



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:14 AM UTC

PDB ID : 5JFK / pdb_00005jfk
Title : Crystal structure of a TDR receptor
Authors : Li, Z.; Xu, G.
Deposited on : 2016-04-19
Resolution : 2.65 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

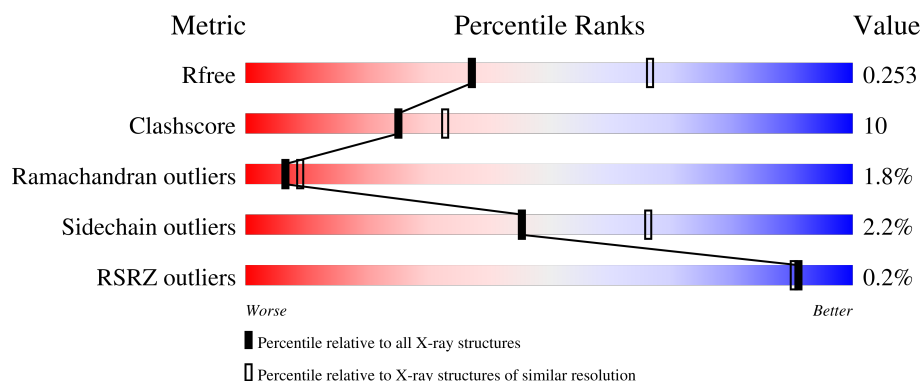
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	2053 (2.66-2.62)
Clashscore	190562	2097 (2.66-2.62)
Ramachandran outliers	187476	2066 (2.66-2.62)
Sidechain outliers	187428	2066 (2.66-2.62)
RSRZ outliers	180081	2052 (2.66-2.62)

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	613	 74% 17% • 6%
1	B	613	 75% 17% • 6%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 9211 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 Leucine-rich repeat receptor-like protein kinase TDR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	577	Total	C	N	O	S	0	0	0
			4463	2859	745	847	12			
1	B	577	Total	C	N	O	S	0	0	0
			4463	2859	745	847	12			

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	66	Total	O	0	0
			66	66		
3	B	79	Total	O	0	0
			79	79		

4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	92.34Å 92.34Å 250.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.17 – 2.65 46.17 – 2.65	Depositor EDS
% Data completeness (in resolution range)	88.1 (46.17-2.65) 88.0 (46.17-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 2.65Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.222 , 0.250 0.227 , 0.253	Depositor DCC
R_{free} test set	1721 reflections (2.84%)	wwPDB-VP
Wilson B-factor (Å ²)	54.6	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 44.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.457 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9211	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.83% 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

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

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	0.40	1/4571 (0.0%)	0.84	9/6214 (0.1%)
1	B	0.32	0/4571	0.79	8/6214 (0.1%)
All	All	0.36	1/9142 (0.0%)	0.82	17/12428 (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	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	74	VAL	CA-CB	6.48	1.61	1.54

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	78	ASN	N-CA-C	6.27	124.15	110.80
1	A	68	TRP	N-CA-C	5.79	117.88	109.07
1	A	68	TRP	CA-C-N	5.78	132.58	121.54
1	A	68	TRP	C-N-CA	5.78	132.58	121.54
1	A	488	ALA	CA-C-N	5.74	124.94	118.97
1	A	488	ALA	C-N-CA	5.74	124.94	118.97
1	B	58	VAL	CA-C-N	-5.61	112.83	119.84
1	B	58	VAL	C-N-CA	-5.61	112.83	119.84
1	A	74	VAL	N-CA-C	-5.45	105.19	110.42
1	B	488	ALA	CA-C-N	5.42	125.07	119.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	488	ALA	C-N-CA	5.42	125.07	119.05
1	B	559	LEU	CA-C-N	5.41	125.23	119.28
1	B	559	LEU	C-N-CA	5.41	125.23	119.28
1	B	68	TRP	N-CA-C	5.33	116.95	108.79
1	A	559	LEU	CA-C-N	5.18	124.98	119.28
1	A	559	LEU	C-N-CA	5.18	124.98	119.28
1	A	475	ASN	N-CA-C	5.01	121.58	114.16

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	78	ASN	Peptide

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	4463	0	4360	90	1
1	B	4463	0	4359	80	1
2	A	70	0	65	2	0
2	B	70	0	65	2	0
3	A	66	0	0	9	0
3	B	79	0	0	13	0
All	All	9211	0	8849	173	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 10.

