



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:27 AM UTC

PDB ID : 1PS3 / pdb_00001ps3
Title : Golgi alpha-mannosidase II in complex with kifunensine
Authors : Shah, N.; Kuntz, D.A.; Rose, D.R.
Deposited on : 2003-06-20
Resolution : 1.80 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

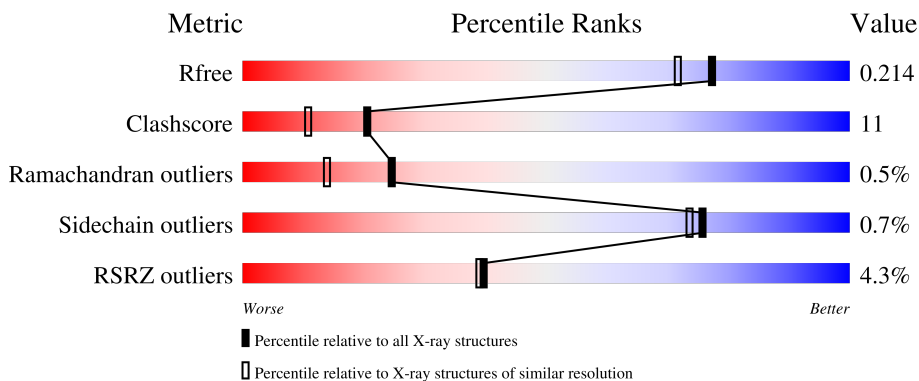
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

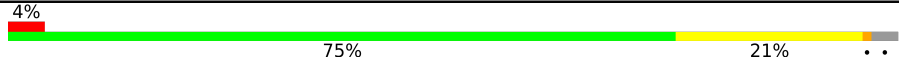
The reported resolution of this entry is 1.80 Å.

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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	1045	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 9204 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 Alpha-mannosidase II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1014	8181	5202	1434	1506	39	0	0	0

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

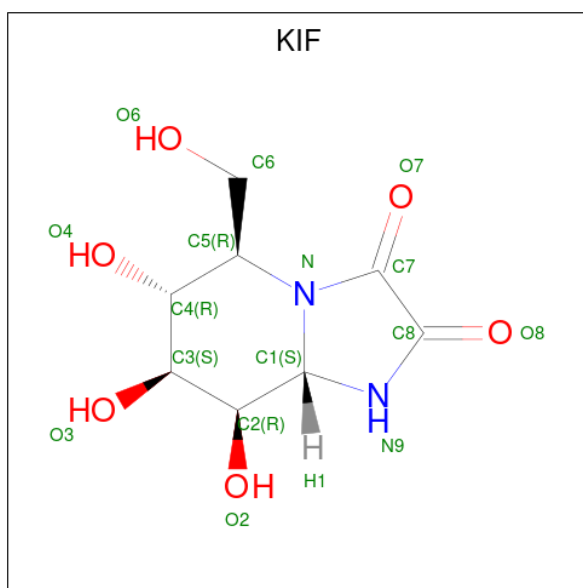


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	15	8	1	6	0	0

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

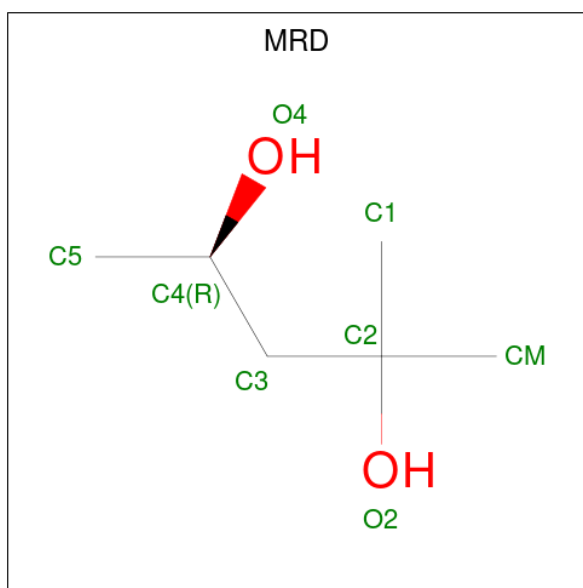
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is KIFUNENSINE (CCD ID: KIF) (formula: $C_8H_{12}N_2O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
			Total	C	N			O
4	A	1	16	8	2	6	0	0

