



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 04:10 PM GMT

PDB ID : 1JS8
Title : Structure of a Functional Unit from Octopus Hemocyanin
Authors : Cuff, M.E.; Miller, K.I.; van Holde, K.E.; Hendrickson, W.A.
Deposited on : 2001-08-16
Resolution : 2.30 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>

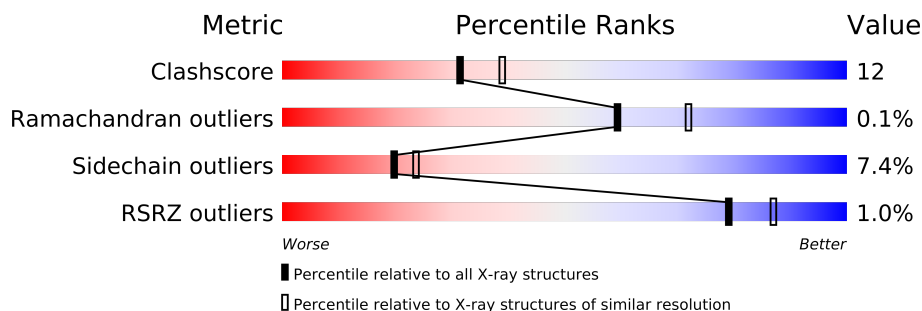
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance



The reported resolution of this entry is 2.30 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))
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

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	394	
1	B	394	

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

Mol	Type	Chain	Res	Geometry	Electron density
4	MAN	A	992	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6593 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 Hemocyanin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	382	Total	C	N	O	S	0	0	0
			3067	1959	521	573	14			
1	B	382	Total	C	N	O	S	0	0	0
			3067	1959	521	573	14			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2843	LEU	PRO	see remark 999	? O61363
B	2843	LEU	PRO	see remark 999	? O61363

- Molecule 2 is a polymer of unknown type called SUGAR (7-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	7	Total	C	N	O	0	0
			83	46	2	35		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2843	LEU	PRO	see remark 999	? O61363

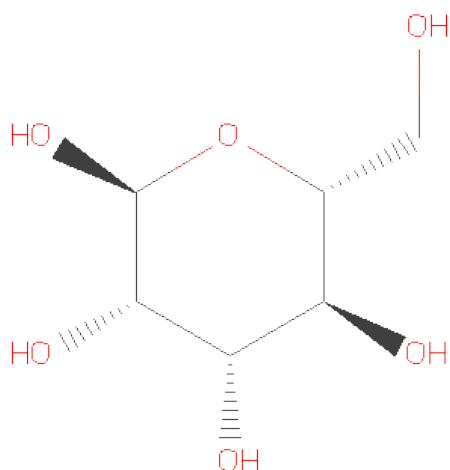
- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	2	Total	C	N	O	0	0
			28	16	2	10		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	2843	LEU	PRO	see remark 999	? O61363

- Molecule 4 is SUGAR (ALPHA-D-MANNOSE) (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			11	6	5		

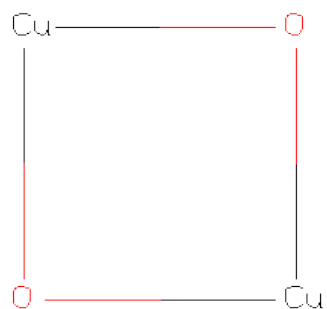
- Molecule 5 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	3	Total	C	O	0	0
			33	18	15		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	2843	LEU	PRO	see remark 999	? O61363

- Molecule 6 is CU2-O2 CLUSTER (three-letter code: CUO) (formula: Cu_2O_2).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	Cu	O	0	0
			4	2	2		
6	B	1	Total	Cu	O	0	0
			4	2	2		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	175	Total	O	0	0
			175	175		
7	B	121	Total	O	0	0
			121	121		

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.

