



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 11:16 PM UTC

PDB ID : 5CNA / pdb_00005cna
Title : REFINED STRUCTURE OF CONCAVALIN A COMPLEXED WITH A
LPHA-METHYL-D-MANNOPYRANOSIDE AT 2.0 ANGSTROMS RESO-
LUTION AND COMPARISON WITH THE SACCHARIDE-FREE STRUC-
TURE
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Hunter, W.N.; Raftery, J.; Kalb(Gilboa), A.J.; Yariv, J.
Deposited on : 1994-02-11
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)

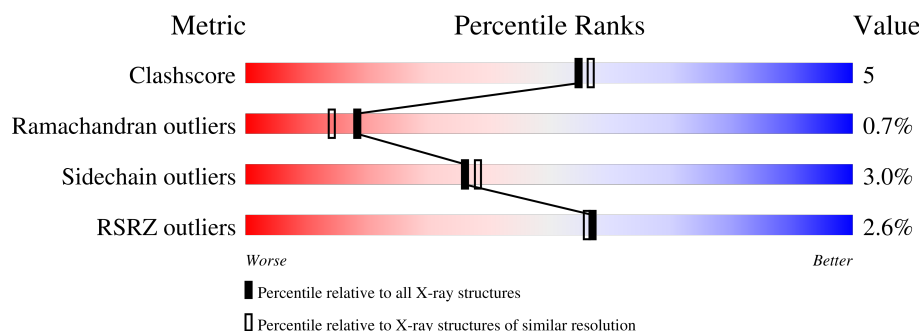
1 Overall quality at a glance

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	3% 68% 28% .
1	B	237	3% 74% 24% .
1	C	237	2% 65% 30% 5%
1	D	237	3% 73% 24% .

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7830 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.

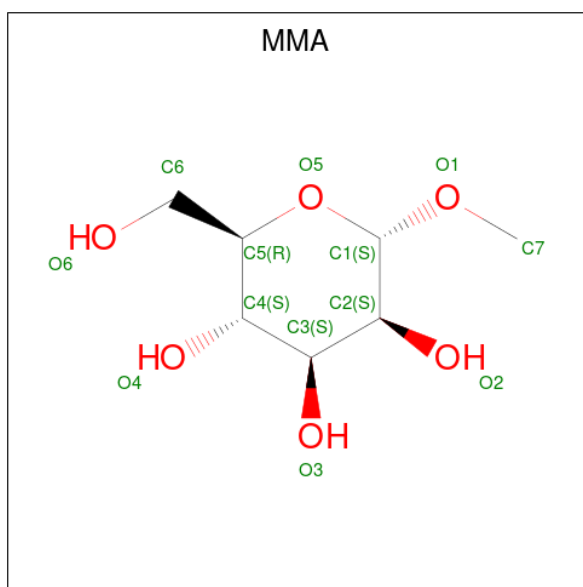
- Molecule 1 is a protein called CONCANAVALIN A.

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			
1	C	237	Total	C	N	O	S	0	0	0
			1809	1141	302	364	2			
1	D	237	Total	C	N	O	S	0	0	0
			1809	1141	302	364	2			

There are 8 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
C	151	ASP	GLU	conflict	UNP P02866
C	155	GLU	ARG	conflict	UNP P02866
D	151	ASP	GLU	conflict	UNP P02866
D	155	GLU	ARG	conflict	UNP P02866

- Molecule 2 is methyl alpha-D-mannopyranoside (CCD ID: MMA) (formula: C₇H₁₄O₆).