All (173) 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:68:TRP:CZ3	1:A:72:SER:HB3	2.03	0.91
1:B:80:THR:HG22	1:B:82:GLN:H	1.39	0.87
1:A:72:SER:OG	1:A:75:VAL:HB	1.81	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:VAL:O	3:B:801:HOH:O	1.99	0.79
1:A:619:LEU:HD23	1:A:620:CYS:H	1.45	0.79
1:A:77:ASP:OD1	1:A:78:ASN:N	2.15	0.79
1:A:151:LYS:NZ	3:A:804:HOH:O	2.15	0.78
1:A:395:LEU:HD11	1:A:398:LEU:HB2	1.68	0.76
1:B:597:ILE:HG22	1:B:616:ASN:HD22	1.51	0.75
1:B:308:GLN:NE2	3:B:805:HOH:O	2.16	0.75
1:B:64:ASN:O	1:B:66:ALA:N	2.20	0.74
1:A:63:GLN:CD	1:A:64:ASN:H	1.95	0.74
1:A:65:ASP:OD2	3:A:801:HOH:O	2.06	0.73
1:B:63:GLN:CD	1:B:64:ASN:H	1.97	0.73
1:B:236:HIS:O	3:B:802:HOH:O	2.07	0.72
1:A:99:ILE:HD12	1:A:124:SER:HB3	1.72	0.71
1:A:132:THR:HG23	1:A:133:THR:HG23	1.73	0.70
1:B:597:ILE:HG22	1:B:616:ASN:ND2	2.06	0.70
1:A:255:ASP:OD2	3:A:802:HOH:O	2.08	0.70
1:A:72:SER:C	1:A:74:VAL:H	2.00	0.69
1:B:132:THR:HG23	1:B:133:THR:HG23	1.73	0.69
1:B:61:ASN:O	3:B:803:HOH:O	2.13	0.67
1:A:421:ARG:HG2	1:A:445:PHE:HB3	1.77	0.66
1:A:72:SER:C	1:A:74:VAL:N	2.53	0.66
1:A:201:GLN:N	1:A:201:GLN:OE1	2.30	0.65
1:B:204:LYS:HA	1:B:227:LEU:HA	1.79	0.65
1:A:64:ASN:O	1:A:66:ALA:N	2.29	0.65
1:A:71:TRP:O	3:A:803:HOH:O	2.14	0.64
1:A:62:GLY:HA2	1:A:71:TRP:CZ2	2.32	0.64
1:A:616:ASN:O	1:A:617:GLU:HG3	1.99	0.63
1:B:42:LEU:HA	1:B:91:ARG:HH22	1.64	0.63
1:A:70:SER:O	3:A:805:HOH:O	2.15	0.63
1:B:373:THR:HG23	1:B:397:LYS:HB3	1.80	0.62
1:B:253:TYR:OH	3:B:804:HOH:O	2.15	0.62
1:A:204:LYS:HA	1:A:227:LEU:HA	1.82	0.61
1:B:71:TRP:NE1	3:B:803:HOH:O	2.22	0.61
1:B:78:ASN:OD1	1:B:79:VAL:N	2.34	0.60
1:B:68:TRP:HZ3	1:B:98:PRO:HD3	1.66	0.60
1:B:68:TRP:HE1	1:B:93:LEU:HB3	1.66	0.59
1:B:82:GLN:NE2	3:B:811:HOH:O	2.30	0.59
1:A:72:SER:O	1:A:74:VAL:N	2.30	0.59
1:B:82:GLN:NE2	3:B:813:HOH:O	2.34	0.59
1:B:91:ARG:HB2	1:B:93:LEU:HG	1.85	0.58
1:A:373:THR:HG23	1:A:397:LYS:HB3	1.86	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:TRP:NE1	1:B:93:LEU:HB3	2.18	0.58
1:A:62:GLY:HA2	1:A:71:TRP:CH2	2.39	0.57
1:B:600:ILE:HD12	1:B:618:GLY:HA3	1.86	0.57
1:B:78:ASN:HB2	1:B:80:THR:OG1	2.04	0.57
1:A:68:TRP:CE3	1:A:69:CYS:N	2.71	0.57
1:A:74:VAL:O	1:A:77:ASP:N	2.38	0.56
1:A:436:GLY:N	1:A:460:ASP:OD2	2.34	0.56
1:B:537:LYS:HB2	3:B:817:HOH:O	2.05	0.56
1:B:292:SER:O	1:B:295:ASN:ND2	2.39	0.56
1:A:515:TYR:HA	1:A:538:LEU:HA	1.88	0.56
1:B:42:LEU:HA	1:B:91:ARG:NH2	2.21	0.55
1:A:504:GLU:OE2	3:A:806:HOH:O	2.18	0.55
1:A:82:GLN:NE2	3:A:814:HOH:O	2.39	0.55
1:B:286:THR:O	3:B:806:HOH:O	2.18	0.55