- Molecule 5 is (4R)-2-METHYLPENTANE-2,4-DIOL (CCD ID: MRD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	8	6	2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	983	Total 983	O 983	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	69.09Å 109.80Å 138.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.80 30.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-1.80) 93.7 (30.00-1.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.51 (at 1.50Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.200 , 0.222 0.190 , 0.214	Depositor DCC
R_{free} test set	7152 reflections (4.58%)	wwPDB-VP
Wilson B-factor (Å ²)	11.0	Xtrriage
Anisotropy	0.137	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 44.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9204	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.43% 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 i

5.1 Standard geometry i

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

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	0.38	0/8406	0.91	34/11416 (0.3%)

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	664	TYR	CA-C-N	7.68	128.07	119.32
1	A	664	TYR	C-N-CA	7.68	128.07	119.32
1	A	35	VAL	N-CA-C	7.43	117.49	111.62
1	A	207	GLY	N-CA-C	-7.34	104.98	111.95
1	A	169	ASP	N-CA-C	-7.05	100.57	110.50
1	A	763	VAL	N-CA-C	6.96	117.80	108.27
1	A	266	PHE	N-CA-C	6.72	119.64	109.95
1	A	168	PRO	N-CA-C	6.68	121.83	111.21
1	A	45	MET	N-CA-C	6.52	119.22	111.33
1	A	153	VAL	N-CA-C	-6.34	104.67	110.82
1	A	36	GLN	N-CA-C	6.33	121.08	113.23
1	A	107	THR	N-CA-C	6.29	118.66	111.11
1	A	447	SER	N-CA-C	-6.20	99.55	109.96
1	A	517	PRO	N-CA-C	6.18	120.89	111.19
1	A	330	ARG	N-CA-C	5.91	120.49	113.28
1	A	875	GLU	N-CA-C	5.76	119.51	111.90
1	A	989	THR	CA-C-N	5.74	127.02	119.84
1	A	989	THR	C-N-CA	5.74	127.02	119.84
1	A	1013	THR	N-CA-C	-5.69	103.02	110.53
1	A	780	VAL	N-CA-C	5.66	116.25	107.99
1	A	267	TYR	N-CA-C	5.47	118.01	111.71
1	A	955	GLU	N-CA-C	5.46	118.73	111.75
1	A	167	MET	N-CA-C	-5.43	96.94	108.66
1	A	518	ASP	N-CA-C	-5.33	96.98	107.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	35	VAL	CB-CA-C	-5.31	106.32	111.05
1	A	480	THR	N-CA-C	5.24	117.40	111.11
1	A	354	ARG	N-CA-C	5.18	116.61	111.07
1	A	204	ASP	N-CA-C	5.17	121.22	109.81
1	A	419	TYR	N-CA-C	-5.15	106.83	113.01
1	A	276	GLY	CA-C-N	5.14	124.75	119.56
1	A	276	GLY	C-N-CA	5.14	124.75	119.56
1	A	872	SER	N-CA-C	5.12	117.65	109.81
1	A	300	LYS	N-CA-C	5.12	121.50	113.72
1	A	968	SER	N-CA-C	5.08	117.56	111.71

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	8181	0	7972	179	0
2	A	15	0	15	4	0
3	A	1	0	0	0	0
4	A	16	0	11	0	0
5	A	8	0	14	2	0
6	A	983	0	0	66	0
All	All	9204	0	8012	181	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 11.