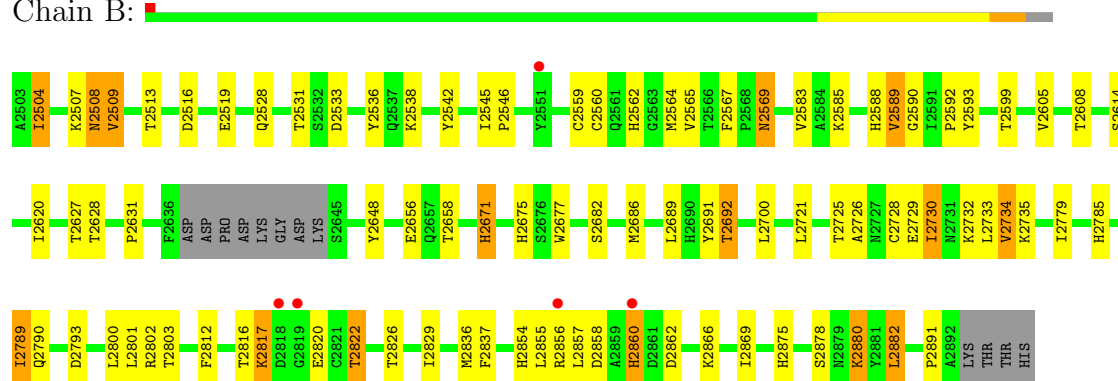
• Molecule 1: Hemocyanin

Chain A:



• Molecule 1: Hemocyanin

Chain B:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	92.86Å 168.39Å 58.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.30 17.95 – 2.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.30) 94.6 (17.95-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.03 (at 2.30Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.202 , 0.262 0.190 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	24.5	Xtriage
Anisotropy	0.475	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 39.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 39114 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6593	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities 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: CUO, BMA, NAG, NDG, MAN

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	0.64	0/3157	0.79	2/4293 (0.0%)
1	B	0.60	0/3157	0.78	0/4293
All	All	0.62	0/6314	0.79	2/8586 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2842	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	A	2802	ARG	NE-CZ-NH2	5.47	123.04	120.30

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	3067	0	2906	69	0
1	B	3067	0	2906	71	0
2	A	83	0	70	0	0
3	B	28	0	25	5	0
4	A	11	0	10	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	33	0	28	1	0
6	A	4	0	0	0	0
6	B	4	0	0	0	0
7	A	175	0	0	5	0
7	B	121	0	0	7	0
All	All	6593	0	5945	140	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 12.