1:A:63:GLN:OE1	1:A:64:ASN:N	2.40	0.55
1:A:619:LEU:CD2	1:A:620:CYS:H	2.17	0.54
1:B:240:ASN:OD1	1:B:241:ILE:N	2.40	0.54
1:A:42:LEU:HA	1:A:91:ARG:HH22	1.73	0.54
1:A:597:ILE:HG22	1:A:617:GLU:OE2	2.08	0.53
1:A:460:ASP:N	1:A:460:ASP:OD1	2.31	0.53
1:B:397:LYS:HE2	1:B:399:ILE:HD11	1.90	0.53
1:A:61:ASN:O	1:A:71:TRP:HZ2	1.92	0.52
1:A:207:HIS:CE1	1:A:209:ALA:HB3	2.45	0.52
1:B:68:TRP:CB	1:B:71:TRP:HB3	2.40	0.52
1:B:170:PRO:O	1:B:173:VAL:HG23	2.10	0.52
1:A:504:GLU:HG3	1:A:526:GLY:HA3	1.92	0.52
1:B:68:TRP:CD1	1:B:93:LEU:HB3	2.45	0.52
1:A:354:ASN:CG	1:A:378:ASN:HD22	2.18	0.51
1:A:458:PRO:HB2	1:A:460:ASP:OD1	2.09	0.51
1:A:240:ASN:OD1	1:A:241:ILE:N	2.44	0.51
1:A:170:PRO:O	1:A:173:VAL:HG23	2.11	0.51
1:B:63:GLN:OE1	1:B:64:ASN:N	2.44	0.51
1:A:292:SER:O	1:A:295:ASN:ND2	2.43	0.51
1:B:70:SER:HA	1:B:73:GLY:HA3	1.94	0.49
1:A:206:ILE:HG22	1:A:227:LEU:HD11	1.94	0.49
1:B:62:GLY:HA2	1:B:71:TRP:HZ2	1.77	0.49
1:B:369:GLY:HA2	1:B:391:HIS:O	2.13	0.49
1:B:597:ILE:HD11	3:B:865:HOH:O	2.12	0.49
1:B:206:ILE:HG22	1:B:227:LEU:HD11	1.94	0.49
1:A:91:ARG:HB2	1:A:93:LEU:HG	1.93	0.49
1:A:180:GLU:HA	1:A:203:LEU:HA	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:575:THR:HA	1:A:597:ILE:O	2.13	0.48
1:A:616:ASN:O	1:A:617:GLU:CG	2.60	0.48
1:B:266:PRO:HG2	1:B:269:LEU:HG	1.95	0.48
1:B:273:SER:C	1:B:275:LEU:H	2.21	0.48
1:B:435:ILE:HG23	1:B:460:ASP:OD2	2.13	0.48
1:A:369:GLY:HA2	1:A:391:HIS:O	2.13	0.48
1:B:207:HIS:CE1	1:B:209:ALA:HB3	2.49	0.48
1:A:68:TRP:CZ2	1:A:98:PRO:HD3	2.49	0.48
1:B:232:ILE:HG13	1:B:256:VAL:HG22	1.96	0.48
1:B:59:PRO:O	1:B:61:ASN:N	2.46	0.48
1:A:273:SER:C	1:A:275:LEU:H	2.22	0.48
1:A:360:VAL:HG13	1:A:361:LEU:O	2.14	0.47
1:A:68:TRP:N	1:A:94:SER:O	2.47	0.47
1:B:118:GLU:HG2	1:B:119:GLY:H	1.78	0.47
1:B:68:TRP:CE3	1:B:72:SER:HB3	2.49	0.47
1:A:225:THR:HG22	1:A:226:GLU:HG2	1.97	0.47
1:B:99:ILE:HD11	1:B:102:ARG:HH21	1.81	0.46
1:B:515:TYR:HA	1:B:538:LEU:HA	1.97	0.46
1:A:232:ILE:HG13	1:A:256:VAL:HG22	1.98	0.46
1:A:42:LEU:HA	1:A:91:ARG:NH2	2.31	0.46
1:B:354:ASN:CG	1:B:378:ASN:HD22	2.24	0.46
1:B:504:GLU:HG3	1:B:526:GLY:HA3	1.98	0.46
1:B:68:TRP:HB2	1:B:71:TRP:HB3	1.98	0.46
1:A:118:GLU:HG2	1:A:119:GLY:H	1.81	0.46
1:B:68:TRP:CZ3	1:B:98:PRO:HD3	2.48	0.46
1:B:360:VAL:HG13	1:B:361:LEU:O	2.16	0.46
1:B:593:TYR:H	1:B:614:SER:HB3	1.80	0.45
2:B:702:NAG:O7	3:B:807:HOH:O	2.20	0.45
1:A:218:PRO:HA	1:A:219:PRO:HD2	1.88	0.45
1:A:559:LEU:HA	1:A:560:PRO:HD3	1.79	0.45
1:B:180:GLU:HA	1:B:203:LEU:HA	1.98	0.45
1:A:397:LYS:HE2	1:A:399:ILE:HD11	1.98	0.45