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

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

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

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

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

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

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total 1	Cl 1	0	0

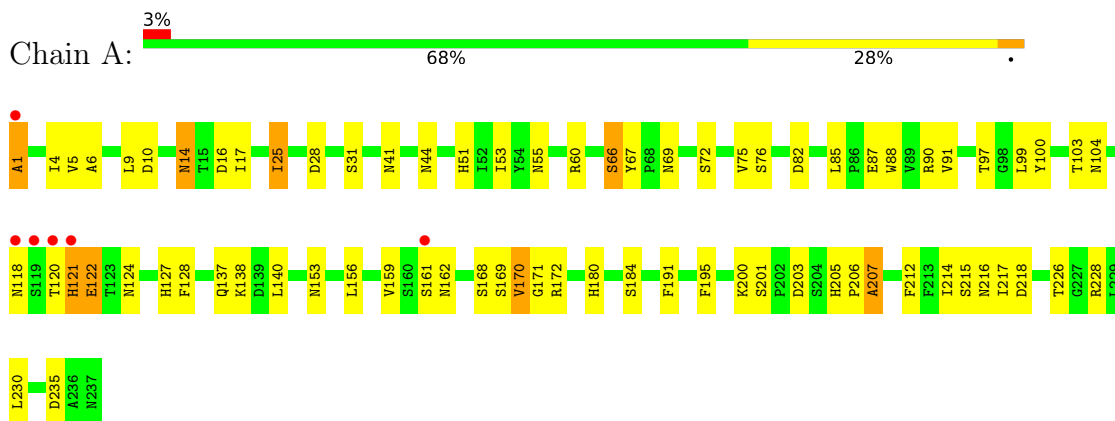
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	148	Total 148	O 148	0	0
6	B	153	Total 153	O 153	0	0
6	C	101	Total 101	O 101	0	0
6	D	131	Total 131	O 131	0	0

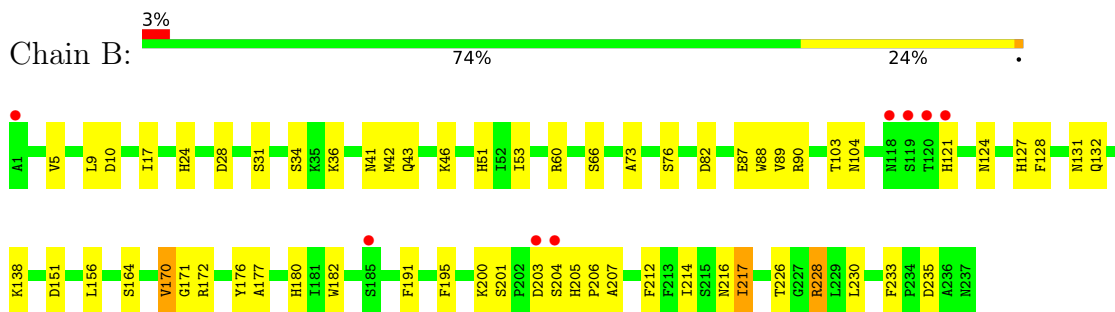
3 Residue-property plots

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.

