WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 28, 2014 – 10:54 AM GMT

PDB ID : 1PS3
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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at http://wwpdb.org/ValidationPDFNotes.html

1 Overall quality at a glance ⓘ

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.

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
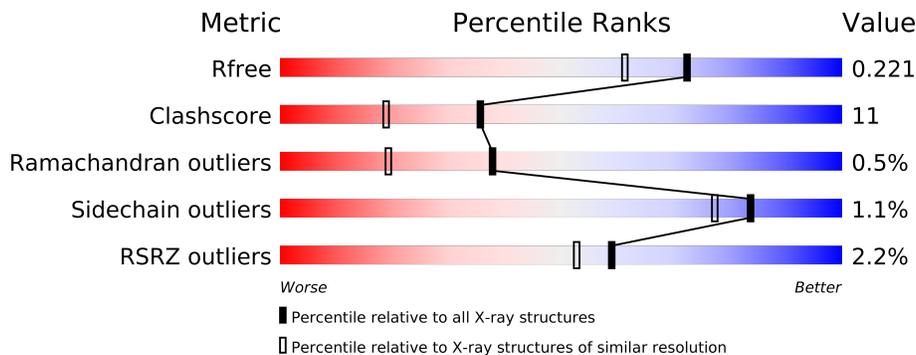
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	3513 (1.80-1.80)
Clashscore	79885	4461 (1.80-1.80)
Ramachandran outliers	78287	4404 (1.80-1.80)
Sidechain outliers	78261	4403 (1.80-1.80)
RSRZ outliers	66119	3515 (1.80-1.80)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	1045	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	NAG	A	1046	-	X
4	KIF	A	1501	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 9204 atoms, of which 0 are hydrogen and 0 are deuterium.

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
1	A	1014	Total 8181	C 5202	N 1434	O 1506	S 39	0	0	0

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).
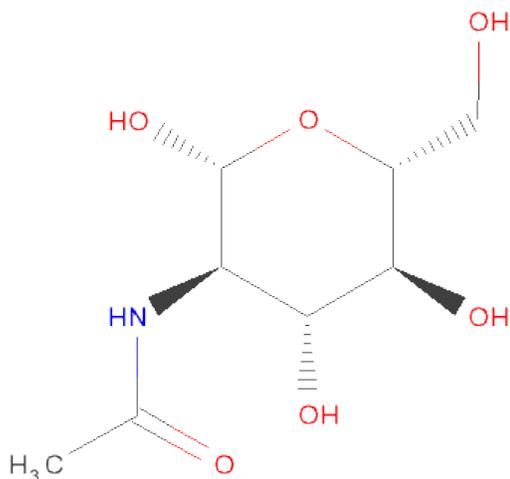
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 15	C 8	N 1	O 6	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 4 is KIFUNENSINE (three-letter code: KIF) (formula: $C_8H_{12}N_2O_6$).
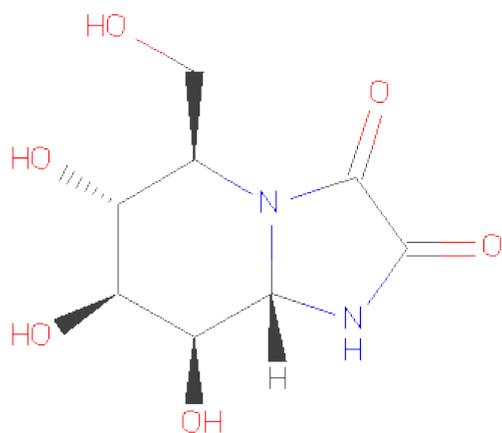
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 16	C 8	N 2	O 6	0	0

- Molecule 5 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula: $C_6H_{14}O_2$).
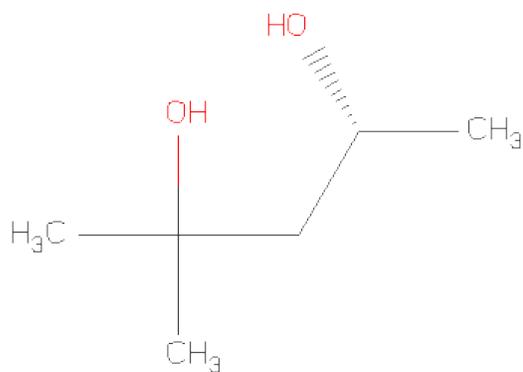
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 8	C 6	O 2	0	0

- Molecule 6 is water.

