Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 03:50 AM BST

PDB ID	:	5JFK
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 following versions of software and data (see references ⓘ) were used in the production of this report:

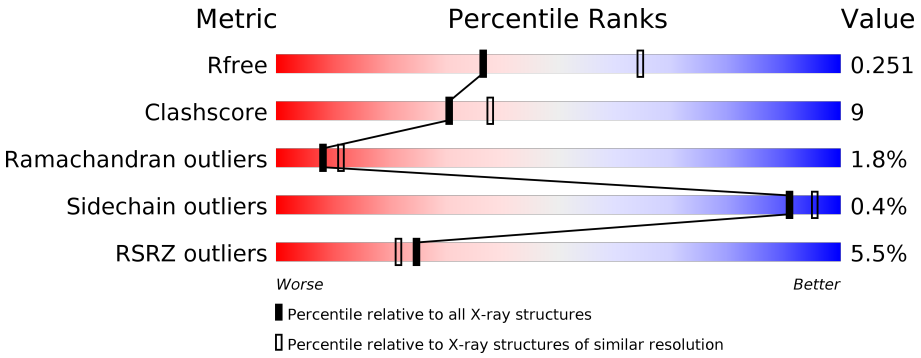
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 2.65 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}	130704	1426 (2.66-2.62)
Clashscore	141614	1472 (2.66-2.62)
Ramachandran outliers	138981	1446 (2.66-2.62)
Sidechain outliers	138945	1446 (2.66-2.62)
RSRZ outliers	127900	1408 (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 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	613	5%, 76%, 17%, • 6%
1	B	613	6%, 77%, 15%, • 6%

2 Entry composition

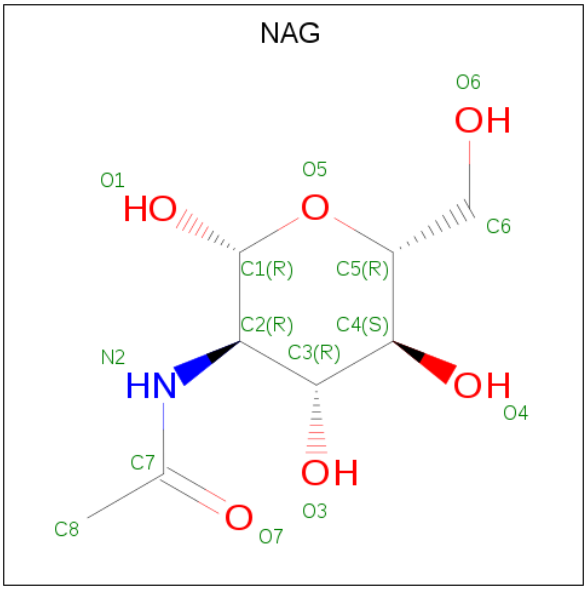
There are 3 unique types of molecules in this entry. The entry contains 9211 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (three-letter code: 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.

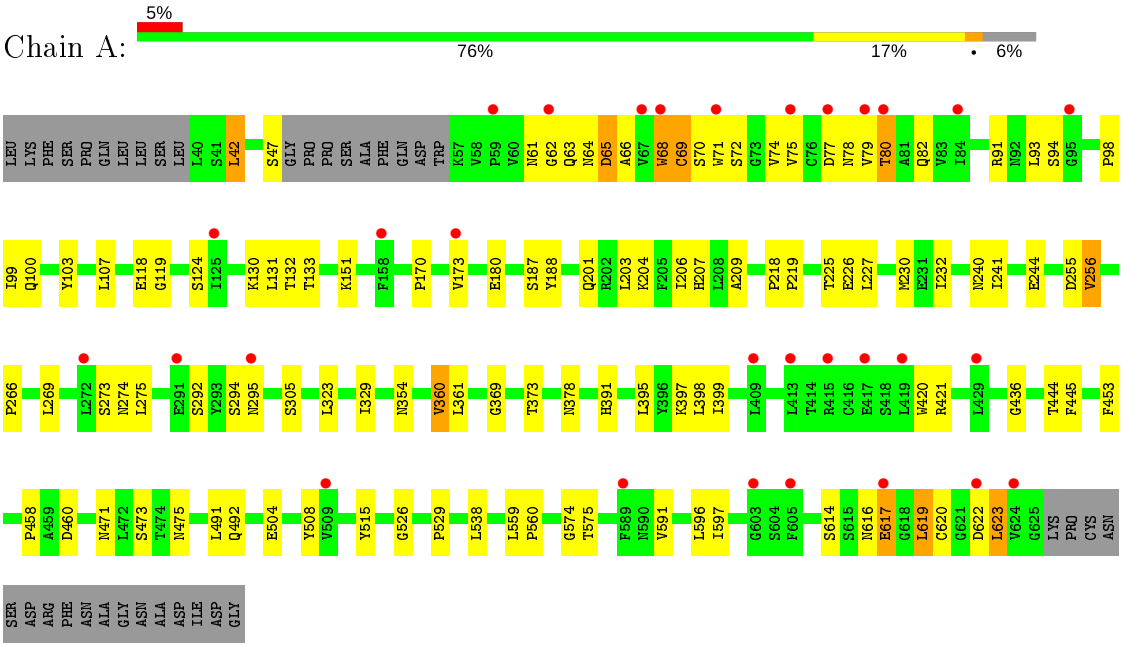
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	66	Total	O	0	0
			66	66		
3	B	79	Total	O	0	0
			79	79		