1:B:130:LYS:HB3	1:B:130:LYS:HE2	1.62	0.45
1:B:484:ASN:HB3	1:B:487:LYS:HG3	1.98	0.45
1:A:453:PHE:O	1:A:475:ASN:O	2.34	0.45
1:A:78:ASN:HB3	1:A:80:THR:HG23	1.98	0.45
1:B:363:HIS:ND1	1:B:364:LYS:HG2	2.32	0.45
1:A:78:ASN:C	1:A:80:THR:N	2.75	0.45
1:A:100:GLN:O	1:A:103:TYR:HD1	1.99	0.45
1:A:130:LYS:HB3	1:A:130:LYS:HE3	1.62	0.45
1:B:273:SER:O	1:B:274:ASN:HB2	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:475:ASN:H	1:B:499:SER:HA	1.81	0.44
1:A:232:ILE:CG1	1:A:256:VAL:HG22	2.47	0.44
1:A:622:ASP:O	1:A:623:LEU:HG	2.17	0.44
1:B:436:GLY:N	1:B:460:ASP:OD2	2.49	0.44
1:B:100:GLN:O	1:B:103:TYR:HD1	1.99	0.44
1:B:232:ILE:CG1	1:B:256:VAL:HG22	2.48	0.44
1:A:273:SER:O	1:A:274:ASN:HB2	2.18	0.44
1:A:47:SER:CB	1:A:80:THR:HG21	2.47	0.44
1:A:62:GLY:HA2	1:A:71:TRP:HZ2	1.80	0.44
1:A:266:PRO:HG2	1:A:269:LEU:HG	1.99	0.44
1:B:68:TRP:HB3	1:B:71:TRP:HB3	1.99	0.43
1:B:218:PRO:HA	1:B:219:PRO:HD2	1.88	0.43
1:B:41:SER:C	1:B:43:LYS:H	2.25	0.43
1:B:471:ASN:OD1	1:B:473:SER:HB3	2.18	0.43
1:A:323:LEU:HD23	1:A:323:LEU:HA	1.83	0.43
1:A:471:ASN:OD1	1:A:473:SER:HB3	2.18	0.43
1:B:495:SER:OG	2:B:703:NAG:H82	2.18	0.43
1:A:611:SER:C	1:A:613:PHE:H	2.26	0.43
1:A:420:TRP:O	1:A:444:THR:HG22	2.19	0.43
1:A:131:LEU:HD23	1:A:131:LEU:HA	1.88	0.43
1:A:591:VAL:CG2	1:A:596:LEU:HD11	2.49	0.43
1:A:305:SER:HB2	1:A:329:ILE:HB	2.01	0.42
1:B:107:LEU:HD12	1:B:128:LEU:HD13	2.02	0.42
1:B:244:GLU:OE1	1:B:244:GLU:N	2.45	0.42
1:A:107:LEU:HD23	1:A:107:LEU:HA	1.87	0.42
2:A:704:NAG:O5	3:A:808:HOH:O	2.22	0.42
1:A:622:ASP:OD1	1:A:622:ASP:N	2.53	0.42
1:A:78:ASN:C	1:A:80:THR:HG23	2.45	0.42
1:B:76:CYS:SG	1:B:101:ILE:HA	2.59	0.42
1:A:227:LEU:HD21	1:A:230:MET:HB2	2.02	0.42
1:B:67:VAL:HG12	1:B:68:TRP:N	2.35	0.42
1:A:230:MET:HE3	1:A:254:PHE:CD1	2.55	0.42
2:A:701:NAG:O4	3:A:807:HOH:O	2.21	0.42
1:A:201:GLN:C	1:A:203:LEU:H	2.28	0.41
1:A:508:TYR:CD2	1:A:529:PRO:HB2	2.55	0.41
1:A:68:TRP:CD2	1:A:69:CYS:N	2.88	0.41
1:A:574:GLY:HA2	1:A:597:ILE:HG12	2.01	0.41
1:B:107:LEU:HD23	1:B:107:LEU:HA	1.85	0.41
1:A:244:GLU:OE1	1:A:244:GLU:N	2.42	0.41
1:A:492:GLN:HB3	1:A:515:TYR:CE2	2.55	0.41
1:B:616:ASN:HB3	1:B:617:GLU:H	1.70	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:ARG:NE	3:B:810:HOH:O	2.29	0.41
1:B:305:SER:HB2	1:B:329:ILE:HB	2.03	0.41
1:B:611:SER:C	1:B:613:PHE:H	2.29	0.41
1:A:187:SER:HB3	1:A:188:TYR:H	1.72	0.40
1:B:80:THR:HG22	1:B:82:GLN:N	2.19	0.40
1:B:230:MET:HE3	1:B:254:PHE:CE1	2.56	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)
1:A:294:SER:OG	1:B:620:CYS:O[3_545]	2.10	0.10

