



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 10:22 PM UTC

PDB ID : 1K2D / pdb_00001k2d
Title : Crystal structure of the autoimmune MHC class II I-Au complexed with myelin basic protein 1-11 at 2.2Å
Authors : He, X.L.; Radu, C.; Ward, E.S.; Garcia, K.C.
Deposited on : 2001-09-26
Resolution : 2.20 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

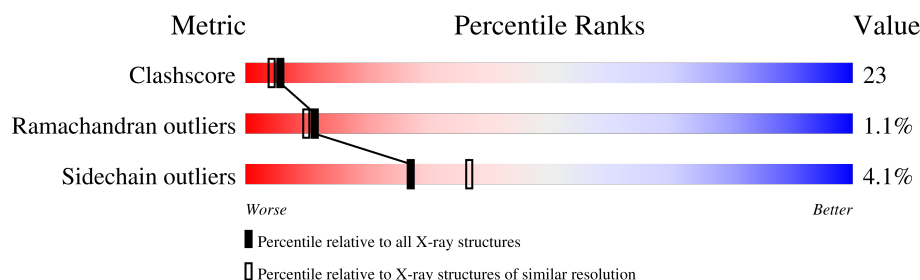
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	189	
2	B	189	
3	P	23	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	A	501	X	-	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3597 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 H-2 class II histocompatibility antigen, A-U alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	182	Total	C	N	O	S	0	0	0
			1463	946	233	281	3			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	HIS	-	cloning artifact	UNP P14438
A	-5	SER	-	cloning artifact	UNP P14438
A	-4	ARG	-	cloning artifact	UNP P14438
A	-3	GLY	-	cloning artifact	UNP P14438
A	-2	GLU	-	cloning artifact	UNP P14438
A	-1	ASP	-	cloning artifact	UNP P14438
A	0	ASP	-	cloning artifact	UNP P14438
A	1	ILE	-	cloning artifact	UNP P14438
A	2	GLU	-	cloning artifact	UNP P14438
A	3	ALA	-	cloning artifact	UNP P14438

- Molecule 2 is a protein called H-2 class II histocompatibility antigen, A-U beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	185	Total	C	N	O	S	0	0	0
			1558	984	279	289	6			

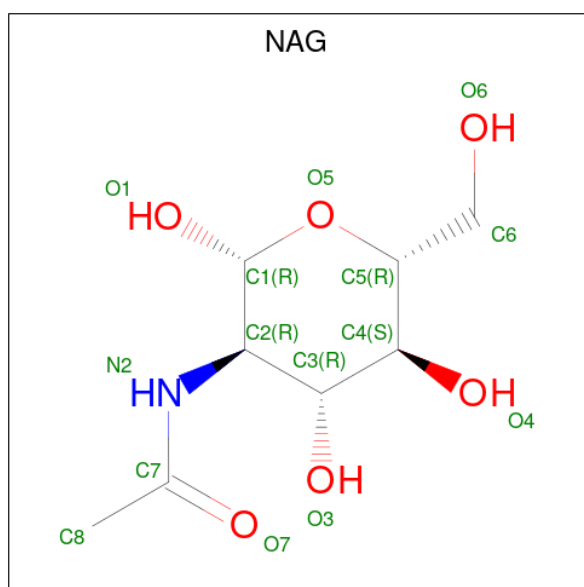
- Molecule 3 is a protein called Myelin Basic Protein peptide with 8 residue linker peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	P	12	Total	C	N	O	0	0	0
			84	49	17	18			

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	-4	HIS	-	cloning artifact	GB 14763906
P	-3	SER	-	cloning artifact	GB 14763906
P	-2	ARG	-	cloning artifact	GB 14763906
P	-1	GLY	-	cloning artifact	GB 14763906
P	0	GLY	MET	conflict	GB 14763906
P	11	GLY	-	linker	GB 14763906
P	12	THR	-	linker	GB 14763906
P	13	GLY	-	linker	GB 14763906
P	14	SER	-	linker	GB 14763906
P	15	GLY	-	linker	GB 14763906
P	16	SER	-	linker	GB 14763906
P	17	GLY	-	linker	GB 14763906
P	18	SER	-	linker	GB 14763906

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 5 is water.