All (181) 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:297:CYS:HB3	6:A:2268:HOH:O	1.58	1.02
1:A:568:LEU:HD12	1:A:770:ARG:HD3	1.48	0.95
1:A:194:ASN:HD21	2:A:1046:NAG:H3	1.31	0.94
1:A:989:THR:HB	1:A:991:GLU:OE2	1.68	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:699:LEU:HG	6:A:2144:HOH:O	1.76	0.84
1:A:883:LEU:HD23	6:A:2113:HOH:O	1.77	0.83
1:A:194:ASN:ND2	2:A:1046:NAG:H3	1.93	0.82
1:A:203:ILE:HG12	6:A:2211:HOH:O	1.80	0.81
1:A:434:HIS:HE1	1:A:930:ASP:OD1	1.66	0.79
1:A:583:LEU:HD22	1:A:944:GLY:N	1.99	0.76
1:A:947:GLY:HA3	6:A:2227:HOH:O	1.84	0.76
1:A:155:ASN:HD21	1:A:157:GLN:HE21	1.33	0.74
1:A:835:MET:HE2	1:A:862:LEU:HD22	1.70	0.74
1:A:254:LYS:HD3	1:A:256:ASP:OD2	1.91	0.71
1:A:869:ARG:HG2	6:A:2113:HOH:O	1.89	0.71
1:A:494:LEU:HA	1:A:497:CYS:SG	2.30	0.71
1:A:641:PRO:HG2	1:A:644:THR:HB	1.72	0.71
1:A:290:MET:CG	1:A:303:PRO:HG2	2.20	0.71
1:A:188:TRP:HB3	6:A:2129:HOH:O	1.92	0.70
1:A:284:GLN:HA	6:A:2186:HOH:O	1.91	0.70
1:A:97:GLN:HG2	6:A:2228:HOH:O	1.92	0.69
1:A:250:ILE:HD11	6:A:2205:HOH:O	1.92	0.69
1:A:989:THR:HG22	1:A:991:GLU:HG3	1.73	0.69
1:A:185:GLY:HA2	6:A:2129:HOH:O	1.93	0.69
1:A:990:PRO:O	1:A:992:GLU:HG3	1.93	0.69
1:A:194:ASN:ND2	2:A:1046:NAG:H83	2.07	0.69
1:A:709:HIS:HB3	6:A:2485:HOH:O	1.93	0.68
1:A:565:ARG:HG2	6:A:2040:HOH:O	1.93	0.68
1:A:96:ILE:HG12	1:A:102:TYR:OH	1.94	0.68
1:A:979:LEU:HD21	1:A:999:VAL:HG11	1.74	0.68
1:A:1008:ARG:HG2	1:A:1042:SER:HB2	1.75	0.68
1:A:770:ARG:NH1	6:A:2371:HOH:O	2.27	0.67
1:A:284:GLN:OE1	1:A:304:ARG:NH2	2.29	0.66
1:A:492:GLU:HG2	6:A:2138:HOH:O	1.95	0.66
1:A:290:MET:HG2	1:A:303:PRO:HG2	1.79	0.65
1:A:950:HIS:CD2	6:A:2227:HOH:O	2.50	0.64
1:A:630:ALA:HB3	6:A:2081:HOH:O	1.99	0.63
1:A:904:ARG:HG2	1:A:985:MET:SD	2.40	0.62
1:A:498:GLN:HE21	1:A:526:LEU:H	1.46	0.62
1:A:583:LEU:HD22	1:A:944:GLY:CA	2.30	0.62
1:A:964:ARG:HH11	1:A:973:GLN:HE21	1.47	0.61
1:A:434:HIS:HD2	1:A:927:ASP:OD1	1.84	0.60
1:A:131:ILE:HG21	6:A:2129:HOH:O	2.02	0.60
1:A:695:LYS:HG3	1:A:709:HIS:CE1	2.36	0.60
1:A:950:HIS:HE1	6:A:2286:HOH:O	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:678:LEU:HD12	1:A:769:MET:HE1	1.85	0.59
1:A:934:PHE:CE2	1:A:936:GLU:HB2	2.38	0.58
1:A:437:ARG:HG3	6:A:2213:HOH:O	2.03	0.58
1:A:144:ASN:HB3	6:A:2184:HOH:O	2.03	0.58
1:A:869:ARG:HH11	1:A:885:ASN:HD22	1.52	0.58
1:A:290:MET:HG3	1:A:303:PRO:HG2	1.85	0.58
1:A:952:SER:H	1:A:995:GLN:NE2	2.02	0.58
1:A:812:GLN:NE2	6:A:2036:HOH:O	2.37	0.57
1:A:265:PRO:HD3	1:A:329:TYR:OH	2.05	0.57
1:A:782:ILE:O	1:A:785:LEU:HD13	2.05	0.57
1:A:628:GLY:CA	6:A:2227:HOH:O	2.53	0.57
1:A:895:VAL:HG12	1:A:897:GLU:HG3	1.87	0.56
1:A:201:TRP:CD1	6:A:2211:HOH:O	2.58	0.56
1:A:1011:ARG:NH1	1:A:1037:ALA:HB1	2.21	0.56
