



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:50 PM UTC

PDB ID : 1RIN / pdb_00001rin
Title : X-RAY CRYSTAL STRUCTURE OF A PEA LECTIN-TRIMANNOSIDE
COMPLEX AT 2.6 ANGSTROMS RESOLUTION
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Deposited on : 1993-01-27
Resolution : 2.60 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

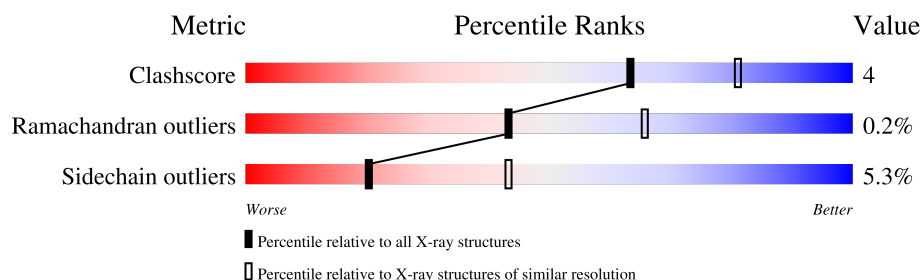
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)

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	180	 71% 24% . .
1	C	180	 69% 27% .
2	B	49	 71% 24% .
2	D	49	 80% 16% .

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 3678 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 PEA LECTIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	180	Total	C	N	O	0	0	0
			1409	899	230	280			
1	C	180	Total	C	N	O	0	0	0
			1409	899	230	280			

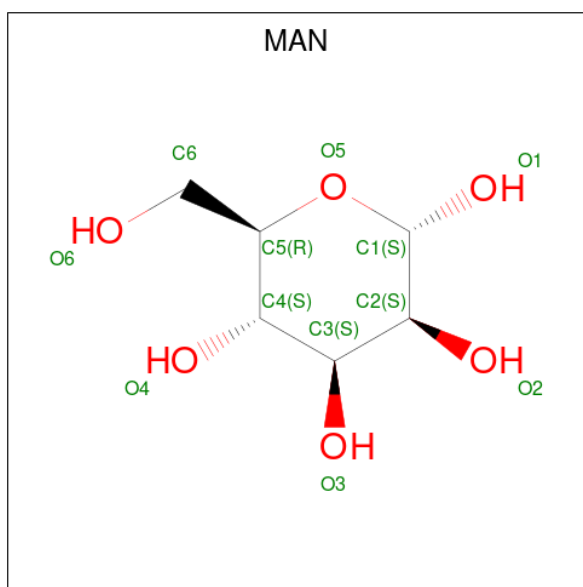
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	114	GLU	GLN	conflict	UNP P02867
C	114	GLU	GLN	conflict	UNP P02867

- Molecule 2 is a protein called PEA LECTIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	47	Total	C	N	O	0	0	0
			367	236	57	74			
2	D	49	Total	C	N	O	0	0	0
			378	242	59	77			

- Molecule 3 is alpha-D-mannopyranose (CCD ID: MAN) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			12	6	6		
3	C	1	Total	C	O	0	0
			12	6	6		

- Molecule 4 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mn	0	0
			1	1		
4	C	1	Total	Mn	0	0
			1	1		

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Ca	0	0
			1	1		
5	C	1	Total	Ca	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	44	Total	O	0	0
			44	44		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	8	Total 8	O 8	0	0
6	C	31	Total 31	O 31	0	0
6	D	4	Total 4	O 4	0	0

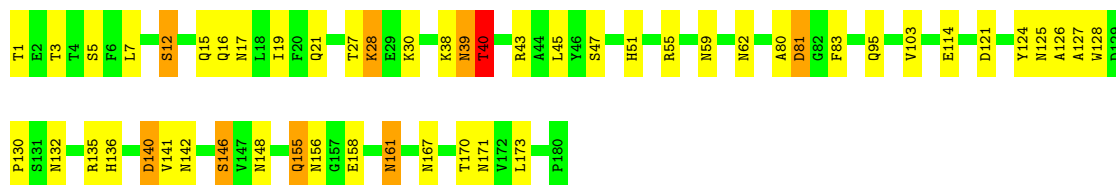
3 Residue-property plots [i](#)

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.