All (140) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:2880:LYS:HB3	1:B:2880:LYS:NZ	1.72	1.01
1:B:2880:LYS:HB3	1:B:2880:LYS:HZ2	1.29	0.93
1:A:2666:GLN:HE22	1:A:2845:LYS:H	1.28	0.80
1:B:2878:SER:OG	1:B:2880:LYS:HB2	1.84	0.76
1:A:2880:LYS:HG2	4:A:992:MAN:O2	1.86	0.74
1:B:2675:HIS:HD1	1:B:2692:THR:HG21	1.53	0.73
1:A:2519:GLU:HG3	1:A:2588:HIS:CE1	2.24	0.73
1:A:2675:HIS:ND1	1:A:2692:THR:HG21	2.03	0.72
1:A:2675:HIS:HD1	1:A:2692:THR:HG21	1.54	0.72
1:B:2533:ASP:HA	1:B:2538:LYS:HG2	1.72	0.72
1:B:2675:HIS:ND1	1:B:2692:THR:HG21	2.06	0.71
1:A:2675:HIS:CE1	1:A:2692:THR:HG21	2.25	0.71
1:B:2686:MET:HA	1:B:2692:THR:HG23	1.74	0.69
1:B:2519:GLU:HG3	1:B:2588:HIS:CE1	2.28	0.69
1:B:2565:VAL:HG11	1:B:2729:GLU:HG3	1.74	0.68
4:A:992:MAN:C5	3:B:991:NAG:H61	2.24	0.68
1:B:2565:VAL:CG1	1:B:2729:GLU:HG3	2.25	0.67
1:B:2816:THR:HG22	1:B:2857:LEU:HD21	1.77	0.67
1:B:2675:HIS:CE1	1:B:2692:THR:HG21	2.30	0.67
1:A:2686:MET:HA	1:A:2692:THR:HG23	1.76	0.66
1:B:2569:ASN:H	1:B:2569:ASN:HD22	1.42	0.66
1:A:2886:THR:HG21	7:B:537:HOH:O	1.95	0.65
1:A:2716:GLN:HE21	1:A:2719:ARG:HH11	1.45	0.65
1:A:2533:ASP:HA	1:A:2538:LYS:HG2	1.77	0.65
1:A:2729:GLU:HG3	7:A:580:HOH:O	1.97	0.64
1:A:2716:GLN:NE2	1:A:2719:ARG:HH11	1.96	0.64
1:A:2859:ALA:HB1	1:B:2730:ILE:HD12	1.80	0.64
1:B:2686:MET:HA	1:B:2692:THR:CG2	2.30	0.61
1:A:2504:ILE:HD11	1:A:2590:GLY:HA2	1.83	0.61
4:A:992:MAN:H5	3:B:991:NAG:H61	1.81	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2793:ASP:OD1	1:A:2891:PRO:HA	2.03	0.59
1:A:2545:ILE:HD11	1:A:2691:TYR:HE1	1.66	0.59
1:B:2880:LYS:HZ3	1:B:2880:LYS:HB3	1.68	0.57
1:A:2803:THR:HG21	7:A:564:HOH:O	2.02	0.57
1:A:2504:ILE:HD12	1:A:2583:VAL:HG21	1.85	0.57
1:B:2592:PRO:HG2	1:B:2700:LEU:HD22	1.87	0.57
1:A:2878:SER:OG	1:A:2880:LYS:HB2	2.06	0.56
1:A:2542:TYR:O	1:A:2559:CYS:HB2	2.05	0.56
1:B:2569:ASN:ND2	1:B:2569:ASN:H	2.03	0.55
1:A:2545:ILE:HD11	1:A:2691:TYR:CE1	2.40	0.55
1:A:2686:MET:HA	1:A:2692:THR:CG2	2.37	0.55
1:A:2817:LYS:HA	1:A:2817:LYS:HE2	1.88	0.54
1:B:2513:THR:O	1:B:2516:ASP:HB2	2.07	0.54
1:B:2817:LYS:HE3	1:B:2817:LYS:HA	1.88	0.54
1:B:2562:HIS:CE1	1:B:2689:LEU:HD11	2.43	0.54
1:B:2812:PHE:HA	1:B:2866:LYS:O	2.07	0.54
1:B:2656:GLU:HG3	1:B:2790:GLN:NE2	2.24	0.53