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

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Alpha-mannosidase II

Chain A:
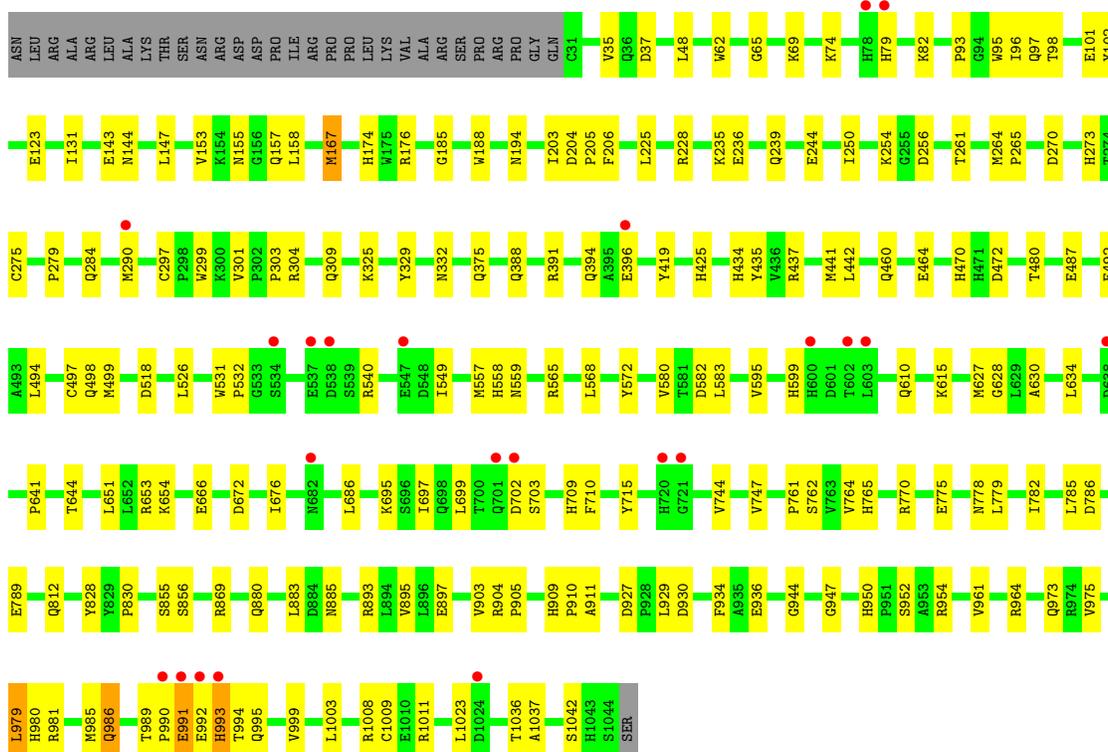
4 Data and refinement statistics (i)

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 29.86　–　1.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-1.80) 83.3 (29.86-1.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.51 (at 1.50Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.200　,　0.222 0.199　,　0.221	Depositor DCC
R_{free} test set	6410 reflections (4.77%)	DCC
Wilson B-factor (Å^2)	11.0	Xtriage
Anisotropy	0.137	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 35.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Outliers	0 of 156264 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9204	wwPDB-VP
Average B, all atoms (Å^2)	14.0	wwPDB-VP

Xtriage'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.*

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[1]Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.33	0/8406	0.63	2/11416 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	167	MET	N-CA-C	-5.21	96.94	111.00
1	A	518	ASP	N-CA-C	-5.19	96.98	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8181	0	7972	169	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	64	0
All	All	9204	0	8012	171	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 11.