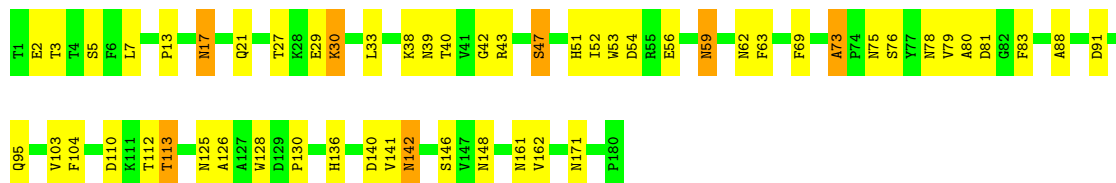
• Molecule 1: PEA LECTIN

Chain A: 



• Molecule 1: PEA LECTIN

Chain C: 



• Molecule 2: PEA LECTIN

Chain B: 



• Molecule 2: PEA LECTIN

Chain D: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	64.30Å 73.40Å 108.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.183 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3678	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

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: MAN, CA, MN

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	0.93	2/1443 (0.1%)	1.85	35/1970 (1.8%)
1	C	0.99	3/1443 (0.2%)	1.90	41/1970 (2.1%)
2	B	1.16	4/377 (1.1%)	1.78	5/515 (1.0%)
2	D	1.23	5/388 (1.3%)	1.71	8/530 (1.5%)
All	All	1.01	14/3651 (0.4%)	1.85	89/4985 (1.8%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	222	HIS	CG-ND1	-6.94	1.30	1.38
1	C	51	HIS	CD2-NE2	-6.60	1.30	1.37
1	C	136	HIS	CD2-NE2	-6.50	1.30	1.37
2	D	222	HIS	CD2-NE2	-6.44	1.30	1.37
2	B	230	HIS	CD2-NE2	-6.19	1.31	1.37
2	D	230	HIS	CD2-NE2	-6.12	1.31	1.37
1	C	136	HIS	CG-ND1	-6.08	1.31	1.38
2	B	222	HIS	CG-ND1	-5.92	1.31	1.38
1	A	51	HIS	CD2-NE2	-5.86	1.31	1.37
1	A	136	HIS	CD2-NE2	-5.63	1.31	1.37
2	D	203	VAL	CA-CB	5.61	1.61	1.54
2	B	230	HIS	CG-ND1	-5.43	1.32	1.38
2	D	230	HIS	CG-ND1	-5.37	1.32	1.38
2	B	222	HIS	CD2-NE2	-5.16	1.32	1.37

