



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 1GIC / pdb_00001gic
Title : CONCAVALIN A COMPLEXED WITH METHYL ALPHA-D-GLUCOPYRANOSIDE
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Deposited on : 1996-08-08
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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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

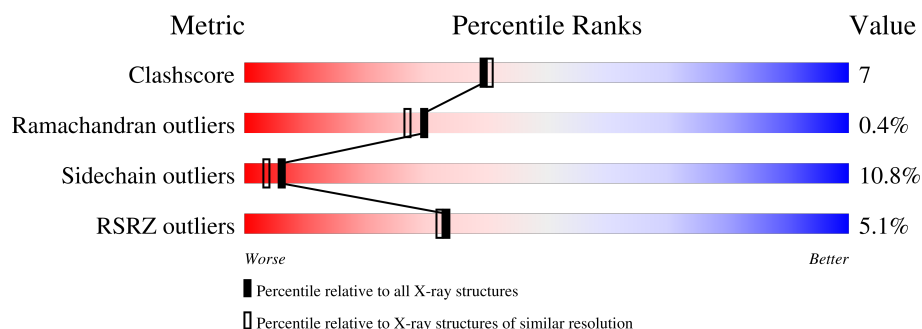
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	237	5% 65% 26% 8% .
1	B	237	5% 62% 28% 9% .

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4008 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.

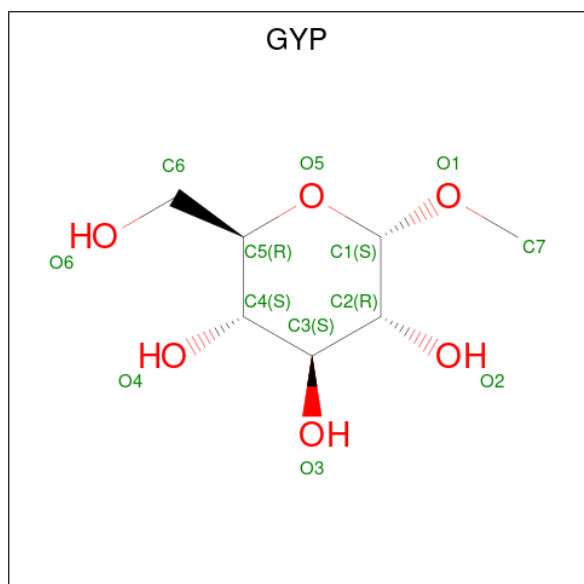
- Molecule 1 is a protein called CONCANAVALIN A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	237	Total	C	N	O	S	0	0	0
			1809	1141	302	364	2			
1	B	237	Total	C	N	O	S	0	0	0
			1809	1141	302	364	2			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	151	ASP	GLU	conflict	UNP P02866
A	155	GLU	ARG	conflict	UNP P02866
B	151	ASP	GLU	conflict	UNP P02866
B	155	GLU	ARG	conflict	UNP P02866

- Molecule 2 is methyl alpha-D-glucopyranoside (CCD ID: GYP) (formula: C₇H₁₄O₆).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 13 7 6	0	0
2	B	1	Total C O 13 7 6	0	0

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mn 1 1	0	0
3	B	1	Total Mn 1 1	0	0

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Ca 1 1	0	0
4	B	1	Total Ca 1 1	0	0

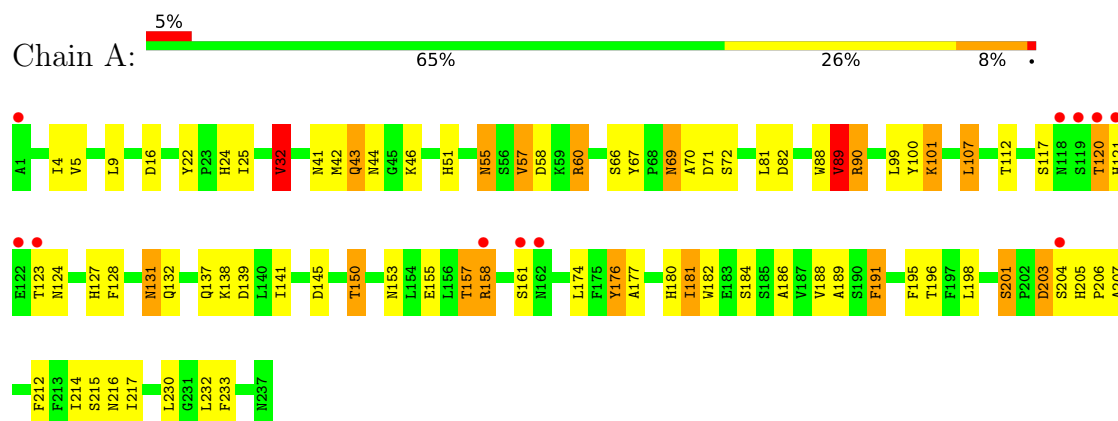
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	186	Total O 186 186	0	0
5	B	174	Total O 174 174	0	0