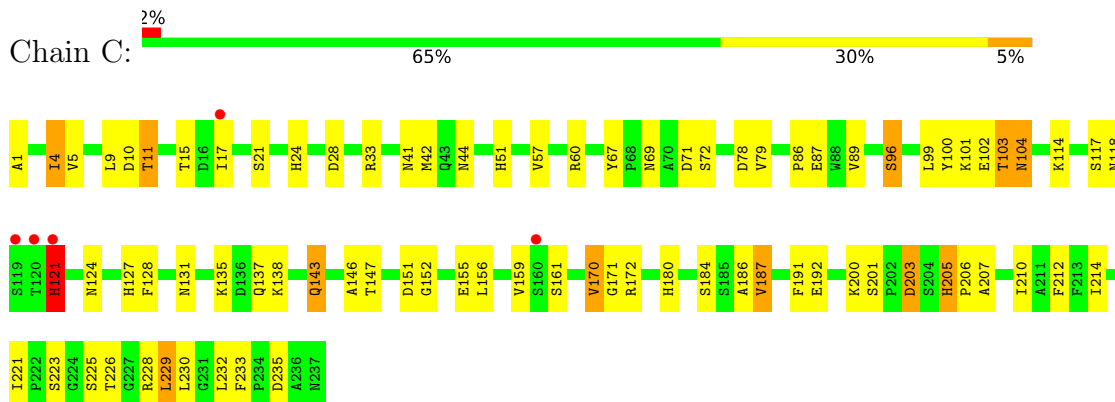
• Molecule 1: CONCAVALIN A



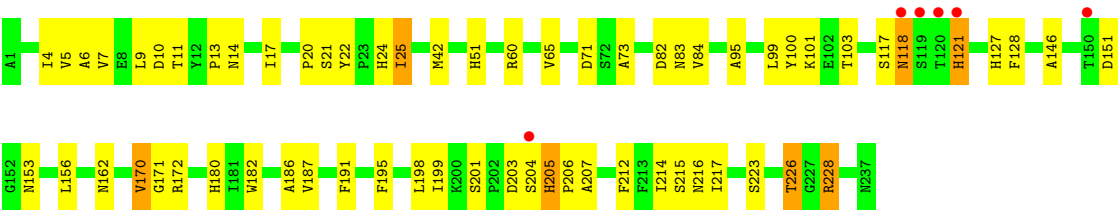
• Molecule 1: CONCAVALIN A



• Molecule 1: CONCAVALIN A



● Molecule 1: CONCAVALIN A



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	123.70Å 128.60Å 67.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.00 8.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.00) 80.4 (8.00-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.67 (at 2.00Å)	Xtriage
Refinement program	X-PLOR 2.1	Depositor
R, R_{free}	0.199 , (Not available) 0.190 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	25.3	Xtriage
Anisotropy	0.339	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 83.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7830	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 26.25 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.7280e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: CA, MN, CL, MMA

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	1.02	10/1851 (0.5%)	1.79	55/2522 (2.2%)
1	B	1.03	9/1851 (0.5%)	1.74	45/2522 (1.8%)
1	C	0.97	8/1851 (0.4%)	1.73	45/2522 (1.8%)
1	D	0.97	7/1851 (0.4%)	1.80	44/2522 (1.7%)
All	All	1.00	34/7404 (0.5%)	1.77	189/10088 (1.9%)

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	127	HIS	CD2-NE2	-7.26	1.29	1.37
1	B	205	HIS	CD2-NE2	-6.98	1.30	1.37
1	C	51	HIS	CD2-NE2	-6.86	1.30	1.37
1	B	180	HIS	CD2-NE2	-6.83	1.30	1.37
1	A	121	HIS	CD2-NE2	-6.78	1.30	1.37
1	C	180	HIS	CD2-NE2	-6.70	1.30	1.37
1	A	180	HIS	CD2-NE2	-6.61	1.30	1.37
1	D	51	HIS	CD2-NE2	-6.60	1.30	1.37
1	D	180	HIS	CD2-NE2	-6.55	1.30	1.37
1	D	205	HIS	CD2-NE2	-6.51	1.30	1.37
1	C	205	HIS	CD2-NE2	-6.42	1.30	1.37
1	C	121	HIS	CD2-NE2	-6.41	1.30	1.37
1	D	121	HIS	CD2-NE2	-6.31	1.30	1.37
1	B	51	HIS	CD2-NE2	-6.24	1.30	1.37
1	C	24	HIS	CD2-NE2	-6.24	1.30	1.37
1	D	24	HIS	CD2-NE2	-6.20	1.31	1.37
1	D	127	HIS	CD2-NE2	-6.09	1.31	1.37
1	B	205	HIS	CG-ND1	-6.08	1.31	1.38
1	B	121	HIS	CD2-NE2	-5.96	1.31	1.37
1	A	51	HIS	CG-ND1	-5.88	1.31	1.38
1	A	205	HIS	CD2-NE2	-5.85	1.31	1.37
1	B	180	HIS	CG-ND1	-5.64	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	180	HIS	CG-ND1	-5.54	1.32	1.38
1	C	24	HIS	CG-ND1	-5.52	1.32	1.38
1	A	51	HIS	CD2-NE2	-5.44	1.31	1.37
1	A	127	HIS	CD2-NE2	-5.42	1.31	1.37
1	C	127	HIS	CD2-NE2	-5.40	1.31	1.37
1	C	79	VAL	CA-CB	5.35	1.61	1.54
1	B	24	HIS	CD2-NE2	-5.33	1.31	1.37
1	A	121	HIS	CG-ND1	-5.21	1.32	1.38
1	B	89	VAL	CA-CB	5.14	1.61	1.54
1	D	24	HIS	CG-ND1	-5.13	1.32	1.38
1	A	205	HIS	CG-ND1	-5.10	1.32	1.38
1	A	91	VAL	CA-CB	5.02	1.61	1.54