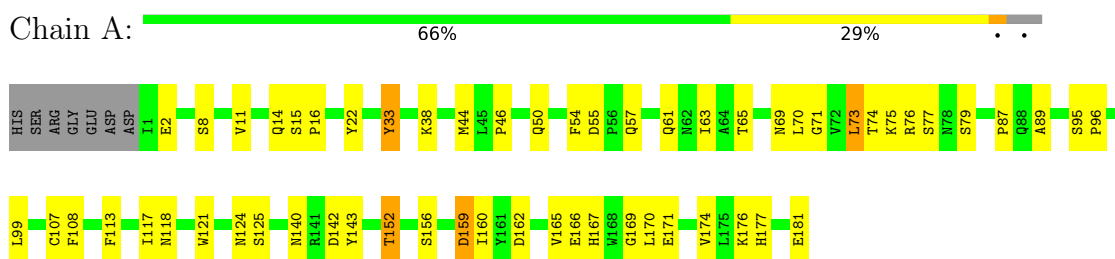
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	225	Total 225	O 225	0	0
5	B	207	Total 207	O 207	0	0
5	P	18	Total 18	O 18	0	0

3 Residue-property plots [i](#)

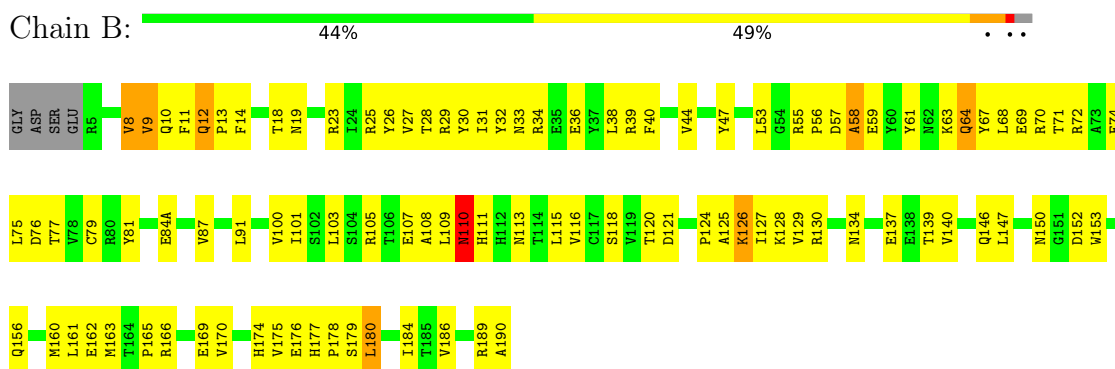
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

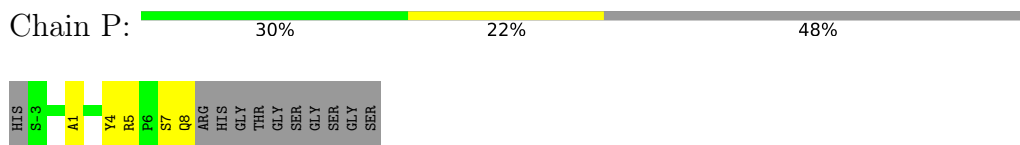
- Molecule 1: H-2 class II histocompatibility antigen, A-U alpha chain



- Molecule 2: H-2 class II histocompatibility antigen, A-U beta chain



- Molecule 3: Myelin Basic Protein peptide with 8 residue linker peptide



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	99.15Å 110.59Å 94.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20	Depositor
% Data completeness (in resolution range)	98.3 (50.00-2.20)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.248 , 0.276	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3597	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

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	0.55	1/1508 (0.1%)	1.00	3/2059 (0.1%)
2	B	0.51	0/1597	0.98	10/2170 (0.5%)
3	P	0.84	0/85	1.59	3/113 (2.7%)
All	All	0.54	1/3190 (0.0%)	1.01	16/4342 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	79	SER	CA-C	-5.22	1.48	1.53