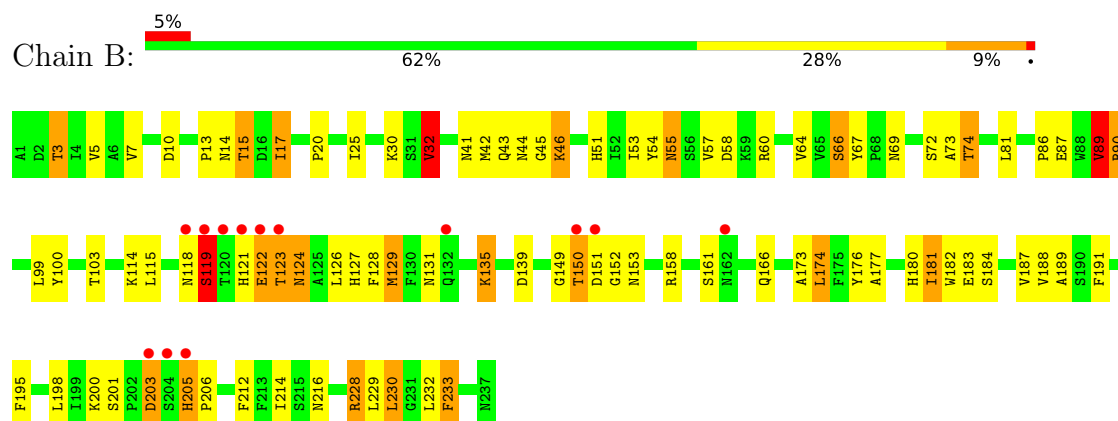
3 Residue-property plots

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 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: CONCANAVALIN A



• Molecule 1: CONCANAVALIN A



4 Data and refinement statistics

Property	Value	Source
Space group	I 21 3	Depositor
Cell constants a, b, c, α , β , γ	167.80Å 167.80Å 167.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 – 2.00 100.00 – 2.02	Depositor EDS
% Data completeness (in resolution range)	64.0 (100.00-2.00) 63.6 (100.00-2.02)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.68 (at 2.01Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.170 , (Not available) 0.176 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	19.8	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 65.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.020 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4008	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.26% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MN, GYP, CA

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	1.11	9/1851 (0.5%)	1.89	58/2522 (2.3%)
1	B	1.15	6/1851 (0.3%)	1.95	61/2522 (2.4%)
All	All	1.13	15/3702 (0.4%)	1.92	119/5044 (2.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	180	HIS	CD2-NE2	-7.68	1.29	1.37
1	A	205	HIS	CD2-NE2	-6.95	1.30	1.37
1	A	181	ILE	CA-CB	6.20	1.62	1.54
1	A	180	HIS	CD2-NE2	-6.14	1.31	1.37
1	A	121	HIS	CD2-NE2	-6.05	1.31	1.37
1	A	51	HIS	CD2-NE2	-5.65	1.31	1.37
1	A	120	THR	CA-CB	5.65	1.62	1.53
1	B	51	HIS	CD2-NE2	-5.65	1.31	1.37
1	B	121	HIS	CD2-NE2	-5.59	1.31	1.37
1	B	127	HIS	CD2-NE2	-5.53	1.31	1.37
1	A	123	THR	CA-CB	5.42	1.61	1.53
1	B	205	HIS	CD2-NE2	-5.41	1.31	1.37
1	A	127	HIS	CD2-NE2	-5.41	1.31	1.37
1	B	181	ILE	CA-CB	5.36	1.61	1.54
1	A	24	HIS	CG-ND1	-5.31	1.32	1.38