All (189) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	82	ASP	CA-CB-CG	12.55	125.15	112.60
1	A	203	ASP	CA-CB-CG	10.62	123.22	112.60
1	D	71	ASP	CA-CB-CG	10.56	123.16	112.60
1	D	128	PHE	CA-CB-CG	9.45	123.25	113.80
1	A	16	ASP	CA-CB-CG	-8.57	104.03	112.60
1	B	176	TYR	N-CA-C	8.55	120.22	111.07
1	A	14	ASN	OD1-CG-ND2	-8.29	114.31	122.60
1	A	51	HIS	ND1-CG-CD2	8.21	114.31	106.10
1	C	128	PHE	CA-CB-CG	8.09	121.89	113.80
1	C	151	ASP	CA-CB-CG	8.05	120.65	112.60
1	C	71	ASP	CA-CB-CG	7.95	120.55	112.60
1	C	87	GLU	CA-CB-CG	7.91	129.92	114.10
1	D	170	VAL	CG1-CB-CG2	-7.77	93.70	110.80
1	A	41	ASN	OD1-CG-ND2	-7.61	114.99	122.60
1	B	5	VAL	N-CA-C	-7.51	96.65	107.77
1	C	4	ILE	N-CA-C	7.49	118.66	108.17
1	B	121	HIS	CA-CB-CG	7.48	121.28	113.80
1	A	124	ASN	OD1-CG-ND2	-7.45	115.15	122.60
1	B	151	ASP	CA-CB-CG	7.43	120.03	112.60
1	B	217	ILE	N-CA-C	7.40	119.06	110.62
1	B	235	ASP	CA-CB-CG	7.39	119.99	112.60
1	D	212	PHE	N-CA-C	-7.24	97.44	109.24
1	C	124	ASN	N-CA-C	-7.23	97.96	109.59
1	A	138	LYS	N-CA-C	7.20	121.16	112.38
1	A	87	GLU	CA-CB-CG	7.19	128.47	114.10
1	A	172	ARG	CB-CG-CD	-7.18	94.78	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	69	ASN	OD1-CG-ND2	-7.18	115.42	122.60
1	D	5	VAL	N-CA-C	-7.17	97.29	107.75
1	C	5	VAL	N-CA-C	-7.09	98.18	108.11
1	A	205	HIS	CA-CB-CG	-7.08	106.72	113.80
1	D	204	SER	N-CA-C	7.02	120.95	112.38
1	C	191	PHE	CA-CB-CG	7.02	120.82	113.80
1	A	195	PHE	CA-CB-CG	6.94	120.74	113.80
1	A	153	ASN	OD1-CG-ND2	-6.92	115.68	122.60
1	B	172	ARG	CB-CG-CD	-6.91	95.41	111.30
1	B	73	ALA	N-CA-C	-6.83	98.59	109.59
1	D	162	ASN	OD1-CG-ND2	-6.80	115.80	122.60
1	D	121	HIS	CB-CG-CD2	-6.73	122.46	131.20
1	D	73	ALA	N-CA-C	-6.72	97.40	108.76
1	D	84	VAL	N-CA-CB	-6.71	106.14	111.64
1	A	99	LEU	N-CA-C	-6.70	104.06	111.36
1	A	44	ASN	OD1-CG-ND2	-6.70	115.90	122.60
1	B	124	ASN	N-CA-C	-6.69	98.50	109.40
1	A	122	GLU	CB-CG-CD	6.65	123.90	112.60
1	D	14	ASN	OD1-CG-ND2	-6.65	115.95	122.60
1	D	195	PHE	CA-CB-CG	6.65	120.45	113.80
1	C	172	ARG	CB-CG-CD	-6.61	96.11	111.30
1	D	83	ASN	OD1-CG-ND2	-6.55	116.05	122.60
1	B	51	HIS	CB-CG-CD2	-6.52	122.72	131.20
1	B	216	ASN	OD1-CG-ND2	-6.51	116.09	122.60
1	D	7	VAL	N-CA-C	-6.51	98.25	107.75
1	B	216	ASN	N-CA-C	-6.49	101.53	110.35
1	C	101	LYS	N-CA-C	6.47	118.36	109.18
1	C	212	PHE	N-CA-C	-6.47	99.16	109.76
1	A	124	ASN	N-CA-C	-6.46	99.19	109.59
1	B	82	ASP	CA-CB-CG	6.43	119.03	112.60
1	C	232	LEU	N-CA-C	6.42	121.52	113.43
1	C	137	GLN	OE1-CD-NE2	-6.39	116.21	122.60
1	B	138	LYS	N-CA-C	6.38	120.33	112.54
1	B	131	ASN	OD1-CG-ND2	-6.38	116.22	122.60
1	B	212	PHE	N-CA-C	-6.34	98.90	109.24
1	A	104	ASN	N-CA-C	-6.30	100.91	109.54