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	109	LEU	N-CA-C	7.75	122.94	113.17
1	A	33	TYR	N-CA-C	-7.62	97.73	109.24
3	P	5	ARG	N-CA-C	6.86	118.29	109.65
1	A	70	LEU	N-CA-C	-6.50	101.34	110.50
2	B	64	GLN	N-CA-C	6.12	119.22	111.69
2	B	120	THR	N-CA-C	6.05	119.07	109.81
2	B	12	GLN	CA-C-N	5.89	127.20	119.84
2	B	12	GLN	C-N-CA	5.89	127.20	119.84
1	A	117	ILE	N-CA-C	5.76	115.93	107.75
2	B	146	GLN	N-CA-C	-5.55	103.21	110.53
2	B	121	ASP	N-CA-C	5.45	118.96	111.54
2	B	180	LEU	N-CA-C	5.43	118.09	109.24
2	B	163	MET	N-CA-C	5.29	115.22	108.24
2	B	39	ARG	N-CA-C	5.28	117.10	108.55
3	P	5	ARG	CG-CD-NE	-5.13	100.70	112.00
3	P	5	ARG	NE-CZ-NH1	-5.00	116.50	121.50

There are no chirality outliers.

There are no planarity outliers.

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	1463	0	1389	52	0
2	B	1558	0	1499	99	0
3	P	84	0	75	7	0
4	A	28	0	26	1	0
4	B	14	0	13	3	0
5	A	225	0	0	10	0
5	B	207	0	0	10	0
5	P	18	0	0	1	0
All	All	3597	0	3002	143	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 23.