5:A:1602:MRD:H1C1	6:A:2546:HOH:O	2.05	0.55
1:A:143:GLU:OE2	1:A:147:LEU:HG	2.07	0.55
1:A:1011:ARG:HH12	1:A:1037:ALA:CB	2.19	0.55
1:A:470:HIS:CE1	1:A:472:ASP:HB2	2.42	0.55
1:A:975:VAL:HG21	1:A:1003:LEU:CD1	2.37	0.55
1:A:765:HIS:HE1	6:A:2281:HOH:O	1.89	0.55
1:A:62:TRP:CD2	1:A:65:GLY:HA3	2.42	0.55
1:A:396:GLU:N	1:A:396:GLU:OE1	2.40	0.54
1:A:229:THR:HG21	1:A:263:MET:HE2	1.88	0.54
1:A:990:PRO:O	1:A:991:GLU:C	2.51	0.54
1:A:435:TYR:HB3	1:A:497:CYS:SG	2.46	0.54
1:A:499:MET:HG3	6:A:2521:HOH:O	2.07	0.54
1:A:480:THR:H	1:A:880:GLN:HE22	1.56	0.54
1:A:1026:MET:HE3	6:A:2401:HOH:O	2.08	0.54
1:A:235:LYS:O	1:A:239:GLN:HG3	2.08	0.53
1:A:686:LEU:HD22	1:A:697:ILE:HG12	1.89	0.53
1:A:309:GLN:HB3	6:A:2513:HOH:O	2.09	0.53
1:A:203:ILE:HG23	6:A:2211:HOH:O	2.08	0.53
1:A:583:LEU:O	1:A:583:LEU:HG	2.08	0.53
1:A:651:LEU:CD1	1:A:653:ARG:HG2	2.39	0.53
1:A:192:PHE:O	1:A:193:MET:HE2	2.08	0.53
1:A:131:ILE:CG2	6:A:2129:HOH:O	2.57	0.53
1:A:1009:CYS:SG	1:A:1023:LEU:HD12	2.49	0.53
1:A:666:GLU:HB2	6:A:2320:HOH:O	2.08	0.52
1:A:299:TRP:N	6:A:2268:HOH:O	2.36	0.52
1:A:460:GLN:O	1:A:464:GLU:HG2	2.10	0.52
1:A:980:HIS:HD2	1:A:1036:THR:OG1	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:LYS:HE2	6:A:1832:HOH:O	2.09	0.52
1:A:765:HIS:HD2	1:A:778:ASN:OD1	1.93	0.52
1:A:869:ARG:HG3	1:A:885:ASN:ND2	2.25	0.52
1:A:595:VAL:HG21	1:A:615:LYS:HG2	1.92	0.51
1:A:158:LEU:C	1:A:158:LEU:HD13	2.36	0.51
1:A:174:HIS:CE1	1:A:176:ARG:HD3	2.44	0.51
1:A:1011:ARG:HH12	1:A:1037:ALA:HB2	1.75	0.51
1:A:986:GLN:HG2	6:A:1765:HOH:O	2.11	0.51
1:A:666:GLU:OE1	6:A:2320:HOH:O	2.20	0.50
1:A:610:GLN:HG2	6:A:2135:HOH:O	2.10	0.50
1:A:388:GLN:HG2	1:A:391:ARG:HH21	1.76	0.49
1:A:786:ASP:HB3	6:A:2562:HOH:O	2.11	0.49
1:A:98:THR:OG1	1:A:101:GLU:HG3	2.13	0.49
5:A:1602:MRD:H1C3	6:A:2369:HOH:O	2.11	0.49
1:A:654:LYS:HE3	1:A:672:ASP:OD1	2.13	0.49
1:A:188:TRP:CB	6:A:2129:HOH:O	2.57	0.49
1:A:954:ARG:NH1	1:A:981:ARG:NH2	2.60	0.49
1:A:531:TRP:HA	1:A:532:PRO:C	2.38	0.48
1:A:559:ASN:O	1:A:627:MET:HA	2.13	0.48
1:A:961:VAL:HA	6:A:2213:HOH:O	2.13	0.48
1:A:980:HIS:HE1	6:A:1682:HOH:O	1.96	0.48
1:A:441:MET:HB3	6:A:2259:HOH:O	2.12	0.48
1:A:301:VAL:HG23	1:A:301:VAL:O	2.13	0.48
1:A:1011:ARG:NH1	1:A:1037:ALA:CB	2.77	0.47
1:A:74:LYS:HD2	6:A:2344:HOH:O	2.14	0.47
1:A:419:TYR:CE2	1:A:830:PRO:HG3	2.49	0.47
1:A:225:LEU:C	1:A:225:LEU:HD23	2.40	0.47
1:A:194:ASN:CG	2:A:1046:NAG:H83	2.39	0.47
1:A:558:HIS:HB3	1:A:930:ASP:HB2	1.96	0.47
1:A:572:TYR:CD2	1:A:615:LYS:HD3	2.50	0.47
1:A:869:ARG:HG3	1:A:885:ASN:HD21	1.79	0.47
1:A:986:GLN:HB3	6:A:2175:HOH:O	2.14	0.47
1:A:678:LEU:CD1	1:A:769:MET:HE1	2.45	0.47
1:A:203:ILE:N	6:A:2211:HOH:O	2.26	0.46
1:A:582:ASP:HB2	6:A:2028:HOH:O	2.15	0.46
1:A:869:ARG:CG	6:A:2113:HOH:O	2.58	0.46