3 Residue-property plots (i)

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.

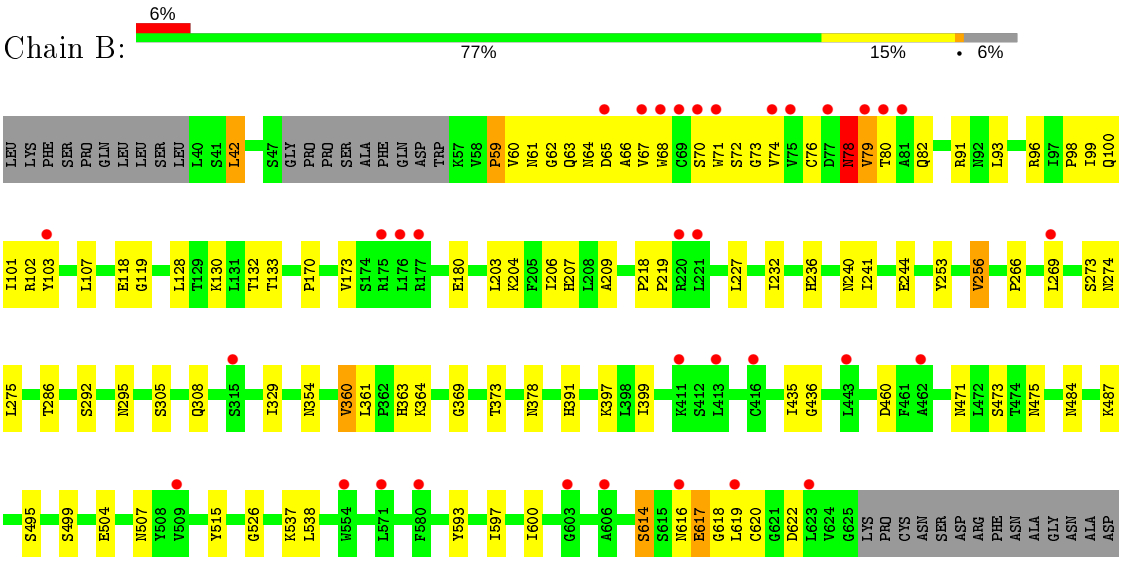
- Molecule 1: Leucine-rich repeat receptor-like protein kinase TDR

Chain A:



- Molecule 1: Leucine-rich repeat receptor-like protein kinase TDR

Chain B:




ILE
ASP
GLY

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	1.67 (at 2.65Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.222 , 0.250 0.225 , 0.251	Depositor DCC
R_{free} test set	1721 reflections (3.05%)	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 , 39.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.457 for h,-k,-l	Xtriage
F_o,F_c correlation	0.93	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.*

[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

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	0.32	0/4571	0.55	1/6214 (0.0%)
1	B	0.26	0/4571	0.50	0/6214
All	All	0.29	0/9142	0.52	1/12428 (0.0%)

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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	619	LEU	CA-CB-CG	5.40	127.72	115.30

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	85	1
1	B	4463	0	4359	77	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	165	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 9.