All (119) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	89	VAL	N-CA-CB	-17.60	92.08	112.32
1	B	89	VAL	N-CA-CB	-12.94	93.07	112.35
1	B	17	ILE	N-CA-CB	-9.56	99.51	111.94
1	A	195	PHE	CA-CB-CG	8.64	122.44	113.80
1	B	5	VAL	N-CA-C	-8.63	95.15	107.75
1	A	121	HIS	CA-CB-CG	8.21	122.00	113.80
1	A	207	ALA	O-C-N	-8.20	114.29	123.48
1	B	55	ASN	OD1-CG-ND2	-7.85	114.75	122.60
1	A	69	ASN	CA-CB-CG	7.84	120.44	112.60
1	A	5	VAL	N-CA-C	-7.80	97.19	108.11
1	B	176	TYR	N-CA-C	7.75	120.41	111.11
1	B	184	SER	N-CA-C	7.47	121.31	111.75
1	B	216	ASN	N-CA-C	-7.45	100.22	110.35
1	B	41	ASN	OD1-CG-ND2	-7.37	115.23	122.60
1	A	176	TYR	N-CA-C	7.24	119.79	111.11
1	B	203	ASP	CA-CB-CG	7.09	119.69	112.60
1	B	139	ASP	CA-CB-CG	6.95	119.55	112.60
1	A	138	LYS	N-CA-C	6.80	120.84	112.54
1	A	89	VAL	CB-CA-C	6.78	120.81	110.91
1	B	191	PHE	CA-CB-CG	6.77	120.57	113.80
1	B	184	SER	CA-CB-OG	-6.64	97.81	111.10
1	A	191	PHE	CA-CB-CG	6.62	120.42	113.80
1	B	212	PHE	N-CA-C	-6.61	98.47	109.24
1	B	10	ASP	CA-CB-CG	6.53	119.13	112.60
1	A	82	ASP	CA-CB-CG	6.50	119.10	112.60
1	B	89	VAL	O-C-N	-6.47	115.76	122.95
1	A	153	ASN	CA-CB-CG	6.47	119.07	112.60
1	A	121	HIS	CB-CG-CD2	-6.37	122.92	131.20
1	B	121	HIS	N-CA-C	-6.36	103.39	111.92
1	A	90	ARG	N-CA-C	-6.36	99.45	109.50
1	B	128	PHE	CA-CB-CG	6.35	120.15	113.80
1	A	107	LEU	CD1-CG-CD2	-6.33	96.88	110.80
1	A	44	ASN	OD1-CG-ND2	-6.30	116.30	122.60
1	B	69	ASN	CA-CB-CG	6.29	118.89	112.60
1	B	17	ILE	CA-CB-CG2	6.26	121.14	110.50
1	B	114	LYS	CB-CG-CD	-6.25	96.92	111.30
1	A	131	ASN	OD1-CG-ND2	-6.24	116.36	122.60
1	A	217	ILE	N-CA-C	6.22	118.83	111.05
1	B	90	ARG	CA-CB-CG	-6.17	101.75	114.10
1	A	99	LEU	N-CA-C	-6.16	104.47	112.23
1	B	67	TYR	N-CA-C	-6.08	99.67	109.58
1	A	212	PHE	N-CA-C	-6.08	99.33	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	182	TRP	CA-CB-CG	6.07	125.14	113.60
1	B	127	HIS	CB-CG-CD2	-6.07	123.31	131.20
1	B	89	VAL	CB-CA-C	6.07	120.04	110.52
1	B	153	ASN	OD1-CG-ND2	-6.05	116.55	122.60
1	B	124	ASN	N-CA-C	-5.99	99.94	109.59
1	A	128	PHE	CA-CB-CG	5.96	119.76	113.80
1	B	149	GLY	CA-C-O	-5.96	113.07	119.27
1	B	151	ASP	CA-CB-CG	5.93	118.53	112.60
1	A	32	VAL	CB-CA-C	-5.92	98.32	111.77
1	B	3	THR	N-CA-C	-5.91	98.88	108.52
1	A	145	ASP	N-CA-C	5.91	120.11	113.02
1	B	119	SER	N-CA-C	-5.91	98.07	108.23
1	B	17	ILE	CB-CA-C	5.89	120.43	112.36
1	B	233	PHE	CA-C-N	5.89	125.43	119.19
1	B	233	PHE	C-N-CA	5.89	125.43	119.19
1	A	60	ARG	N-CA-CB	-5.85	101.59	110.77
1	B	195	PHE	CA-CB-CG	5.82	119.61	113.80