1:B:2793:ASP:OD1	1:B:2891:PRO:HA	2.08	0.53
1:B:2732:LYS:HB3	7:B:664:HOH:O	2.08	0.53
1:A:2565:VAL:HG23	1:A:2660:PHE:CE2	2.44	0.52
4:A:992:MAN:O5	3:B:991:NAG:H61	2.10	0.52
1:B:2789:ILE:HG22	1:B:2790:GLN:HG3	1.92	0.51
1:A:2557:TYR:HE2	1:A:2836:MET:CE	2.24	0.51
1:B:2565:VAL:HG11	1:B:2728:CYS:SG	2.52	0.50
1:B:2631:PRO:HA	1:B:2677:TRP:O	2.11	0.50
1:B:2508:ASN:HD22	1:B:2509:VAL:N	2.10	0.50
1:A:2816:THR:HG22	1:A:2857:LEU:HD21	1.94	0.49
1:A:2671:HIS:CE1	1:A:2672:ASN:OD1	2.65	0.49
1:B:2560:CYS:SG	1:B:2689:LEU:HD11	2.52	0.49
1:B:2605:VAL:HA	1:B:2608:THR:OG1	2.12	0.49
1:A:2715:LEU:O	1:A:2719:ARG:HG3	2.12	0.49
1:A:2648:TYR:OH	1:A:2785:HIS:CE1	2.66	0.49
1:B:2545:ILE:HD11	1:B:2691:TYR:CE1	2.47	0.49
1:B:2802:ARG:NH1	7:B:512:HOH:O	2.45	0.49
1:B:2648:TYR:OH	1:B:2785:HIS:NE2	2.45	0.49
1:B:2822:THR:HG21	1:B:2855:LEU:HG	1.95	0.48
1:A:2812:PHE:HA	1:A:2866:LYS:O	2.12	0.48
1:A:2734:VAL:HG11	1:B:2860:HIS:O	2.13	0.48
1:A:2565:VAL:HG23	1:A:2660:PHE:HE2	1.79	0.48
1:B:2620:ILE:HD11	1:B:2627:THR:HG22	1.96	0.48
1:A:2656:GLU:HG3	1:A:2790:GLN:NE2	2.28	0.48
1:A:2729:GLU:OE2	1:A:2732:LYS:HE3	2.14	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:A:992:MAN:C5	3:B:991:NAG:C6	2.90	0.48
1:B:2542:TYR:O	1:B:2559:CYS:HB2	2.14	0.48
1:B:2509:VAL:HG22	1:B:2593:TYR:O	2.13	0.47
1:B:2816:THR:OG1	1:B:2820:GLU:HB3	2.15	0.47
1:B:2822:THR:CG2	1:B:2855:LEU:HG	2.45	0.47
4:A:992:MAN:C6	3:B:991:NAG:O6	2.63	0.47
1:A:2717:LYS:HD2	1:A:2723:TYR:CZ	2.49	0.47
1:B:2628:THR:HB	1:B:2682:SER:HB2	1.97	0.47
1:A:2513:THR:O	1:A:2516:ASP:HB2	2.16	0.46
1:A:2557:TYR:CE2	1:A:2836:MET:CE	2.99	0.46
1:B:2822:THR:HG22	1:B:2855:LEU:HD11	1.96	0.46
1:B:2789:ILE:HD13	7:B:552:HOH:O	2.14	0.46
1:A:2880:LYS:HB3	1:A:2880:LYS:NZ	2.31	0.46
1:B:2858:ASP:OD1	1:B:2860:HIS:CE1	2.69	0.46
1:B:2779:ILE:HD13	7:B:501:HOH:O	2.14	0.46
1:B:2507:LYS:HE3	1:B:2589:VAL:HG21	1.97	0.45
1:B:2658:THR:HB	1:B:2721:LEU:HD13	1.98	0.45
1:B:2802:ARG:HD2	7:B:529:HOH:O	2.16	0.45
1:A:2747:ASN:ND2	1:A:2750:THR:H	2.15	0.45
1:B:2504:ILE:HD12	1:B:2583:VAL:HG21	1.97	0.45
1:A:2551:TYR:HE2	7:A:657:HOH:O	1.99	0.45
1:A:2569:ASN:HD22	1:A:2569:ASN:H	1.64	0.45
1:B:2817:LYS:CE	1:B:2817:LYS:HA	2.48	0.44
1:A:2735:LYS:NZ	1:B:2862:ASP:OD1	2.48	0.44