1:A:69:LYS:HE2	6:A:2087:HOH:O	2.16	0.46
1:A:284:GLN:NE2	1:A:301:VAL:HG21	2.31	0.46
1:A:301:VAL:HG22	6:A:1718:HOH:O	2.15	0.46
1:A:48:LEU:HD11	1:A:236:GLU:HG2	1.98	0.46
1:A:580:VAL:HG22	1:A:634:LEU:CD2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:VAL:HG22	1:A:158:LEU:HD12	1.98	0.45
1:A:992:GLU:O	1:A:994:THR:HG23	2.17	0.45
1:A:425:HIS:HE1	1:A:487:GLU:OE1	2.00	0.45
1:A:761:PRO:O	1:A:762:SER:HB2	2.15	0.45
1:A:79:HIS:CE1	1:A:332:ASN:HB3	2.52	0.45
1:A:929:LEU:HD11	6:A:2040:HOH:O	2.16	0.45
1:A:389:ALA:HB1	1:A:394:GLN:CD	2.42	0.45
1:A:93:PRO:HD2	1:A:470:HIS:CD2	2.52	0.44
1:A:400:LEU:HD23	1:A:400:LEU:C	2.42	0.44
1:A:82:LYS:NZ	6:A:2245:HOH:O	2.50	0.44
1:A:299:TRP:HB2	6:A:2268:HOH:O	2.17	0.44
1:A:715:TYR:HB2	1:A:789:GLU:HB2	1.99	0.44
1:A:279:PRO:HB2	1:A:299:TRP:CZ2	2.53	0.44
1:A:883:LEU:CD2	6:A:2113:HOH:O	2.50	0.44
1:A:909:HIS:CE1	1:A:911:ALA:HB3	2.52	0.44
1:A:628:GLY:HA3	6:A:2227:HOH:O	2.16	0.44
1:A:989:THR:CG2	1:A:991:GLU:HG3	2.45	0.44
1:A:37:ASP:HB2	6:A:2204:HOH:O	2.18	0.43
1:A:131:ILE:HD11	6:A:2220:HOH:O	2.18	0.43
1:A:785:LEU:HD12	1:A:785:LEU:N	2.33	0.43
1:A:442:LEU:HG	6:A:2259:HOH:O	2.17	0.43
1:A:995:GLN:HG3	6:A:2224:HOH:O	2.17	0.43
1:A:480:THR:HG23	6:A:2236:HOH:O	2.19	0.43
1:A:244:GLU:HA	1:A:261:THR:O	2.17	0.43
1:A:653:ARG:HD3	1:A:744:VAL:HG22	1.99	0.43
1:A:775:GLU:HA	1:A:893:ARG:HD2	2.01	0.43
1:A:986:GLN:CG	6:A:1765:HOH:O	2.67	0.43
1:A:676:ILE:HD13	1:A:747:VAL:HG21	2.01	0.43
1:A:641:PRO:HG2	1:A:644:THR:CB	2.47	0.43
1:A:557:MET:HA	1:A:930:ASP:O	2.18	0.42
1:A:903:VAL:HB	1:A:986:GLN:HG3	2.01	0.42
1:A:990:PRO:HB3	1:A:992:GLU:OE2	2.19	0.42
1:A:301:VAL:CG2	6:A:1718:HOH:O	2.67	0.42
1:A:332:ASN:H	1:A:394:GLN:NE2	2.18	0.42
1:A:460:GLN:NE2	6:A:2240:HOH:O	2.53	0.42
1:A:225:LEU:HD21	1:A:264:MET:SD	2.60	0.42
1:A:332:ASN:H	1:A:394:GLN:HE22	1.66	0.42
1:A:964:ARG:HH11	1:A:973:GLN:NE2	2.16	0.41
1:A:270:ASP:OD1	1:A:273:HIS:HD2	2.03	0.41
1:A:703:SER:HB2	6:A:1967:HOH:O	2.21	0.41
1:A:989:THR:HA	1:A:990:PRO:HD3	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:875:GLU:CD	6:A:2008:HOH:O	2.64	0.41
1:A:251:TRP:CD1	1:A:251:TRP:C	2.98	0.41
1:A:540:ARG:HG3	1:A:572:TYR:CE2	2.55	0.41
1:A:679:ARG:HH12	1:A:701:GLN:CD	2.28	0.41
1:A:205:PRO:O	1:A:228:ARG:HB2	2.21	0.41
1:A:498:GLN:NE2	1:A:526:LEU:H	2.15	0.41
1:A:1008:ARG:HG3	6:A:1763:HOH:O	2.21	0.41
1:A:435:TYR:CE2	1:A:526:LEU:HD13	2.56	0.41
1:A:599:HIS:CD2	1:A:610:GLN:OE1	2.73	0.41
1:A:855:SER:OG	1:A:856:SER:N	2.54	0.41
1:A:909:HIS:HA	1:A:910:PRO:HD3	1.93	0.41
1:A:35:VAL:HG13	1:A:905:PRO:HG3	2.02	0.40
1:A:764:VAL:HB	1:A:779:LEU:HB3	2.02	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	1012/1045 (97%)	973 (96%)	34 (3%)	5 (0%)	24 14