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	161	ASN	OD1-CG-ND2	-11.42	111.18	122.60
1	C	75	ASN	OD1-CG-ND2	-9.73	112.87	122.60
1	C	80	ALA	O-C-N	-9.52	113.23	123.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	171	ASN	OD1-CG-ND2	-9.31	113.29	122.60
1	C	39	ASN	OD1-CG-ND2	-8.74	113.86	122.60
1	A	95	GLN	OE1-CD-NE2	-8.67	113.93	122.60
1	A	140	ASP	CA-CB-CG	8.28	120.88	112.60
1	C	161	ASN	OD1-CG-ND2	-8.10	114.50	122.60
1	A	167	ASN	OD1-CG-ND2	-8.08	114.52	122.60
1	C	112	THR	CA-CB-OG1	-7.91	97.73	109.60
1	A	171	ASN	OD1-CG-ND2	-7.79	114.81	122.60
1	C	78	ASN	OD1-CG-ND2	-7.72	114.88	122.60
1	A	161	ASN	CB-CG-ND2	7.51	127.66	116.40
1	A	148	ASN	OD1-CG-ND2	-7.48	115.12	122.60
1	A	80	ALA	O-C-N	-7.47	114.73	123.25
1	A	127	ALA	N-CA-C	7.32	120.31	111.82
1	A	142	ASN	OD1-CG-ND2	-7.25	115.35	122.60
1	A	81	ASP	CA-CB-CG	-7.21	105.39	112.60
1	A	17	ASN	OD1-CG-ND2	-7.14	115.46	122.60
2	B	219	TYR	N-CA-C	7.03	118.86	108.60
1	C	110	ASP	CA-CB-CG	6.99	119.59	112.60
1	C	81	ASP	CA-CB-CG	-6.98	105.62	112.60
1	A	15	GLN	OE1-CD-NE2	-6.93	115.67	122.60
1	A	62	ASN	CA-CB-CG	6.74	119.34	112.60
1	A	59	ASN	OD1-CG-ND2	-6.62	115.98	122.60
1	A	121	ASP	CA-CB-CG	6.57	119.17	112.60
1	C	148	ASN	OD1-CG-ND2	-6.55	116.05	122.60
2	B	230	HIS	ND1-CG-CD2	6.49	112.59	106.10
2	D	230	HIS	ND1-CG-CD2	6.47	112.57	106.10
1	C	83	PHE	CA-CB-CG	6.45	120.25	113.80
1	C	171	ASN	CB-CG-ND2	6.43	126.05	116.40
1	A	132	ASN	OD1-CG-ND2	-6.41	116.19	122.60
2	B	200	LYS	CB-CG-CD	-6.29	96.83	111.30
1	A	12	SER	O-C-N	-6.21	115.61	121.20
1	C	95	GLN	OE1-CD-NE2	-6.19	116.41	122.60
1	A	47	SER	N-CA-C	6.18	118.82	111.71
1	C	30	LYS	N-CA-C	6.16	119.06	109.52
1	A	155	GLN	OE1-CD-NE2	-6.11	116.49	122.60
1	C	140	ASP	CA-CB-CG	6.08	118.68	112.60
2	B	190	SER	N-CA-C	6.07	118.92	109.52
1	A	83	PHE	CA-CB-CG	6.06	119.86	113.80
2	D	222	HIS	ND1-CG-CD2	5.98	112.08	106.10
1	C	39	ASN	CB-CG-ND2	5.98	125.37	116.40
1	C	63	PHE	CA-CB-CG	5.97	119.77	113.80
1	A	128	TRP	CG-CD2-CE3	5.93	139.83	133.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	59	ASN	OD1-CG-ND2	-5.85	116.75	122.60
1	C	112	THR	CA-CB-CG2	5.84	120.42	110.50
2	D	202	VAL	N-CA-CB	-5.79	105.84	111.57
1	C	75	ASN	CA-CB-CG	-5.74	106.86	112.60
1	A	125	ASN	OD1-CG-ND2	-5.74	116.86	122.60
2	D	200	LYS	CB-CG-CD	-5.73	98.11	111.30
1	A	146	SER	N-CA-C	5.72	118.53	110.23
1	C	136	HIS	N-CA-C	5.70	117.73	109.07
1	C	128	TRP	CG-CD2-CE3	5.70	139.60	133.90
1	A	125	ASN	CB-CG-ND2	5.70	124.94	116.40
1	A	103	VAL	CB-CA-C	-5.69	105.07	110.65
1	C	79	VAL	N-CA-C	5.66	116.09	108.17
2	D	234	SER	CB-CA-C	-5.62	98.57	109.76
1	C	128	TRP	CE2-CD2-CG	-5.62	100.46	107.20
1	A	95	GLN	CG-CD-NE2	5.61	124.81	116.40
1	C	125	ASN	OD1-CG-ND2	-5.59	117.01	122.60
1	A	16	GLN	OE1-CD-NE2	-5.55	117.05	122.60
1	C	62	ASN	OD1-CG-ND2	-5.51	117.09	122.60
1	C	91	ASP	CA-CB-CG	5.48	118.08	112.60
1	A	135	ARG	CA-CB-CG	-5.47	103.16	114.10
1	C	73	ALA	CA-C-N	5.45	124.79	118.85
1	C	73	ALA	C-N-CA	5.45	124.79	118.85
1	A	30	LYS	N-CA-C	5.45	118.94	110.17
1	C	88	ALA	N-CA-C	5.44	114.39	108.14
1	C	17	ASN	OD1-CG-ND2	-5.38	117.22	122.60
1	C	54	ASP	CA-CB-CG	5.38	117.98	112.60
2	B	222	HIS	ND1-CG-CD2	5.37	111.47	106.10
2	D	219	TYR	N-CA-C	5.36	117.22	109.07
1	A	39	ASN	OD1-CG-ND2	-5.36	117.24	122.60
1	C	75	ASN	CB-CG-ND2	5.35	124.42	116.40
1	A	55	ARG	CA-CB-CG	5.33	124.76	114.10
2	D	200	LYS	CA-CB-CG	5.22	124.54	114.10
1	C	79	VAL	O-C-N	-5.21	117.71	123.18
1	A	156	ASN	OD1-CG-ND2	-5.20	117.40	122.60
1	A	40	THR	CA-CB-OG1	-5.18	101.84	109.60
1	C	126	ALA	N-CA-C	5.17	117.58	111.33
1	C	88	ALA	O-C-N	-5.14	117.17	121.54
1	C	142	ASN	OD1-CG-ND2	-5.13	117.47	122.60
1	C	161	ASN	CA-CB-CG	-5.10	107.50	112.60
1	C	56	GLU	CA-CB-CG	-5.09	103.92	114.10
1	C	141	VAL	O-C-N	-5.08	117.79	122.71
1	C	53	TRP	CE2-CD2-CG	-5.07	101.12	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	234	SER	N-CA-CB	5.05	118.12	110.45
1	A	21	GLN	OE1-CD-NE2	-5.04	117.56	122.60

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	1409	0	1358	18	0
1	C	1409	0	1358	12	0
2	B	367	0	346	7	0
2	D	378	0	356	3	0
3	A	12	0	12	0	0
3	C	12	0	12	0	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
6	A	44	0	0	2	0
6	B	8	0	0	0	0
6	C	31	0	0	0	0
6	D	4	0	0	1	0
All	All	3678	0	3442	28	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 4.

