B	383/417 (92%)	372 (97%)	11 (3%)	0	100	100
All	All	768/834 (92%)	744 (97%)	24 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	274/320 (86%)	244 (89%)	30 (11%)	6	13
1	B	297/320 (93%)	277 (93%)	20 (7%)	15	31
All	All	571/640 (89%)	521 (91%)	50 (9%)	9	20

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

Mol	Chain	Res	Type
1	A	24	ASN
1	A	44	GLU
1	A	45	THR
1	A	59	ASP
1	A	82	ASN
1	A	85	SER
1	A	90	LYS
1	A	93	ASP
1	A	114	LYS
1	A	148	ILE
1	A	154	ASP
1	A	159	LYS
1	A	160	VAL
1	A	173	LYS
1	A	188	PRO
1	A	206	LYS
1	A	235	LEU
1	A	249	ASN
1	A	270	LYS
1	A	279	VAL
1	A	282	LYS
1	A	286	CYS
1	A	312	ASN
1	A	369	ASP
1	A	374	SER

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Mol	Chain	Res	Type
1	A	379	THR
1	A	381	LEU
1	A	399	GLN
1	A	407	LYS
1	A	414	LYS
1	B	24	ASN
1	B	31	LEU
1	B	33	TRP
1	B	41	LYS
1	B	43	VAL
1	B	72	THR
1	B	130	ASP
1	B	182	LEU
1	B	196	GLU
1	B	206	LYS
1	B	242	ASN
1	B	270	LYS
1	B	282	LYS
1	B	285	GLN
1	B	310	ASP
1	B	342	VAL
1	B	347	ASP
1	B	363	LYS
1	B	377	MET
1	B	381	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	GLN
1	A	132	HIS
1	A	184	HIS
1	A	249	ASN
1	A	318	ASN
1	A	330	GLN
1	A	399	GLN
1	B	82	ASN
1	B	184	HIS
1	B	190	GLN
1	B	209	HIS
1	B	249	ASN
1	B	312	ASN

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Mol	Chain	Res	Type
1	B	330	GLN
1	B	336	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 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	389/417 (93%)	0.63	31 (7%) 18 16	11, 28, 63, 84	0
1	B	387/417 (92%)	0.60	21 (5%) 31 27	17, 32, 55, 66	0
All	All	776/834 (93%)	0.61	52 (6%) 24 21	11, 30, 57, 84	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	336	ASN	7.3
1	A	280	ALA	7.1
1	A	91	GLY	6.5
1	B	336	ASN	5.8
1	A	279	VAL	5.0
1	A	90	LYS	4.6
1	A	73	VAL	4.0
1	A	92	PRO	3.9
1	A	337	LYS	3.9
1	B	377	MET	3.7
1	A	281	GLY	3.6
1	A	63	ALA	3.6
1	B	25	PRO	3.4
1	B	91	GLY	3.4
1	B	376	GLY	3.2
1	A	45	THR	3.0
1	B	33	TRP	2.9
1	A	89	ILE	2.8
1	A	33	TRP	2.8
1	A	282	LYS	2.8
1	B	280	ALA	2.7
1	A	35	THR	2.7
1	A	311	ALA	2.6
1	B	42	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	37	GLY	2.6
1	B	60	ASN	2.6
1	A	57	TRP	2.6
1	A	79	ILE	2.5
1	B	174	LEU	2.4
1	B	50	ILE	2.4
1	A	56	ILE	2.4
1	B	250	ILE	2.4
1	A	65	GLY	2.3
1	B	100	LEU	2.3
1	A	76	THR	2.3
1	B	45	THR	2.3
1	B	279	VAL	2.3
1	A	360	ALA	2.3
1	A	46	LEU	2.3
1	B	99	ALA	2.3
1	A	38	GLY	2.2
1	A	59	ASP	2.2
1	A	283	ASP	2.1
1	A	36	SER	2.1
1	B	92	PRO	2.1
1	A	62	VAL	2.1
1	A	54	GLY	2.1
1	B	43	VAL	2.0
1	B	252	ALA	2.0
1	A	278	LYS	2.0
1	B	378	ALA	2.0
1	B	129	TYR	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 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.