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	95	TRP
1	A	991	GLU
1	A	993	HIS
1	A	204	ASP
1	A	549	ILE

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	901/928 (97%)	895 (99%)	6 (1%)	76 73

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	123	GLU
1	A	275	CYS
1	A	702	ASP
1	A	828	TYR
1	A	979	LEU
1	A	986	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	ASN
1	A	148	GLN
1	A	157	GLN
1	A	191	GLN
1	A	194	ASN
1	A	223	ASN
1	A	240	GLN
1	A	273	HIS
1	A	309	GLN
1	A	380	GLN
1	A	394	GLN
1	A	425	HIS
1	A	434	HIS
1	A	460	GLN
1	A	470	HIS
1	A	488	GLN
1	A	498	GLN
1	A	554	HIS
1	A	585	ASN

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Mol	Chain	Res	Type
1	A	608	HIS
1	A	682	ASN
1	A	698	GLN
1	A	709	HIS
1	A	765	HIS
1	A	778	ASN
1	A	809	ASN
1	A	812	GLN
1	A	866	GLN
1	A	880	GLN
1	A	885	ASN
1	A	919	HIS
1	A	945	GLN
1	A	950	HIS
1	A	973	GLN
1	A	980	HIS
1	A	986	GLN
1	A	993	HIS
1	A	995	GLN
1	A	1005	ASN
1	A	1018	GLN

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](#)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 for Mogul analysis.