All (165) 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
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:65:ASP:OD2	3:A:801:HOH:O	2.06	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:B:132:THR:HG23	1:B:133:THR:HG23	1.73	0.69
1:A:63:GLN:CD	1:A:64:ASN:H	1.95	0.68
1:B:63:GLN:CD	1:B:64:ASN:H	1.97	0.68
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:201:GLN:OE1	1:A:201:GLN:N	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:72:SER:C	1:A:74:VAL:H	2.00	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:72:SER:C	1:A:74:VAL:N	2.53	0.61
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
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:436:GLY:N	1:A:460:ASP:OD2	2.34	0.56
1:A:74:VAL:O	1:A:77:ASP:N	2.38	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:207:HIS:CE1	1:A:209:ALA:HB3	2.45	0.52
1:A:61:ASN:O	1:A:71:TRP:HZ2	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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: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:A:354:ASN:CG	1:A:378:ASN:HD22	2.18	0.47
1:B:515:TYR:HA	1:B:538:LEU:HA	1.97	0.46
1:B:99:ILE:HD11	1:B:102:ARG:HH21	1.81	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: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:360:VAL:HG13	1:B:361:LEU:O	2.16	0.46
1:B:68:TRP:CZ3	1:B:98:PRO:HD3	2.48	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HE2	1:B:130:LYS:HB3	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:100:GLN:O	1:A:103:TYR:HD1	1.99	0.45
1:A:130:LYS:HE3	1:A:130:LYS:HB3	1.62	0.45
1:B:273:SER:O	1:B:274:ASN:HB2	2.16	0.45
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:266:PRO:HG2	1:A:269:LEU:HG	1.99	0.44
1:A:62:GLY:HA2	1:A:71:TRP:HZ2	1.80	0.44
1:B:273:SER:C	1:B:275:LEU:H	2.21	0.44
1:B:218:PRO:HA	1:B:219:PRO:HD2	1.88	0.43
1:B:68:TRP:HB3	1:B:71:TRP:HB3	1.99	0.43
1:B:471:ASN:OD1	1:B:473:SER:HB3	2.18	0.43
1:A:323:LEU:HA	1:A:323:LEU:HD23	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:420:TRP:O	1:A:444:THR:HG22	2.19	0.43
1:A:131:LEU:HA	1:A:131:LEU:HD23	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:A:273:SER:C	1:A:275:LEU:H	2.22	0.42
1:A:622:ASP:OD1	1:A:622:ASP:N	2.53	0.42
1:B:244:GLU:N	1:B:244:GLU:OE1	2.45	0.42
1:A:107:LEU:HA	1:A:107:LEU:HD23	1.87	0.42
2:A:704:NAG:O5	3:A:808:HOH:O	2.22	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:A:701:NAG:O4	3:A:807:HOH:O	2.21	0.42
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:HA	1:B:107:LEU:HD23	1.85	0.41
1:B:354:ASN:CG	1:B:378:ASN:HD22	2.24	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
1:B:305:SER:HB2	1:B:329:ILE:HB	2.03	0.41
1:B:96:ARG:NE	3:B:810:HOH:O	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

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%)	9	12
1	B	573/613 (94%)	499 (87%)	63 (11%)	11 (2%)	8	10
All	All	1146/1226 (94%)	997 (87%)	128 (11%)	21 (2%)	8	11

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
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 (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	505/544 (93%)	503 (100%)	2 (0%)	91 95
1	B	505/544 (93%)	503 (100%)	2 (0%)	91 95
All	All	1010/1088 (93%)	1006 (100%)	4 (0%)	91 95