1:A:2509:VAL:HG22	1:A:2593:TYR:O	2.17	0.44
1:B:2726:ALA:HB3	1:B:2733:LEU:HD11	1.99	0.44
1:A:2747:ASN:HD22	1:A:2747:ASN:C	2.20	0.44
1:A:2822:THR:HG22	1:A:2855:LEU:HD11	1.99	0.44
1:A:2545:ILE:HA	1:A:2546:PRO:C	2.38	0.44
1:A:2569:ASN:H	1:A:2569:ASN:ND2	2.15	0.44
1:B:2545:ILE:HD11	1:B:2691:TYR:HE1	1.82	0.44
1:B:2567:PHE:CZ	1:B:2671:HIS:CE1	3.06	0.44
1:B:2878:SER:C	1:B:2880:LYS:H	2.21	0.43
1:B:2686:MET:CA	1:B:2692:THR:HG23	2.47	0.43
1:A:2849:THR:O	1:A:2853:LYS:HG2	2.19	0.43
1:A:2731:ASN:O	1:A:2734:VAL:HG22	2.18	0.43
1:A:2577:GLN:HE21	1:A:2750:THR:HG21	1.83	0.43
1:A:2717:LYS:HA	7:A:682:HOH:O	2.19	0.43
1:B:2729:GLU:O	1:B:2732:LYS:HB2	2.19	0.42
1:A:2742:LEU:O	1:A:2751:LYS:HE3	2.19	0.42
1:A:2860:HIS:O	1:B:2734:VAL:HG21	2.19	0.42
1:A:2686:MET:O	1:A:2692:THR:HG23	2.19	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:2801:LEU:HD22	1:B:2829:ILE:HD11	2.00	0.42
1:A:2572:ARG:NH1	1:A:2760:PHE:O	2.52	0.42
1:B:2837:PHE:HD1	5:B:994:MAN:HO6	1.63	0.42
1:B:2528:GLN:HA	1:B:2536:TYR:HB2	2.00	0.42
1:A:2733:LEU:O	1:A:2757:ALA:N	2.52	0.42
1:A:2576:LYS:HZ2	1:A:2580:ASP:CG	2.22	0.42
1:A:2631:PRO:HA	1:A:2677:TRP:O	2.20	0.42
1:B:2585:LYS:HD3	1:B:2585:LYS:HA	1.83	0.42
1:A:2816:THR:OG1	1:A:2820:GLU:HB3	2.19	0.42
1:A:2747:ASN:ND2	1:A:2749:VAL:H	2.18	0.42
1:A:2635:LEU:HD23	1:A:2636:PHE:CZ	2.55	0.42
1:B:2504:ILE:HD11	1:B:2590:GLY:HA2	2.02	0.41
1:B:2656:GLU:HG3	1:B:2790:GLN:HE21	1.85	0.41
1:A:2886:THR:HG22	1:A:2887:VAL:N	2.35	0.41
1:B:2869:ILE:HD11	1:B:2882:LEU:HB2	2.02	0.41
1:A:2675:HIS:HD1	1:A:2692:THR:CG2	2.28	0.41
1:A:2565:VAL:HG12	7:A:593:HOH:O	2.21	0.41
1:A:2504:ILE:HD12	1:A:2583:VAL:CG2	2.50	0.41
1:A:2585:LYS:HD3	1:A:2585:LYS:HA	1.92	0.41
1:B:2565:VAL:HG13	1:B:2729:GLU:HG3	2.02	0.41
1:B:2628:THR:CB	1:B:2682:SER:HB2	2.51	0.41
1:A:2862:ASP:OD1	1:B:2735:LYS:HE3	2.21	0.41
1:B:2803:THR:HG21	7:B:548:HOH:O	2.20	0.40
1:B:2545:ILE:HA	1:B:2546:PRO:C	2.40	0.40
1:A:2577:GLN:NE2	1:A:2750:THR:OG1	2.49	0.40
1:A:2880:LYS:HB3	1:A:2880:LYS:HE3	1.90	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	378/394 (96%)	368 (97%)	9 (2%)	1 (0%)	50	60
1	B	378/394 (96%)	364 (96%)	14 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	756/788 (96%)	732 (97%)	23 (3%)	1 (0%)	59	72