1	A	121	HIS	CB-CG-ND1	5.79	131.38	122.70
1	B	90	ARG	O-C-N	-5.79	115.67	123.19
1	B	14	ASN	OD1-CG-ND2	-5.78	116.83	122.60
1	B	90	ARG	NE-CZ-NH2	-5.76	114.02	119.20
1	A	141	ILE	N-CA-C	-5.72	99.64	107.99
1	A	201	SER	CA-C-N	5.71	125.39	119.05
1	A	201	SER	C-N-CA	5.71	125.39	119.05
1	A	203	ASP	N-CA-C	-5.68	101.79	110.14
1	B	152	GLY	N-CA-C	-5.65	106.20	114.90
1	B	44	ASN	OD1-CG-ND2	-5.63	116.97	122.60
1	A	196	THR	N-CA-C	-5.62	100.25	109.40
1	B	180	HIS	CB-CG-CD2	-5.61	123.91	131.20
1	B	149	GLY	N-CA-C	5.60	121.74	115.08
1	B	17	ILE	CA-CB-CG1	-5.58	100.91	110.40
1	B	173	ALA	O-C-N	-5.56	116.82	123.27
1	B	73	ALA	N-CA-C	-5.53	99.88	108.90
1	A	214	ILE	N-CA-C	-5.53	100.16	108.12
1	A	67	TYR	N-CA-C	-5.51	100.60	109.58
1	B	124	ASN	O-C-N	-5.51	116.22	123.21
1	B	99	LEU	N-CA-C	-5.49	105.21	111.14
1	B	32	VAL	N-CA-C	-5.49	104.87	112.50
1	A	22	TYR	CA-C-O	-5.46	115.48	120.50
1	A	71	ASP	CA-CB-CG	5.43	118.03	112.60
1	B	214	ILE	N-CA-C	-5.39	100.36	108.12
1	A	216	ASN	N-CA-C	-5.37	103.04	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	189	ALA	N-CA-C	-5.37	99.69	108.76
1	B	25	ILE	N-CA-C	-5.37	100.73	108.89
1	A	43	GLN	OE1-CD-NE2	-5.35	117.25	122.60
1	A	155	GLU	CA-C-O	-5.34	114.99	120.54
1	B	15	THR	N-CA-CB	-5.34	102.05	110.06
1	A	25	ILE	N-CA-C	-5.33	100.81	108.48
1	B	44	ASN	CA-CB-CG	-5.31	107.29	112.60
1	B	230	LEU	N-CA-C	5.29	119.04	112.47
1	A	16	ASP	CA-CB-CG	5.29	117.89	112.60
1	A	158	ARG	CB-CG-CD	-5.28	99.15	111.30
1	A	5	VAL	O-C-N	-5.28	117.56	123.26
1	B	90	ARG	N-CA-C	-5.28	101.28	109.72
1	A	70	ALA	N-CA-C	-5.28	101.05	109.07
1	A	88	TRP	CG-CD2-CE3	5.26	139.16	133.90
1	A	189	ALA	O-C-N	-5.25	117.17	123.31
1	A	57	VAL	N-CA-C	-5.24	105.74	110.82
1	A	180	HIS	CA-C-O	-5.20	115.76	121.58
1	B	7	VAL	N-CA-C	-5.20	99.02	107.28
1	B	51	HIS	CA-C-O	-5.17	114.78	120.36
1	B	177	ALA	CA-C-N	5.12	125.12	119.90
1	B	177	ALA	C-N-CA	5.12	125.12	119.90
1	A	137	GLN	OE1-CD-NE2	-5.11	117.49	122.60
1	A	180	HIS	CB-CG-CD2	-5.10	124.57	131.20
1	B	32	VAL	CB-CA-C	-5.06	97.77	111.34
1	B	118	ASN	CA-CB-CG	5.05	117.65	112.60
1	A	182	TRP	CE2-CD2-CG	-5.05	101.14	107.20
1	A	41	ASN	OD1-CG-ND2	-5.04	117.56	122.60
1	A	55	ASN	CA-CB-CG	5.04	117.64	112.60
1	A	9	LEU	N-CA-C	-5.03	96.63	107.49
1	A	157	THR	CA-C-N	5.03	127.91	120.82
1	A	157	THR	C-N-CA	5.03	127.91	120.82
1	A	101	LYS	N-CA-C	5.02	115.67	108.74
1	B	103	THR	N-CA-C	-5.02	103.05	110.48
1	A	177	ALA	CA-C-N	5.01	125.00	119.89
1	A	177	ALA	C-N-CA	5.01	125.00	119.89