All (28) 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:C:17:ASN:O	1:C:47:SER:HB2	2.04	0.57
1:C:33:LEU:O	1:C:42:GLY:HA3	2.06	0.56
1:A:7:LEU:HB3	1:C:3:THR:HB	1.91	0.53
1:A:27:THR:HG23	1:A:28:LYS:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:GLU:O	2:B:203:VAL:HG12	2.10	0.51
1:C:21:GLN:HB2	1:C:43:ARG:HB2	1.93	0.51
1:C:38:LYS:HG3	2:D:219:TYR:CD2	2.48	0.48
1:A:28:LYS:HD3	1:A:28:LYS:H	1.79	0.48
1:C:69:PHE:HE1	1:C:162:VAL:HG21	1.80	0.47
1:A:43:ARG:HD2	2:B:212:SER:HB3	1.98	0.46
1:C:113:THR:HB	1:C:142:ASN:HD22	1.81	0.46
1:A:130:PRO:HD2	6:A:255:HOH:O	2.15	0.46
2:D:234:SER:HB3	2:D:236:THR:HG23	1.97	0.45
1:C:73:ALA:HB1	6:D:23:HOH:O	2.16	0.45
1:C:103:VAL:HG23	1:C:104:PHE:CD2	2.51	0.45
1:A:141:VAL:HG13	2:B:202:VAL:HG11	1.99	0.44
1:C:59:ASN:HD21	2:D:236:THR:H	1.64	0.44
1:A:7:LEU:O	1:C:2:GLU:HA	2.18	0.43
1:A:114:GLU:HB3	2:B:204:PRO:HD3	2.00	0.43
1:A:1:THR:HA	2:B:233:LEU:O	2.19	0.42
1:A:19:ILE:HB	1:A:45:LEU:HB2	2.01	0.42
1:A:3:THR:HB	1:C:7:LEU:HB3	2.01	0.42
1:A:38:LYS:HG2	1:A:39:ASN:ND2	2.35	0.42
1:A:40:THR:HG22	2:B:215:THR:OG1	2.20	0.41
1:A:155:GLN:HB3	1:A:158:GLU:HG3	2.03	0.41
1:A:173:LEU:O	2:B:194:SER:HA	2.21	0.41
1:A:124:TYR:CZ	1:A:126:ALA:HA	2.55	0.41
1:A:140:ASP:HA	6:A:264:HOH:O	2.19	0.41

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	178/180 (99%)	165 (93%)	13 (7%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	178/180 (99%)	169 (95%)	8 (4%)	1 (1%)	21	42
2	B	45/49 (92%)	44 (98%)	1 (2%)	0	100	100
2	D	47/49 (96%)	45 (96%)	2 (4%)	0	100	100
All	All	448/458 (98%)	423 (94%)	24 (5%)	1 (0%)	43	66

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	29	GLU

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	155/155 (100%)	147 (95%)	8 (5%)	21	44
1	C	155/155 (100%)	144 (93%)	11 (7%)	13	31
2	B	41/42 (98%)	41 (100%)	0	100	100
2	D	42/42 (100%)	40 (95%)	2 (5%)	23	47
All	All	393/394 (100%)	372 (95%)	21 (5%)	20	43

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	SER
1	A	12	SER
1	A	28	LYS
1	A	40	THR
1	A	81	ASP
1	A	146	SER
1	A	161	ASN
1	A	170	THR
1	C	5	SER
1	C	13	PRO

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Mol	Chain	Res	Type
1	C	27	THR
1	C	30	LYS
1	C	40	THR
1	C	47	SER
1	C	52	ILE
1	C	76	SER
1	C	113	THR
1	C	130	PRO
1	C	146	SER
2	D	190	SER
2	D	198	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	39	ASN
1	A	155	GLN
1	A	161	ASN
1	C	59	ASN
1	C	105	ASN
1	C	142	ASN

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 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	$\# Z > 2$
3	MAN	A	250	-	12,12,12	0.74	0	17,17,17	0.76	0
3	MAN	C	250	-	12,12,12	0.64	0	17,17,17	0.88	1 (5%)

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
3	MAN	A	250	-	-	0/2/22/22	0/1/1/1
3	MAN	C	250	-	-	0/2/22/22	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(°)
3	C	250	MAN	O1-C1-C2	2.06	114.95	108.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.