1	B	191	PHE	CA-CB-CG	6.28	120.08	113.80
1	D	121	HIS	N-CA-C	6.25	120.69	113.38
1	C	67	TYR	N-CA-C	-6.21	100.77	110.14
1	A	67	TYR	N-CA-C	-6.20	100.61	110.10
1	B	127	HIS	CB-CG-CD2	-6.20	123.14	131.20
1	D	216	ASN	OD1-CG-ND2	-6.19	116.41	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	195	PHE	CA-CB-CG	6.19	119.99	113.80
1	A	5	VAL	N-CA-C	-6.18	98.72	107.75
1	C	72	SER	N-CA-C	-6.14	99.89	109.72
1	C	159	VAL	N-CA-C	-6.14	99.28	108.12
1	C	214	ILE	N-CA-C	-6.13	99.53	108.11
1	A	41	ASN	CB-CG-ND2	6.11	125.57	116.40
1	D	118	ASN	CA-CB-CG	6.08	118.68	112.60
1	C	138	LYS	N-CA-C	6.07	120.15	112.87
1	B	170	VAL	CG1-CB-CG2	-6.07	97.45	110.80
1	C	152	GLY	N-CA-C	-6.05	106.36	115.32
1	A	90	ARG	N-CA-C	-6.04	99.95	109.50
1	D	103	THR	N-CA-C	-6.04	101.55	110.48
1	A	235	ASP	CA-CB-CG	6.04	118.64	112.60
1	D	9	LEU	N-CA-C	-6.03	95.23	107.41
1	C	57	VAL	N-CA-C	-6.03	104.43	111.00
1	A	10	ASP	CA-CB-CG	6.00	118.60	112.60
1	D	203	ASP	CA-CB-CG	6.00	118.60	112.60
1	C	180	HIS	CB-CG-CD2	-5.99	123.42	131.20
1	A	212	PHE	N-CA-C	-5.97	99.50	109.24
1	A	51	HIS	CG-CD2-NE2	-5.96	101.24	107.20
1	C	9	LEU	N-CA-C	-5.94	97.03	107.73
1	C	69	ASN	OD1-CG-ND2	-5.91	116.69	122.60
1	B	205	HIS	CB-CG-CD2	-5.90	123.53	131.20
1	A	162	ASN	OD1-CG-ND2	-5.89	116.71	122.60
1	B	34	SER	N-CA-C	5.88	119.01	110.42
1	A	6	ALA	N-CA-C	5.87	118.11	109.24
1	C	28	ASP	CA-CB-CG	5.87	118.47	112.60
1	A	207	ALA	O-C-N	-5.85	117.36	123.56
1	B	132	GLN	OE1-CD-NE2	-5.83	116.77	122.60
1	D	216	ASN	CB-CG-ND2	5.81	125.12	116.40
1	D	214	ILE	N-CA-C	-5.81	99.75	108.12
1	A	55	ASN	CA-CB-CG	5.80	118.40	112.60
1	A	118	ASN	OD1-CG-ND2	-5.79	116.81	122.60
1	A	128	PHE	CA-CB-CG	5.78	119.58	113.80
1	B	230	LEU	N-CA-C	5.76	119.62	112.47
1	C	41	ASN	OD1-CG-ND2	-5.72	116.88	122.60
1	A	184	SER	N-CA-C	5.71	117.18	111.07
1	B	124	ASN	OD1-CG-ND2	-5.71	116.89	122.60
1	A	169	SER	N-CA-CB	-5.70	101.73	110.85
1	C	10	ASP	CA-CB-CG	5.69	118.29	112.60
1	B	121	HIS	CB-CG-CD2	-5.68	123.82	131.20
1	B	104	ASN	OD1-CG-ND2	-5.67	116.93	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	9	LEU	N-CA-C	-5.67	95.97	107.41
1	A	216	ASN	OD1-CG-ND2	-5.65	116.95	122.60
1	D	172	ARG	CB-CG-CD	-5.64	98.33	111.30
1	D	22	TYR	CA-C-N	5.63	125.63	119.89
1	D	22	TYR	C-N-CA	5.63	125.63	119.89
1	D	127	HIS	CB-CG-CD2	-5.62	123.89	131.20
1	A	82	ASP	CA-CB-CG	5.62	118.22	112.60
1	D	118	ASN	OD1-CG-ND2	-5.60	117.00	122.60
1	A	103	THR	N-CA-C	-5.56	102.66	110.50
1	D	199	ILE	CA-C-O	5.55	126.47	120.53
1	A	161	SER	N-CA-CB	-5.55	101.68	109.94
1	A	14	ASN	CB-CG-ND2	5.54	124.70	116.40
1	C	127	HIS	CB-CG-CD2	-5.51	124.04	131.20
1	B	10	ASP	N-CA-C	5.49	117.17	108.67
1	C	170	VAL	CG1-CB-CG2	-5.48	98.74	110.80