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	100	TYR	Sidechain

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	1809	0	1755	20	0
1	B	1809	0	1755	31	0
2	A	13	0	14	0	0
2	B	13	0	14	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	186	0	0	3	0
5	B	174	0	0	4	0
All	All	4008	0	3538	48	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 7.

All (48) 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:B:55:ASN:HD22	1:B:57:VAL:H	1.30	0.79
1:B:129:MET:HG3	5:B:408:HOH:O	1.94	0.66
1:B:201:SER:HB2	1:B:206:PRO:HB3	1.79	0.64
1:B:55:ASN:ND2	1:B:58:ASP:H	1.95	0.64
1:B:55:ASN:HD21	1:B:58:ASP:H	1.43	0.64
1:A:124:ASN:ND2	1:B:131:ASN:H	1.97	0.62
1:A:55:ASN:HD22	1:A:57:VAL:H	1.52	0.58
1:B:42:MET:HE1	1:B:206:PRO:HG3	1.87	0.56
1:B:187:VAL:HG23	1:B:188:VAL:HG23	1.88	0.56
1:A:157:THR:HB	5:A:332:HOH:O	2.05	0.56
1:A:43:GLN:HE21	1:A:46:LYS:HG3	1.71	0.55
1:B:54:TYR:HD2	5:B:389:HOH:O	1.88	0.55
1:B:43:GLN:HB3	1:B:46:LYS:HG3	1.90	0.53
1:A:201:SER:HB2	1:A:206:PRO:HB3	1.90	0.51
1:A:107:LEU:HD12	1:A:107:LEU:N	2.26	0.50
1:A:150:THR:HB	5:A:415:HOH:O	2.11	0.50
1:B:55:ASN:HD22	1:B:57:VAL:N	2.05	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:SER:HB3	1:B:72:SER:HB3	1.94	0.49
1:B:150:THR:HG21	5:B:279:HOH:O	2.12	0.49
1:A:117:SER:HA	1:A:186:ALA:HA	1.94	0.48
1:B:100:TYR:HB3	1:B:205:HIS:O	2.14	0.48
1:B:119:SER:O	1:B:122:GLU:HB2	2.13	0.48
1:B:13:PRO:HB3	1:B:20:PRO:O	2.14	0.48
1:A:112:THR:O	1:A:191:PHE:HA	2.13	0.48
1:B:86:PRO:HG2	1:B:89:VAL:HG23	1.96	0.47
1:B:115:LEU:O	1:B:123:THR:HA	2.14	0.47
1:B:228:ARG:HD3	5:B:256:HOH:O	2.15	0.47
1:A:131:ASN:H	1:B:124:ASN:ND2	2.12	0.47
1:A:32:VAL:HG13	1:A:233:PHE:CD2	2.51	0.45
1:B:32:VAL:HG13	1:B:233:PHE:CD2	2.51	0.45
1:B:90:ARG:HB3	1:B:174:LEU:HD12	1.98	0.45
1:B:3:THR:HG23	1:B:30:LYS:HD3	1.98	0.45
1:A:60:ARG:NH1	5:A:389:HOH:O	2.50	0.44
1:A:124:ASN:HD21	1:B:131:ASN:H	1.64	0.44
1:A:42:MET:HE1	1:A:206:PRO:CG	2.49	0.43
1:A:55:ASN:ND2	1:A:58:ASP:H	2.15	0.43
1:A:139:ASP:O	1:A:176:TYR:HB2	2.19	0.43
1:B:135:LYS:HB3	1:B:135:LYS:NZ	2.34	0.43
1:A:43:GLN:HB3	1:A:46:LYS:HG3	2.01	0.42
1:B:158:ARG:HH21	1:B:166:GLN:HG3	1.84	0.42
1:A:66:SER:HB3	1:A:72:SER:HB3	2.02	0.42
1:B:45:GLY:HA2	1:B:200:LYS:HB3	2.02	0.41
1:B:64:VAL:HG13	1:B:74:THR:HG22	2.02	0.41
1:B:55:ASN:ND2	1:B:57:VAL:HB	2.36	0.41
1:B:87:GLU:HG3	1:B:182:TRP:O	2.21	0.41
1:A:89:VAL:HG22	1:A:215:SER:O	2.21	0.40
1:B:205:HIS:HA	1:B:206:PRO:HD2	1.82	0.40
1:A:90:ARG:HB3	1:A:174:LEU:HD23	2.03	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	235/237 (99%)	224 (95%)	10 (4%)	1 (0%)	30	27
1	B	235/237 (99%)	223 (95%)	11 (5%)	1 (0%)	30	27
All	All	470/474 (99%)	447 (95%)	21 (4%)	2 (0%)	30	27