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2730	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	332/343 (97%)	309 (93%)	23 (7%)	22	27
1	B	332/343 (97%)	306 (92%)	26 (8%)	18	22
All	All	664/686 (97%)	615 (93%)	49 (7%)	20	24

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2504	ILE
1	A	2507	LYS
1	A	2508	ASN
1	A	2509	VAL
1	A	2531	THR
1	A	2552	GLU
1	A	2565	VAL
1	A	2589	VAL
1	A	2599	THR
1	A	2671	HIS
1	A	2692	THR
1	A	2729	GLU
1	A	2747	ASN
1	A	2759	SER
1	A	2784	GLU
1	A	2789	ILE
1	A	2803	THR
1	A	2817	LYS

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Mol	Chain	Res	Type
1	A	2826	THR
1	A	2856	ARG
1	A	2875	HIS
1	A	2880	LYS
1	A	2882	LEU
1	B	2504	ILE
1	B	2508	ASN
1	B	2509	VAL
1	B	2531	THR
1	B	2564	MET
1	B	2569	ASN
1	B	2589	VAL
1	B	2599	THR
1	B	2614	SER
1	B	2671	HIS
1	B	2692	THR
1	B	2725	THR
1	B	2730	ILE
1	B	2734	VAL
1	B	2789	ILE
1	B	2800	LEU
1	B	2817	LYS
1	B	2822	THR
1	B	2826	THR
1	B	2836	MET
1	B	2854	HIS
1	B	2856	ARG
1	B	2860	HIS
1	B	2875	HIS
1	B	2880	LYS
1	B	2882	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2508	ASN
1	A	2569	ASN
1	A	2577	GLN
1	A	2666	GLN
1	A	2704	ASN
1	A	2713	GLN
1	A	2716	GLN

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Mol	Chain	Res	Type
1	A	2724	ASN
1	A	2747	ASN
1	A	2773	ASN
1	A	2775	HIS
1	A	2785	HIS
1	A	2790	GLN
1	B	2508	ASN
1	B	2569	ASN
1	B	2577	GLN
1	B	2704	ASN
1	B	2724	ASN
1	B	2773	ASN
1	B	2775	HIS
1	B	2790	GLN

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 ⓘ

12 carbohydrates 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	NDG	A	890	2	12,14,15	1.35	1 (8%)	15,19,21	0.73	0
2	NAG	A	891	2	12,14,15	0.70	0	15,19,21	0.93	0
2	BMA	A	892	2	10,11,12	0.95	1 (10%)	11,15,17	1.84	1 (9%)
2	MAN	A	893	2	10,11,12	0.59	0	11,15,17	0.97	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MAN	A	894	2	10,11,12	0.55	0	11,15,17	0.84	0
2	MAN	A	895	2	10,11,12	0.49	0	11,15,17	0.64	0
2	BMA	A	896	2	10,11,12	1.02	0	11,15,17	1.24	2 (18%)
3	NAG	B	990	1,3	12,14,15	1.00	1 (8%)	15,19,21	1.64	4 (26%)
3	NAG	B	991	3	12,14,15	1.42	3 (25%)	15,19,21	1.27	1 (6%)
5	MAN	B	993	5	10,11,12	0.61	0	11,15,17	1.08	1 (9%)
5	MAN	B	994	5	10,11,12	0.80	0	11,15,17	0.70	0
5	BMA	B	995	5	10,11,12	1.04	0	11,15,17	1.11	1 (9%)

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	NDG	A	890	2	-	0/6/23/26	0/1/1/1
2	NAG	A	891	2	-	0/6/23/26	0/1/1/1
2	BMA	A	892	2	-	0/2/19/22	0/1/1/1
2	MAN	A	893	2	-	0/2/19/22	0/1/1/1
2	MAN	A	894	2	-	0/2/19/22	0/1/1/1
2	MAN	A	895	2	-	0/2/19/22	0/1/1/1
2	BMA	A	896	2	-	0/2/19/22	0/1/1/1
3	NAG	B	990	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	991	3	-	0/6/23/26	0/1/1/1
5	MAN	B	993	5	-	0/2/19/22	0/1/1/1
5	MAN	B	994	5	-	0/2/19/22	0/1/1/1
5	BMA	B	995	5	-	0/2/19/22	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	890	NDG	C2-N2	-3.44	1.42	1.46
3	B	991	NAG	C3-C2	2.64	1.58	1.52
3	B	990	NAG	C4-C5	2.60	1.58	1.53
3	B	991	NAG	C8-C7	2.38	1.55	1.50
2	A	892	BMA	O3-C3	2.08	1.48	1.43
3	B	991	NAG	O5-C5	-2.04	1.41	1.45