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	573/613 (94%)	498 (87%)	65 (11%)	10 (2%)	7	9
1	B	573/613 (94%)	499 (87%)	63 (11%)	11 (2%)	6	8
All	All	1146/1226 (94%)	997 (87%)	128 (11%)	21 (2%)	6	9

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	65	ASP
1	A	80	THR
1	A	617	GLU
1	A	623	LEU
1	B	65	ASP
1	B	78	ASN
1	B	79	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	619	LEU
1	A	69	CYS
1	A	614	SER
1	B	617	GLU
1	B	622	ASP
1	A	491	LEU
1	B	42	LEU
1	B	614	SER
1	A	42	LEU
1	B	59	PRO
1	B	60	VAL
1	A	79	VAL
1	A	256	VAL
1	B	256	VAL

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	505/544 (93%)	492 (97%)	13 (3%)	40	61
1	B	505/544 (93%)	496 (98%)	9 (2%)	51	71
All	All	1010/1088 (93%)	988 (98%)	22 (2%)	45	66

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	TRP
1	A	82	GLN
1	A	173	VAL
1	A	177	ARG
1	A	201	GLN
1	A	204	LYS
1	A	225	THR
1	A	291	GLU
1	A	360	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	413	LEU
1	A	460	ASP
1	A	509	VAL
1	A	584	LYS
1	B	82	GLN
1	B	173	VAL
1	B	204	LYS
1	B	360	VAL
1	B	413	LEU
1	B	487	LYS
1	B	507	ASN
1	B	584	LYS
1	B	624	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	238	ASN
1	A	490	ASN
1	B	426	ASN
1	B	450	ASN
1	B	490	ASN
1	B	507	ASN
1	B	616	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