All (143) 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)
2:B:72:ARG:HA	5:B:576:HOH:O	1.69	0.93
2:B:125:ALA:HB1	2:B:147:LEU:HD21	1.54	0.87
2:B:126:LYS:C	2:B:126:LYS:HE2	1.98	0.87
4:A:502:NAG:H62	5:A:589:HOH:O	1.82	0.80
1:A:160:ILE:HG23	1:A:177:HIS:CE1	2.17	0.79
2:B:18:THR:HG22	2:B:19:ASN:HD22	1.48	0.77
4:B:503:NAG:H4	5:B:677:HOH:O	1.84	0.75
2:B:126:LYS:HE2	2:B:127:ILE:N	2.01	0.75
1:A:14:GLN:HG3	2:B:8:VAL:HG22	1.68	0.74
2:B:11:PHE:HE1	2:B:28:THR:HG23	1.53	0.73
2:B:150:ASN:HD21	2:B:156:GLN:HE21	1.34	0.73
1:A:170:LEU:HD13	1:A:174:VAL:HG23	1.70	0.73
2:B:11:PHE:CE1	2:B:28:THR:HG23	2.24	0.73
2:B:55:ARG:HB3	2:B:56:PRO:HD3	1.70	0.72
2:B:10:GLN:HB2	2:B:31:ILE:HB	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:190:ALA:HB2	5:B:637:HOH:O	1.90	0.70
2:B:177:HIS:CD2	2:B:179:SER:H	2.10	0.69
1:A:96:PRO:HG2	2:B:100:VAL:HG21	1.74	0.69
2:B:177:HIS:HD2	2:B:179:SER:H	1.40	0.69
1:A:75:LYS:HE2	5:A:724:HOH:O	1.93	0.68
2:B:18:THR:HB	2:B:23:ARG:HB3	1.77	0.67
2:B:137:GLU:H	2:B:137:GLU:CD	2.03	0.66
2:B:134:ASN:HD21	2:B:169:GLU:HG2	1.66	0.61
2:B:59:GLU:CG	2:B:63:LYS:HE2	2.31	0.60
1:A:118:ASN:HB2	1:A:166:GLU:HB2	1.81	0.60
1:A:71:GLY:HA2	1:A:74:THR:HB	1.84	0.60
2:B:70:ARG:HD2	5:B:622:HOH:O	2.01	0.59
2:B:27:VAL:HG12	2:B:28:THR:N	2.17	0.59
2:B:74:GLU:HA	2:B:77:THR:OG1	2.03	0.58
2:B:75:LEU:HD23	2:B:75:LEU:O	2.03	0.58
2:B:30:TYR:HB2	2:B:38:LEU:HB3	1.85	0.58
2:B:110:ASN:CG	2:B:166:ARG:HH12	2.12	0.57
3:P:8:GLN:HB2	5:P:134:HOH:O	2.04	0.57
2:B:70:ARG:HG2	5:B:586:HOH:O	2.03	0.57
2:B:26:TYR:HB3	2:B:75:LEU:HD12	1.86	0.57
1:A:8:SER:HA	2:B:13:PRO:O	2.05	0.57
2:B:152:ASP:O	2:B:153:TRP:HB2	2.05	0.57
2:B:128:LYS:HE2	2:B:176:GLU:OE1	2.05	0.56
1:A:118:ASN:CB	1:A:166:GLU:HB2	2.36	0.56
2:B:126:LYS:NZ	5:B:535:HOH:O	2.38	0.56
1:A:143:TYR:OH	2:B:29:ARG:HD3	2.06	0.55
2:B:32:TYR:CE2	2:B:33:ASN:ND2	2.75	0.55
2:B:87:VAL:HA	2:B:91:LEU:HD12	1.87	0.55
2:B:166:ARG:HB2	2:B:169:GLU:OE2	2.06	0.55
2:B:166:ARG:HH11	2:B:166:ARG:HG2	1.72	0.54
2:B:170:VAL:HG22	2:B:189:ARG:NE	2.22	0.54
1:A:87:PRO:HD2	1:A:170:LEU:HD21	1.88	0.54
2:B:125:ALA:HB1	2:B:147:LEU:CD2	2.32	0.54
2:B:124:PRO:O	2:B:177:HIS:HE1	1.91	0.54
2:B:27:VAL:CG1	2:B:28:THR:N	2.70	0.53
2:B:72:ARG:HH11	2:B:72:ARG:HG2	1.72	0.53
2:B:101:ILE:HD12	2:B:186:VAL:HG12	1.91	0.53
1:A:76:ARG:HH22	2:B:57:ASP:CG	2.17	0.52
1:A:160:ILE:HG23	1:A:177:HIS:ND1	2.24	0.52
2:B:105:ARG:HB2	2:B:113:ASN:ND2	2.24	0.52
2:B:26:TYR:HE1	2:B:74:GLU:HB2	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:134:ASN:ND2	2:B:169:GLU:HG2	2.25	0.52
1:A:152:THR:HG22	5:A:668:HOH:O	2.09	0.52
2:B:36:GLU:HG3	5:B:544:HOH:O	2.09	0.51
1:A:11:VAL:HG13	1:A:63:ILE:HD13	1.93	0.51
1:A:167:HIS:CD2	1:A:169:GLY:H	2.29	0.50
1:A:75:LYS:HD2	5:A:713:HOH:O	2.10	0.50
1:A:69:ASN:O	1:A:73:LEU:HB2	2.11	0.50
1:A:152:THR:CG2	5:A:668:HOH:O	2.60	0.50
1:A:171:GLU:HG2	5:A:693:HOH:O	2.10	0.50
1:A:124:ASN:O	1:A:125:SER:OG	2.28	0.49
1:A:143:TYR:HB2	2:B:34:ARG:HG3	1.94	0.49
2:B:32:TYR:O	2:B:33:ASN:HB2	2.13	0.49
1:A:76:ARG:NH1	2:B:57:ASP:OD2	2.38	0.49
2:B:150:ASN:ND2	2:B:156:GLN:HE21	2.06	0.49
2:B:116:VAL:HG22	2:B:160:MET:HG3	1.94	0.49
2:B:11:PHE:HB2	3:P:4:TYR:CZ	2.48	0.48
1:A:140:ASN:HB3	5:A:579:HOH:O	2.13	0.48