1	C	103	THR	N-CA-C	-5.48	102.77	110.50
1	A	191	PHE	CA-CB-CG	5.46	119.25	113.80
1	D	205	HIS	CB-CG-CD2	-5.44	124.12	131.20
1	B	90	ARG	N-CA-C	-5.44	100.90	109.50
1	C	143	GLN	CA-C-O	-5.43	114.48	120.24
1	D	10	ASP	CA-CB-CG	5.42	118.02	112.60
1	B	121	HIS	N-CA-CB	-5.41	104.02	112.41
1	D	25	ILE	N-CA-C	-5.40	100.68	108.89
1	A	1	ALA	N-CA-C	-5.39	95.91	111.00
1	D	191	PHE	CA-CB-CG	5.39	119.19	113.80
1	D	146	ALA	N-CA-C	5.39	118.25	110.28
1	A	85	LEU	CA-C-N	5.38	125.68	119.92
1	A	85	LEU	C-N-CA	5.38	125.68	119.92
1	C	203	ASP	CA-CB-CG	5.36	117.96	112.60
1	C	124	ASN	OD1-CG-ND2	-5.35	117.25	122.60
1	C	229	LEU	N-CA-C	5.34	119.78	113.16
1	A	97	THR	O-C-N	-5.32	116.25	122.96
1	B	103	THR	N-CA-C	-5.32	102.60	110.48
1	A	168	SER	N-CA-C	5.32	118.78	111.54
1	D	180	HIS	CB-CG-CD2	-5.32	124.29	131.20
1	B	214	ILE	N-CA-C	-5.31	100.48	108.12
1	C	235	ASP	CA-CB-CG	5.31	117.91	112.60
1	D	83	ASN	N-CA-C	-5.31	106.85	113.38
1	C	180	HIS	CB-CG-ND1	5.30	130.65	122.70
1	C	210	ILE	O-C-N	-5.28	117.49	123.03
1	D	153	ASN	OD1-CG-ND2	-5.27	117.33	122.60
1	B	216	ASN	CB-CG-ND2	5.26	124.30	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	87	GLU	CA-CB-CG	5.26	124.63	114.10
1	C	96	SER	N-CA-C	5.25	116.12	108.14
1	A	230	LEU	N-CA-C	5.25	118.97	112.47
1	C	69	ASN	CB-CG-ND2	5.24	124.26	116.40
1	B	128	PHE	CA-CB-CG	5.24	119.04	113.80
1	C	131	ASN	CA-CB-CG	-5.24	107.36	112.60
1	B	207	ALA	O-C-N	-5.21	117.64	123.48
1	D	99	LEU	N-CA-C	-5.21	105.68	111.36
1	D	207	ALA	O-C-N	-5.21	118.04	123.56
1	A	9	LEU	N-CA-C	-5.21	96.25	107.49
1	B	10	ASP	CA-CB-CG	5.20	117.80	112.60
1	D	6	ALA	N-CA-C	5.19	117.07	109.24
1	B	41	ASN	OD1-CG-ND2	-5.17	117.43	122.60
1	C	104	ASN	OD1-CG-ND2	-5.17	117.43	122.60
1	A	25	ILE	CG1-CB-CG2	-5.17	95.20	110.70
1	D	217	ILE	N-CA-C	5.16	120.08	109.34
1	B	164	SER	N-CA-C	5.15	116.16	109.72
1	B	182	TRP	CA-CB-CG	5.14	123.37	113.60
1	C	187	VAL	N-CA-C	-5.14	105.40	111.00
1	A	170	VAL	CB-CA-C	-5.14	101.80	111.30
1	C	11	THR	N-CA-C	5.14	119.60	113.23
1	D	187	VAL	N-CA-C	-5.12	105.42	111.00
1	B	177	ALA	CA-C-N	5.11	125.04	119.78
1	B	177	ALA	C-N-CA	5.11	125.04	119.78
1	B	233	PHE	CA-C-N	5.11	124.42	118.85
1	B	233	PHE	C-N-CA	5.11	124.42	118.85
1	A	172	ARG	NE-CZ-NH2	-5.10	114.61	119.20
1	C	207	ALA	O-C-N	-5.08	117.80	123.48
1	A	218	ASP	CA-CB-CG	5.06	117.66	112.60
1	A	66	SER	N-CA-C	5.05	116.75	109.07
1	A	214	ILE	N-CA-C	-5.04	100.86	108.12
1	C	99	LEU	N-CA-C	-5.04	105.86	111.36
1	D	182	TRP	CG-CD2-CE3	5.04	138.94	133.90
1	A	69	ASN	CB-CG-ND2	5.03	123.94	116.40
1	C	121	HIS	CB-CG-CD2	-5.03	124.66	131.20
1	A	159	VAL	N-CA-C	-5.02	100.30	107.78
1	D	182	TRP	CE2-CD2-CG	-5.02	101.17	107.20