10 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	B	704	1	14,14,15	1.12	1 (7%)	17,19,21	1.34	1 (5%)
2	NAG	A	705	1	14,14,15	0.55	0	17,19,21	0.58	0
2	NAG	A	703	1	14,14,15	0.61	0	17,19,21	0.55	0
2	NAG	B	701	1	14,14,15	0.44	0	17,19,21	0.58	0
2	NAG	A	701	1	14,14,15	0.52	0	17,19,21	0.59	0
2	NAG	B	702	1	14,14,15	0.31	0	17,19,21	0.41	0
2	NAG	B	705	1	14,14,15	0.50	0	17,19,21	0.56	0
2	NAG	A	702	1	14,14,15	0.24	0	17,19,21	0.38	0
2	NAG	B	703	1	14,14,15	0.70	0	17,19,21	0.55	0
2	NAG	A	704	1	14,14,15	0.53	0	17,19,21	0.47	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	704	1	-	3/6/23/26	0/1/1/1
2	NAG	A	705	1	-	1/6/23/26	0/1/1/1
2	NAG	A	703	1	-	2/6/23/26	0/1/1/1
2	NAG	B	701	1	-	2/6/23/26	0/1/1/1
2	NAG	A	701	1	-	2/6/23/26	0/1/1/1
2	NAG	B	702	1	-	2/6/23/26	0/1/1/1
2	NAG	B	705	1	-	0/6/23/26	0/1/1/1
2	NAG	A	702	1	-	1/6/23/26	0/1/1/1
2	NAG	B	703	1	-	2/6/23/26	0/1/1/1
2	NAG	A	704	1	-	4/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	704	NAG	O5-C1	3.90	1.50	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	704	NAG	C1-O5-C5	5.13	119.07	112.19

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	703	NAG	O5-C5-C6-O6
2	B	701	NAG	O5-C5-C6-O6
2	A	701	NAG	O5-C5-C6-O6
2	A	703	NAG	O5-C5-C6-O6
2	A	704	NAG	O5-C5-C6-O6
2	B	703	NAG	C4-C5-C6-O6
2	B	701	NAG	C4-C5-C6-O6
2	A	701	NAG	C4-C5-C6-O6
2	A	703	NAG	C4-C5-C6-O6
2	A	704	NAG	C8-C7-N2-C2
2	A	704	NAG	O7-C7-N2-C2
2	B	704	NAG	C8-C7-N2-C2
2	B	704	NAG	O7-C7-N2-C2
2	A	704	NAG	C4-C5-C6-O6
2	B	702	NAG	O5-C5-C6-O6
2	B	702	NAG	C4-C5-C6-O6
2	A	702	NAG	O5-C5-C6-O6
2	A	705	NAG	O5-C5-C6-O6
2	B	704	NAG	C4-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	NAG	1	0
2	B	702	NAG	1	0
2	B	703	NAG	1	0
2	A	704	NAG	1	0

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	577/613 (94%)	-0.93	0 100 100	37, 61, 93, 121	0
1	B	577/613 (94%)	-0.94	2 (0%) 90 89	35, 61, 94, 118	0
All	All	1154/1226 (94%)	-0.93	2 (0%) 91 90	35, 61, 93, 121	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	80	THR	2.1
1	B	46	LEU	2.1

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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	A	702	14/15	0.97	0.07	73,94,104,108	0
2	NAG	A	704	14/15	0.97	0.06	65,82,97,99	0
2	NAG	B	702	14/15	0.97	0.07	75,94,104,104	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	B	704	14/15	0.97	0.08	66,79,89,89	0
2	NAG	A	701	14/15	0.98	0.06	31,61,72,72	0
2	NAG	B	701	14/15	0.99	0.04	31,62,71,71	0
2	NAG	A	703	14/15	0.99	0.04	34,41,55,56	0
2	NAG	B	703	14/15	0.99	0.03	28,42,58,58	0
2	NAG	A	705	14/15	0.99	0.04	57,72,79,88	0
2	NAG	B	705	14/15	0.99	0.05	58,77,88,99	0

6.5 Other polymers [i](#)

There are no such residues in this entry.