1:A:95:SER:HB2	1:A:96:PRO:CD	2.43	0.48
2:B:11:PHE:HE1	2:B:28:THR:CG2	2.24	0.48
2:B:128:LYS:HE3	2:B:130:ARG:HD3	1.95	0.48
1:A:15:SER:HA	1:A:16:PRO:C	2.38	0.48
2:B:31:ILE:HD12	2:B:31:ILE:N	2.29	0.48
1:A:95:SER:HB2	1:A:96:PRO:HD2	1.95	0.47
2:B:126:LYS:HE2	2:B:127:ILE:CA	2.43	0.47
2:B:180:LEU:HD13	2:B:184:ILE:HG12	1.96	0.47
2:B:61:TYR:HE2	3:P:7:SER:HA	1.80	0.47
2:B:11:PHE:HB2	3:P:4:TYR:CE1	2.49	0.47
2:B:176:GLU:HG3	5:B:547:HOH:O	2.15	0.47
1:A:75:LYS:HG3	5:A:689:HOH:O	2.14	0.47
1:A:162:ASP:OD1	1:A:177:HIS:HB2	2.15	0.46
2:B:28:THR:HG22	2:B:30:TYR:HE1	1.80	0.46
1:A:113:PHE:CD1	2:B:34:ARG:HD3	2.51	0.46
2:B:107:GLU:HG3	2:B:108:ALA:N	2.30	0.46
1:A:50:GLN:NE2	5:A:523:HOH:O	2.50	0.45
2:B:81:TYR:O	2:B:84(A):GLU:HB2	2.17	0.45
2:B:103:LEU:HD13	2:B:115:LEU:HD23	1.99	0.45
2:B:129:VAL:HG13	2:B:175:VAL:HG22	1.99	0.45
2:B:180:LEU:CD1	2:B:184:ILE:HG12	2.47	0.44
2:B:59:GLU:HG3	2:B:63:LYS:HE2	1.99	0.44
1:A:38:LYS:HE2	5:A:597:HOH:O	2.16	0.44
1:A:75:LYS:C	1:A:77:SER:N	2.75	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:CYS:HB2	1:A:121:TRP:CH2	2.53	0.44
2:B:40:PHE:CD1	2:B:71:THR:HG21	2.53	0.44
2:B:40:PHE:CG	2:B:71:THR:HG21	2.52	0.44
1:A:89:ALA:HA	1:A:108:PHE:O	2.17	0.44
1:A:96:PRO:HG2	2:B:100:VAL:CG2	2.43	0.44
2:B:130:ARG:HH21	2:B:174:HIS:CD2	2.36	0.44
2:B:69:GLU:HB3	5:B:586:HOH:O	2.18	0.43
2:B:74:GLU:C	2:B:76:ASP:N	2.75	0.43
2:B:111:HIS:O	2:B:165:PRO:HD2	2.19	0.43
2:B:166:ARG:HG2	2:B:166:ARG:NH1	2.33	0.43
1:A:11:VAL:HB	2:B:11:PHE:HB3	2.00	0.43
1:A:142:ASP:OD1	1:A:142:ASP:C	2.60	0.43
2:B:105:ARG:HB2	2:B:113:ASN:HD21	1.83	0.43
2:B:162:GLU:OE1	2:B:162:GLU:HA	2.19	0.42
2:B:31:ILE:HG22	2:B:32:TYR:N	2.33	0.42
1:A:156:SER:OG	1:A:159:ASP:OD1	2.36	0.42
1:A:160:ILE:HG23	1:A:177:HIS:HE1	1.77	0.42
4:B:503:NAG:H3	4:B:503:NAG:H82	2.01	0.42
1:A:22:TYR:O	1:A:33:TYR:HA	2.19	0.42
1:A:54:PHE:CE1	3:P:1:ALA:HB2	2.55	0.42
1:A:55:ASP:OD1	1:A:57:GLN:HG3	2.19	0.42
2:B:12:GLN:HB3	2:B:14:PHE:CE2	2.54	0.42
1:A:65:THR:HG21	3:P:4:TYR:O	2.20	0.41
1:A:44:MET:O	1:A:46:PRO:HD3	2.19	0.41
2:B:8:VAL:HG12	2:B:9:VAL:N	2.36	0.41
2:B:100:VAL:HG22	2:B:118:SER:HB2	2.00	0.41
1:A:54:PHE:HE1	3:P:1:ALA:HB2	1.85	0.41
1:A:113:PHE:CZ	2:B:34:ARG:HB2	2.55	0.41
1:A:159:ASP:C	1:A:160:ILE:HD12	2.45	0.41
2:B:27:VAL:HA	2:B:40:PHE:O	2.20	0.41
2:B:57:ASP:O	2:B:58:ALA:C	2.62	0.41
2:B:40:PHE:HB2	2:B:47:TYR:CE1	2.56	0.41
1:A:76:ARG:NH1	2:B:53:LEU:O	2.52	0.41
1:A:176:LYS:HD3	1:A:176:LYS:HA	1.86	0.41
2:B:25:ARG:HD2	5:B:560:HOH:O	2.20	0.41
2:B:129:VAL:HA	2:B:174:HIS:O	2.21	0.41
2:B:177:HIS:CG	2:B:178:PRO:HD2	2.56	0.41
2:B:23:ARG:HG2	2:B:23:ARG:O	2.20	0.41
2:B:26:TYR:CD2	2:B:26:TYR:C	2.98	0.41
2:B:44:VAL:HG12	2:B:44:VAL:O	2.22	0.40
2:B:74:GLU:C	2:B:76:ASP:H	2.29	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:19:ASN:OD1	4:B:503:NAG:H2	2.22	0.40
2:B:28:THR:HG22	2:B:30:TYR:CE1	2.56	0.40
2:B:161:LEU:HD12	2:B:162:GLU:N	2.36	0.40
1:A:181:GLU:O	1:A:181:GLU:HG2	2.21	0.40
1:A:118:ASN:O	1:A:165:VAL:HA	2.22	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	180/189 (95%)	171 (95%)	9 (5%)	0	100	100
2	B	183/189 (97%)	159 (87%)	20 (11%)	4 (2%)	5	3
3	P	10/23 (44%)	8 (80%)	2 (20%)	0	100	100
All	All	373/401 (93%)	338 (91%)	31 (8%)	4 (1%)	11	10