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	1046	-	15,15,15	0.55	0	21,21,21	0.85	0
5	MRD	A	1602	-	7,7,7	0.48	0	9,10,10	0.26	0
4	KIF	A	1501	3	15,17,17	2.79	6 (40%)	14,26,26	2.25	4 (28%)

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	1046	-	-	6/6/26/26	0/1/1/1
5	MRD	A	1602	-	-	2/5/5/5	-
4	KIF	A	1501	3	-	0/2/38/38	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1501	KIF	O2-C2	-9.01	1.20	1.43
4	A	1501	KIF	C5-N	2.54	1.52	1.48
4	A	1501	KIF	C8-N9	-2.50	1.31	1.35
4	A	1501	KIF	C4-C5	2.49	1.58	1.53
4	A	1501	KIF	C3-C4	2.25	1.58	1.52
4	A	1501	KIF	C6-C5	2.02	1.55	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1501	KIF	O2-C2-C3	5.58	123.53	110.38
4	A	1501	KIF	C2-C3-C4	4.03	117.91	110.83
4	A	1501	KIF	C7-C8-N9	2.44	107.70	105.30
4	A	1501	KIF	C6-C5-C4	-2.34	109.40	112.93

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1046	NAG	C3-C2-N2-C7
2	A	1046	NAG	C8-C7-N2-C2
2	A	1046	NAG	O7-C7-N2-C2
5	A	1602	MRD	C2-C3-C4-O4
2	A	1046	NAG	C4-C5-C6-O6
2	A	1046	NAG	O5-C5-C6-O6
5	A	1602	MRD	C2-C3-C4-C5
2	A	1046	NAG	C1-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1046	NAG	4	0
5	A	1602	MRD	2	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, 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	1014/1045 (97%)	0.12	44 (4%) 40 39	6, 12, 25, 47	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	993	HIS	5.9
1	A	990	PRO	5.3
1	A	991	GLU	4.9
1	A	534	SER	4.7
1	A	602	THR	4.5
1	A	682	ASN	4.5
1	A	497	CYS	4.1
1	A	702	ASP	3.8
1	A	603	LEU	3.5
1	A	1008	ARG	3.4
1	A	600	HIS	3.4
1	A	992	GLU	3.3
1	A	638	ASP	3.2
1	A	583	LEU	3.1
1	A	986	GLN	3.0
1	A	290	MET	3.0
1	A	601	ASP	3.0
1	A	547	GLU	3.0
1	A	396	GLU	3.0
1	A	721	GLY	2.9
1	A	537	GLU	2.9
1	A	538	ASP	2.9
1	A	304	ARG	2.9
1	A	79	HIS	2.8
1	A	1024	ASP	2.8
1	A	451	MET	2.7
1	A	720	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	701	GLN	2.6
1	A	139	HIS	2.6
1	A	704	PRO	2.6
1	A	116	ARG	2.6
1	A	144	ASN	2.6
1	A	994	THR	2.5
1	A	316	ASP	2.5
1	A	703	SER	2.5
1	A	1044	SER	2.4
1	A	785	LEU	2.4
1	A	739	GLU	2.3
1	A	76	ASN	2.3
1	A	301	VAL	2.2
1	A	784	SER	2.1
1	A	742	GLN	2.1
1	A	771	GLY	2.0
1	A	613	THR	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](#)

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(\AA^2)	Q<0.9
2	NAG	A	1046	15/15	0.47	0.25	71,71,71,71	0
5	MRD	A	1602	8/8	0.86	0.12	14,16,17,18	0
4	KIF	A	1501	16/16	0.91	0.08	13,17,20,22	0
3	ZN	A	1601	1/1	1.00	0.01	8,8,8,8	0

6.5 Other polymers [i](#)

There are no such residues in this entry.