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	892	BMA	O3-C3-C2	5.03	119.14	109.94
3	B	990	NAG	C3-C2-N2	-3.41	106.57	111.76
3	B	990	NAG	O4-C4-C3	-3.36	102.82	110.35
5	B	995	BMA	C3-C4-C5	3.29	116.08	110.20
3	B	991	NAG	C6-C5-C4	2.98	120.19	113.00
5	B	993	MAN	C4-C3-C2	2.44	113.78	110.50
2	A	896	BMA	C3-C4-C5	-2.19	106.30	110.20
3	B	990	NAG	C8-C7-N2	-2.17	111.86	116.11
2	A	896	BMA	O5-C5-C6	2.17	109.26	106.98
3	B	990	NAG	O5-C5-C6	-2.03	104.85	106.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.6 Ligand geometry ⓘ

3 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	$\# Z > 2$
6	CUO	A	888	1	0,4,4	0.00	-	0,4,4	0.00	-
4	MAN	A	992	-	10,11,12	1.15	0	11,15,17	1.54	2 (18%)
6	CUO	B	999	1	0,4,4	0.00	-	0,4,4	0.00	-

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
6	CUO	A	888	1	-	0/0/4/4	0/0/1/1
4	MAN	A	992	-	-	0/2/19/22	0/1/1/1
6	CUO	B	999	1	-	0/0/4/4	0/0/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	A	992	MAN	C4-C3-C2	-3.96	105.19	110.50
4	A	992	MAN	C3-C4-C5	-2.36	105.98	110.20

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	382/394 (96%)	-0.33	1 (0%) 91 96	4, 17, 38, 51	0
1	B	382/394 (96%)	-0.19	5 (1%) 74 82	5, 19, 40, 53	0
All	All	764/788 (96%)	-0.26	6 (0%) 79 90	4, 18, 39, 53	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2860	HIS	4.4
1	B	2856	ARG	2.5
1	A	2818	ASP	2.3
1	B	2819	GLY	2.3
1	B	2551	TYR	2.2
1	B	2818	ASP	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 ⓘ

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
2	MAN	A	895	11/12	0.20	15.36	40,44,49,50	0
5	BMA	B	995	11/12	0.36	6.55	62,65,68,72	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	MAN	B	994	11/12	0.20	1.56	39,43,48,60	0
2	NDG	A	890	14/15	0.13	0.61	18,21,27,31	0
5	MAN	B	993	11/12	0.16	0.60	32,37,46,56	0
3	NAG	B	990	14/15	0.21	-0.16	41,47,52,52	0
2	MAN	A	893	11/12	0.11	-0.18	16,21,28,35	0
2	MAN	A	894	11/12	0.12	-0.56	19,27,35,39	0
2	NAG	A	891	14/15	0.11	-0.62	26,30,33,36	0
2	BMA	A	892	11/12	0.12	-	31,33,39,41	0
2	BMA	A	896	11/12	0.45	-	37,39,44,45	0
3	NAG	B	991	14/15	0.29	-	45,52,54,58	0

6.4 Ligands

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(\AA^2)	Q<0.9
4	MAN	A	992	11/12	0.72	5.99	34,36,39,40	0
6	CUO	A	888	4/4	0.07	-0.86	9,10,11,12	0
6	CUO	B	999	4/4	0.07	-0.95	11,15,17,22	0

6.5 Other polymers

There are no such residues in this entry.