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	1809	0	1755	16	0
1	B	1809	0	1755	14	0
1	C	1809	0	1755	26	0
1	D	1809	0	1755	15	0
2	A	13	0	14	0	0
2	B	13	0	14	1	0
2	C	13	0	14	0	0
2	D	13	0	14	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	1	0	0	0	0
6	A	148	0	0	3	0
6	B	153	0	0	1	0
6	C	101	0	0	2	0
6	D	131	0	0	0	0
All	All	7830	0	7076	69	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 5.

All (69) 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:170:VAL:HG23	1:B:226:THR:HG22	1.73	0.71
1:B:43:GLN:HE21	1:B:46:LYS:HG3	1.57	0.70
1:A:17:ILE:HD13	1:A:228:ARG:HD3	1.75	0.68
1:C:117:SER:HA	1:C:186:ALA:HA	1.77	0.65
1:D:117:SER:HA	1:D:186:ALA:HA	1.78	0.64
1:C:170:VAL:HG12	1:C:221:ILE:HD13	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:SER:HB2	1:A:206:PRO:HB3	1.80	0.63
1:A:14:ASN:HA	6:A:303:HOH:O	1.99	0.60
1:B:201:SER:HB2	1:B:206:PRO:HB3	1.82	0.59
1:C:96:SER:OG	1:C:230:LEU:HA	2.02	0.59
1:C:201:SER:HB2	1:C:206:PRO:HB3	1.84	0.59
1:A:170:VAL:HG23	1:A:226:THR:HG22	1.86	0.58
1:D:4:ILE:HD13	1:D:215:SER:HB3	1.84	0.58
1:B:36:LYS:HD2	1:B:76:SER:O	2.05	0.57
1:D:201:SER:HB2	1:D:206:PRO:HB3	1.85	0.56
1:B:60:ARG:HD3	1:B:76:SER:HB3	1.90	0.53
1:B:66:SER:HA	6:B:336:HOH:O	2.08	0.53
1:B:17:ILE:HD13	1:B:228:ARG:HD3	1.90	0.52
1:C:170:VAL:CG2	1:C:226:THR:HA	2.40	0.51
1:D:13:PRO:HB3	1:D:20:PRO:O	2.11	0.51
1:A:60:ARG:HD3	1:A:76:SER:HB3	1.93	0.49
1:C:143:GLN:O	1:C:221:ILE:HD11	2.12	0.49
1:C:102:GLU:HG3	1:C:104:ASN:ND2	2.27	0.48
1:D:170:VAL:CG2	1:D:226:THR:HA	2.42	0.48
1:B:88:TRP:HB3	1:B:217:ILE:HD11	1.94	0.48
1:C:96:SER:HB3	1:C:170:VAL:HG22	1.96	0.48
1:A:66:SER:HB3	1:A:72:SER:HB3	1.95	0.47
1:D:170:VAL:HG23	1:D:226:THR:HG22	1.95	0.47
1:A:28:ASP:HB3	1:A:31:SER:O	2.14	0.47
1:C:11:THR:HG22	1:C:42:MET:HG3	1.96	0.47
1:A:1:ALA:HB1	6:A:296:HOH:O	2.15	0.47
1:A:60:ARG:NH2	1:C:60:ARG:HH21	2.13	0.47
1:B:42:MET:HB3	1:B:42:MET:HE3	1.67	0.46