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	161	SER
1	B	150	THR

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	203/203 (100%)	185 (91%)	18 (9%)	9	6
1	B	203/203 (100%)	177 (87%)	26 (13%)	4	2
All	All	406/406 (100%)	362 (89%)	44 (11%)	6	3

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	32	VAL
1	A	69	ASN
1	A	81	LEU
1	A	89	VAL
1	A	101	LYS
1	A	120	THR
1	A	132	GLN
1	A	150	THR
1	A	158	ARG
1	A	181	ILE

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Mol	Chain	Res	Type
1	A	184	SER
1	A	188	VAL
1	A	198	LEU
1	A	203	ASP
1	A	204	SER
1	A	230	LEU
1	A	232	LEU
1	B	15	THR
1	B	17	ILE
1	B	32	VAL
1	B	46	LYS
1	B	53	ILE
1	B	60	ARG
1	B	66	SER
1	B	74	THR
1	B	81	LEU
1	B	89	VAL
1	B	119	SER
1	B	122	GLU
1	B	123	THR
1	B	126	LEU
1	B	129	MET
1	B	135	LYS
1	B	161	SER
1	B	174	LEU
1	B	181	ILE
1	B	183	GLU
1	B	198	LEU
1	B	203	ASP
1	B	228	ARG
1	B	229	LEU
1	B	230	LEU
1	B	232	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	GLN
1	A	51	HIS
1	A	55	ASN
1	A	104	ASN
1	A	118	ASN

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Mol	Chain	Res	Type
1	A	124	ASN
1	A	131	ASN
1	A	153	ASN
1	A	162	ASN
1	B	43	GLN
1	B	51	HIS
1	B	55	ASN
1	B	104	ASN
1	B	124	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	$\# Z > 2$
2	GYP	B	238	-	13,13,13	0.76	1 (7%)	18,18,18	0.90	1 (5%)
2	GYP	A	238	-	13,13,13	1.13	1 (7%)	18,18,18	5.07	2 (11%)

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	GYP	B	238	-	-	0/4/24/24	0/1/1/1
2	GYP	A	238	-	-	0/4/24/24	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	238	GYP	O1-C1	3.25	1.45	1.40
2	B	238	GYP	O1-C1	2.39	1.44	1.40

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	238	GYP	C7-O1-C1	21.27	145.58	113.26
2	B	238	GYP	C7-O1-C1	2.45	116.98	113.26
2	A	238	GYP	O4-C4-C3	-2.09	105.44	110.38

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	237/237 (100%)	-0.22	11 (4%) 37 36	8, 17, 47, 70	0
1	B	237/237 (100%)	-0.27	13 (5%) 30 29	6, 15, 46, 76	0
All	All	474/474 (100%)	-0.24	24 (5%) 33 32	6, 16, 47, 76	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	120	THR	5.4
1	B	121	HIS	5.0
1	A	118	ASN	4.9
1	B	118	ASN	4.4
1	A	121	HIS	4.2
1	B	120	THR	4.1
1	B	119	SER	4.1
1	A	122	GLU	3.3
1	A	119	SER	3.2
1	B	122	GLU	3.2
1	A	1	ALA	3.1
1	B	205	HIS	3.0
1	A	161	SER	2.9
1	B	204	SER	2.7
1	B	151	ASP	2.5
1	B	132	GLN	2.5
1	B	123	THR	2.4
1	A	162	ASN	2.4
1	B	203	ASP	2.4
1	B	162	ASN	2.1
1	A	158	ARG	2.0
1	B	150	THR	2.0
1	A	204	SER	2.0
1	A	123	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($\text{\AA}^2$)	Q<0.9
2	GYP	A	238	13/13	0.97	0.05	18,21,24,25	0
2	GYP	B	238	13/13	0.97	0.05	14,17,17,17	0
3	MN	A	239	1/1	0.99	0.02	13,13,13,13	0
4	CA	A	240	1/1	0.99	0.03	13,13,13,13	0
4	CA	B	240	1/1	0.99	0.02	13,13,13,13	0
3	MN	B	239	1/1	1.00	0.02	14,14,14,14	0

6.5 Other polymers [i](#)

There are no such residues in this entry.