All (171) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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
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:869:ARG:HG2	6:A:2113:HOH:O	1.89	0.71
1:A:254:LYS:HD3	1:A:256:ASP:OD2	1.91	0.71
1:A:641:PRO:HG2	1:A:644:THR:HB	1.72	0.71
1:A:494:LEU:HA	1:A:497:CYS:SG	2.30	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:990:PRO:O	1:A:992:GLU:HG3	1.93	0.69
1:A:185:GLY:HA2	6:A:2129:HOH:O	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:1008:ARG:HG2	1:A:1042:SER:HB2	1.75	0.68
1:A:979:LEU:HD21	1:A:999:VAL:HG11	1.74	0.68
1:A:96:ILE:HG12	1:A:102:TYR:OH	1.94	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:950:HIS:HE1	6:A:2286:HOH:O	1.84	0.60
1:A:695:LYS:HG3	1:A:709:HIS:CE1	2.36	0.60
1:A:167:MET:HE1	6:A:2211:HOH:O	2.02	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:782:ILE:O	1:A:785:LEU:HD13	2.05	0.57
1:A:265:PRO:HD3	1:A:329:TYR:OH	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: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:1011:ARG:HH12	1:A:1037:ALA:CB	2.19	0.55
1:A:143:GLU:OE2	1:A:147:LEU:HG	2.07	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: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:583:LEU:O	1:A:583:LEU:HG	2.08	0.53
1:A:686:LEU:HD22	1:A:697:ILE:HG12	1.89	0.53
1:A:235:LYS:O	1:A:239:GLN:HG3	2.08	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:651:LEU:CD1	1:A:653:ARG:HG2	2.39	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
1:A:325:LYS:HE2	6:A:1832:HOH:O	2.09	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:869:ARG:HG3	1:A:885:ASN:ND2	2.25	0.52
1:A:765:HIS:HD2	1:A:778:ASN:OD1	1.93	0.52
1:A:595:VAL:HG21	1:A:615:LYS:HG2	1.92	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:990:PRO:O	1:A:991:GLU:C	2.51	0.49
1:A:786:ASP:HB3	6:A:2562:HOH:O	2.11	0.49
5:A:1602:MRD:H1C3	6:A:2369:HOH:O	2.11	0.49
1:A:98:THR:OG1	1:A:101:GLU:HG3	2.13	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: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:559:ASN:O	1:A:627:MET:HA	2.13	0.48
1:A:441:MET:HB3	6:A:2259:HOH:O	2.12	0.48
1:A:301:VAL:O	1:A:301:VAL:HG23	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: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:158:LEU:HD13	1:A:158:LEU:C	2.36	0.47
1:A:869:ARG:CG	6:A:2113:HOH:O	2.58	0.46
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: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
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:761:PRO:O	1:A:762:SER:HB2	2.15	0.45
1:A:425:HIS:HE1	1:A:487:GLU:OE1	2.00	0.45
1:A:79:HIS:CE1	1:A:332:ASN:HB3	2.52	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:929:LEU:HD11	6:A:2040:HOH:O	2.16	0.45
1:A:93:PRO:HD2	1:A:470:HIS:CD2	2.52	0.44
1:A:299:TRP:HB2	6:A:2268:HOH:O	2.17	0.44
1:A:82:LYS:NZ	6:A:2245:HOH:O	2.50	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:494:LEU:O	1:A:497:CYS:SG	2.73	0.43
1:A:131:ILE:HD11	6:A:2220:HOH:O	2.18	0.43
1:A:37:ASP:HB2	6:A:2204:HOH:O	2.18	0.43
1:A:785:LEU:N	1:A:785:LEU:HD12	2.33	0.43
1:A:995:GLN:HG3	6:A:2224:HOH:O	2.17	0.43
1:A:442:LEU:HG	6:A:2259:HOH:O	2.17	0.43
1:A:480:THR:HG23	6:A:2236:HOH:O	2.19	0.43
1:A:531:TRP:HA	1:A:532:PRO:C	2.38	0.43
1:A:653:ARG:HD3	1:A:744:VAL:HG22	1.99	0.43
1:A:244:GLU:HA	1:A:261:THR:O	2.17	0.43
1:A:986:GLN:CG	6:A:1765:HOH:O	2.67	0.43
1:A:775:GLU:HA	1:A:893:ARG:HD2	2.01	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:225:LEU:HD23	1:A:225:LEU:C	2.40	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:332:ASN:H	1:A:394:GLN:HE22	1.66	0.42
1:A:225:LEU:HD21	1:A:264:MET:SD	2.60	0.42
1:A:194:ASN:CG	2:A:1046:NAG:H83	2.39	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:989:THR:HA	1:A:990:PRO:HD3	1.92	0.41
1:A:703:SER:HB2	6:A:1967:HOH:O	2.21	0.41
1:A:540:ARG:HG3	1:A:572:TYR:CE2	2.55	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:205:PRO:O	1:A:228:ARG:HB2	2.21	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:909:HIS:HA	1:A:910:PRO:HD3	1.93	0.41
1:A:855:SER:OG	1:A:856:SER:N	2.54	0.41
1:A:764:VAL:HB	1:A:779:LEU:HB3	2.02	0.40
1:A:35:VAL:HG13	1:A:905:PRO:HG3	2.02	0.40

There are no symmetry-related clashes.