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	TRP
1	A	360	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	360	VAL
1	B	507	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
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 monosaccharides 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	A	701	1	14,14,15	0.50	0	17,19,21	0.57	0
2	NAG	A	704	1	14,14,15	0.50	0	17,19,21	0.45	0
2	NAG	B	702	1	14,14,15	0.30	0	17,19,21	0.39	0
2	NAG	B	705	1	14,14,15	0.51	0	17,19,21	0.53	0
2	NAG	A	703	1	14,14,15	0.58	0	17,19,21	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	B	703	1	14,14,15	0.68	0	17,19,21	0.55	0
2	NAG	A	702	1	14,14,15	0.24	0	17,19,21	0.36	0
2	NAG	B	704	1	14,14,15	1.16	1 (7%)	17,19,21	1.32	1 (5%)
2	NAG	A	705	1	14,14,15	0.56	0	17,19,21	0.55	0
2	NAG	B	701	1	14,14,15	0.42	0	17,19,21	0.56	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	A	701	1	-	2/6/23/26	0/1/1/1
2	NAG	A	704	1	-	4/6/23/26	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	703	1	-	2/6/23/26	0/1/1/1
2	NAG	B	703	1	-	2/6/23/26	0/1/1/1
2	NAG	A	702	1	-	1/6/23/26	0/1/1/1
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	B	701	1	-	2/6/23/26	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	4.08	1.50	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	704	NAG	C1-O5-C5	5.07	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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	701	NAG	O5-C5-C6-O6
2	A	704	NAG	O5-C5-C6-O6
2	A	703	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	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	703	NAG	C4-C5-C6-O6
2	B	702	NAG	O5-C5-C6-O6
2	A	704	NAG	C4-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	A	704	NAG	1	0
2	B	702	NAG	1	0
2	B	703	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

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	577/613 (94%)	0.56	30 (5%)	27	24	37, 61, 93, 121	0
1	B	577/613 (94%)	0.55	34 (5%)	22	19	35, 61, 94, 118	0
All	All	1154/1226 (94%)	0.55	64 (5%)	25	22	35, 61, 93, 121	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	62	GLY	7.8
1	A	68	TRP	6.6
1	B	68	TRP	6.3
1	A	75	VAL	5.9
1	A	77	ASP	5.2
1	B	77	ASP	5.1
1	A	80	THR	4.9
1	B	623	LEU	4.9
1	B	70	SER	4.3
1	A	84	ILE	4.2
1	B	176	LEU	4.0
1	A	617	GLU	3.8
1	B	75	VAL	3.5
1	B	74	VAL	3.4
1	B	80	THR	3.3
1	B	65	ASP	3.3
1	B	79	VAL	3.2
1	A	59	PRO	3.2
1	B	416	CYS	3.0
1	A	413	LEU	3.0
1	A	291	GLU	3.0
1	B	413	LEU	3.0
1	B	67	VAL	2.9
1	B	221	LEU	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	429	LEU	2.8
1	A	603	GLY	2.8
1	A	158	PHE	2.8
1	B	603	GLY	2.7
1	B	462	ALA	2.7
1	A	71	TRP	2.7
1	B	606	ALA	2.6
1	B	69	CYS	2.6
1	B	71	TRP	2.6
1	A	125	ILE	2.5
1	B	554	TRP	2.5
1	A	622	ASP	2.4
1	A	419	LEU	2.3
1	A	624	VAL	2.3
1	B	509	VAL	2.3
1	A	67	VAL	2.3
1	B	269	LEU	2.3
1	B	315	SER	2.3
1	A	95	GLY	2.3
1	B	103	TYR	2.3
1	A	272	LEU	2.2
1	A	417	GLU	2.2
1	B	220	ARG	2.2
1	B	81	ALA	2.2
1	A	173	VAL	2.2
1	A	415	ARG	2.2
1	A	79	VAL	2.2
1	A	409	LEU	2.2
1	A	509	VAL	2.2
1	B	580	PHE	2.2
1	B	616	ASN	2.1
1	B	175	ARG	2.1
1	A	295	ASN	2.1
1	A	589	PHE	2.1
1	A	605	PHE	2.1
1	B	177	ARG	2.1
1	B	443	LEU	2.0
1	B	411	LYS	2.0
1	B	571	LEU	2.0
1	B	619	LEU	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 monosaccharides 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, 95^{th} 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	B	704	14/15	0.72	0.20	66,79,89,89	0
2	NAG	A	704	14/15	0.76	0.16	65,82,97,99	0
2	NAG	B	701	14/15	0.84	0.16	31,62,71,71	0
2	NAG	B	705	14/15	0.85	0.26	58,77,88,99	0
2	NAG	A	705	14/15	0.86	0.22	57,72,79,88	0
2	NAG	A	701	14/15	0.87	0.17	31,61,72,72	0
2	NAG	B	702	14/15	0.87	0.17	75,94,104,104	0
2	NAG	A	702	14/15	0.88	0.22	73,94,104,108	0
2	NAG	B	703	14/15	0.96	0.18	28,42,58,58	0
2	NAG	A	703	14/15	0.97	0.19	34,41,55,56	0

6.5 Other polymers (i)

There are no such residues in this entry.