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	58	ALA
2	B	79	CYS
2	B	110	ASN
2	B	140	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	163/169 (96%)	157 (96%)	6 (4%)	30	41
2	B	172/175 (98%)	164 (95%)	8 (5%)	23	31
3	P	8/16 (50%)	8 (100%)	0	100	100
All	All	343/360 (95%)	329 (96%)	14 (4%)	27	37

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	61	GLN
1	A	73	LEU
1	A	99	LEU
1	A	152	THR
1	A	159	ASP
2	B	8	VAL
2	B	9	VAL
2	B	64	GLN
2	B	67	TYR
2	B	68	LEU
2	B	110	ASN
2	B	126	LYS
2	B	139	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	GLN
1	A	101	GLN
1	A	167	HIS
2	B	22	GLN
2	B	64	GLN
2	B	96	GLN
2	B	111	HIS
2	B	136	GLN
2	B	146	GLN
2	B	156	GLN
2	B	177	HIS

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](#)

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	$\# Z > 2$
4	NAG	A	501	1	14,14,15	0.71	0	17,19,21	0.67	1 (5%)
4	NAG	B	503	2	14,14,15	0.53	0	17,19,21	0.71	0
4	NAG	A	502	1	14,14,15	0.62	0	17,19,21	0.72	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
4	NAG	A	501	1	1/1/5/7	5/6/23/26	0/1/1/1
4	NAG	B	503	2	-	3/6/23/26	0/1/1/1
4	NAG	A	502	1	-	5/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	501	NAG	C2-N2-C7	-2.12	120.06	122.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	501	NAG	C1

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	501	NAG	C8-C7-N2-C2
4	A	501	NAG	O7-C7-N2-C2
4	A	502	NAG	C3-C2-N2-C7
4	A	502	NAG	C8-C7-N2-C2
4	A	502	NAG	O7-C7-N2-C2
4	B	503	NAG	C1-C2-N2-C7
4	B	503	NAG	C8-C7-N2-C2
4	B	503	NAG	O7-C7-N2-C2
4	A	501	NAG	C4-C5-C6-O6
4	A	501	NAG	O5-C5-C6-O6
4	A	502	NAG	O5-C5-C6-O6
4	A	502	NAG	C4-C5-C6-O6
4	A	501	NAG	C1-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	503	NAG	3	0
4	A	502	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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.