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	1012/1045 (97%)	973 (96%)	34 (3%)	5 (0%)	38	19

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 ⓘ

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%)	891 (99%)	10 (1%)	84	77

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	123	GLU
1	A	206	PHE
1	A	275	CYS
1	A	375	GLN
1	A	702	ASP
1	A	710	PHE
1	A	828	TYR
1	A	979	LEU
1	A	986	GLN
1	A	993	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	ASN
1	A	91	ASN
1	A	121	ASN
1	A	148	GLN
1	A	157	GLN
1	A	191	GLN
1	A	194	ASN
1	A	240	GLN
1	A	249	GLN
1	A	273	HIS
1	A	309	GLN
1	A	347	ASN
1	A	394	GLN
1	A	425	HIS
1	A	434	HIS
1	A	460	GLN
1	A	469	GLN
1	A	470	HIS
1	A	488	GLN
1	A	498	GLN
1	A	554	HIS
1	A	608	HIS
1	A	682	ASN
1	A	698	GLN
1	A	765	HIS
1	A	809	ASN
1	A	880	GLN

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Mol	Chain	Res	Type
1	A	885	ASN
1	A	919	HIS
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
1	A	1022	HIS

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	0.51	0	21,21,21	0.82	0
4	KIF	A	1501	3	17,17,17	4.21	8 (47%)	26,26,26	1.84	5 (19%)
5	MRD	A	1602	-	7,7,7	0.48	0	10,10,10	0.27	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	1046	-	-	0/6/26/26	0/1/1/1
4	KIF	A	1501	3	-	0/2/38/38	0/0/2/2
5	MRD	A	1602	-	-	0/5/5/5	0/0/0/0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1501	KIF	C2-C1	13.45	1.69	1.53
4	A	1501	KIF	O2-C2	-9.24	1.20	1.43
4	A	1501	KIF	C8-N9	-2.38	1.31	1.34
4	A	1501	KIF	C4-C5	2.32	1.58	1.53
4	A	1501	KIF	C5-N	2.23	1.52	1.48
4	A	1501	KIF	C1-N9	2.18	1.46	1.44
4	A	1501	KIF	C3-C4	2.17	1.58	1.52
4	A	1501	KIF	C6-C5	2.04	1.55	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1501	KIF	O2-C2-C3	5.88	123.53	110.35
4	A	1501	KIF	C2-C3-C4	3.84	117.91	110.82
4	A	1501	KIF	C6-C5-C4	-2.52	109.40	113.05
4	A	1501	KIF	C7-C8-N9	2.39	107.70	105.45
4	A	1501	KIF	O8-C8-C7	2.06	129.01	125.27

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7　Other polymers　ⓘ

There are no such residues in this entry.

5.8　Polymer linkage issues

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%)	-0.19	22 (2%)	59	53	6, 12, 25, 47	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	993	HIS	6.9
1	A	602	THR	6.1
1	A	990	PRO	5.1
1	A	991	GLU	3.9
1	A	702	ASP	3.8
1	A	682	ASN	3.8
1	A	78	HIS	3.2
1	A	534	SER	3.2
1	A	603	LEU	3.1
1	A	600	HIS	3.0
1	A	720	HIS	2.9
1	A	992	GLU	2.9
1	A	638	ASP	2.8
1	A	79	HIS	2.8
1	A	701	GLN	2.7
1	A	538	ASP	2.7
1	A	547	GLU	2.6
1	A	1024	ASP	2.4
1	A	290	MET	2.2
1	A	396	GLU	2.2
1	A	721	GLY	2.1
1	A	537	GLU	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors($Å^2$)	Q<0.9
4	KIF	A	1501	16/16	0.14	6.44	13,17,20,22	0
2	NAG	A	1046	15/15	0.39	3.23	71,71,71,71	0
5	MRD	A	1602	8/8	0.13	1.06	14,16,17,18	0
3	ZN	A	1601	1/1	0.03	-4.82	8,8,8,8	0

6.5 Other polymers (i)

There are no such residues in this entry.