1:D:170:VAL:HG23	1:D:226:THR:HA	1.97	0.46
1:A:100:TYR:HB2	1:A:207:ALA:HB3	1.98	0.46
1:C:118:ASN:HA	1:C:187:VAL:HG23	1.97	0.46
1:C:17:ILE:HG22	1:C:33:ARG:NH2	2.30	0.46
1:D:11:THR:HG22	1:D:42:MET:HG3	1.97	0.46
1:A:156:LEU:O	1:A:171:GLY:HA3	2.15	0.46
1:D:17:ILE:HD13	1:D:228:ARG:HD3	1.97	0.46
1:C:114:LYS:HE3	1:C:114:LYS:HB2	1.59	0.45
1:C:100:TYR:HB3	1:C:205:HIS:O	2.16	0.45
1:C:156:LEU:O	1:C:171:GLY:HA3	2.17	0.45
1:A:228:ARG:HD2	6:A:288:HOH:O	2.16	0.45
1:D:156:LEU:O	1:D:171:GLY:HA3	2.16	0.45
1:A:4:ILE:HD13	1:A:215:SER:HB3	2.00	0.44
1:C:86:PRO:HG2	1:C:89:VAL:HG12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:ILE:HG22	1:A:75:VAL:HG11	2.00	0.44
1:B:28:ASP:HB3	1:B:31:SER:O	2.17	0.44
1:A:88:TRP:HB3	1:A:217:ILE:HD11	2.00	0.43
1:B:156:LEU:O	1:B:171:GLY:HA3	2.18	0.43
1:C:225:SER:HB3	1:C:233:PHE:O	2.18	0.43
1:C:1:ALA:N	6:C:278:HOH:O	2.52	0.43
1:B:228:ARG:HG2	2:B:238:MMA:O3	2.18	0.43
1:C:170:VAL:HG23	1:C:226:THR:HG22	2.00	0.43
1:B:60:ARG:NH2	1:D:60:ARG:HH21	2.17	0.43
1:C:118:ASN:HA	1:C:187:VAL:CG2	2.49	0.42
1:C:78:ASP:HB3	6:C:289:HOH:O	2.20	0.42
1:B:200:LYS:HB3	1:B:200:LYS:HE2	1.77	0.42
1:A:137:GLN:HG2	1:A:140:LEU:HD12	2.01	0.41
1:C:225:SER:HA	1:C:229:LEU:HD12	2.03	0.41
1:C:170:VAL:HG21	1:C:226:THR:HA	2.03	0.41
1:C:42:MET:HE1	1:C:44:ASN:HB2	2.03	0.40
1:D:95:ALA:HB3	1:D:156:LEU:HB3	2.03	0.40
1:C:146:ALA:HA	1:C:155:GLU:O	2.21	0.40
1:D:100:TYR:CD1	1:D:205:HIS:HB2	2.56	0.40
1:D:25:ILE:HG21	1:D:65:VAL:HG21	2.03	0.40
1:C:103:THR:OG1	1:C:200:LYS:HG2	2.21	0.40
1:D:228:ARG:HG2	2:D:238:MMA:O3	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	235/237 (99%)	221 (94%)	12 (5%)	2 (1%)	14	9
1	B	235/237 (99%)	222 (94%)	11 (5%)	2 (1%)	14	9
1	C	235/237 (99%)	216 (92%)	17 (7%)	2 (1%)	14	9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	235/237 (99%)	219 (93%)	15 (6%)	1 (0%)	30	27
All	All	940/948 (99%)	878 (93%)	55 (6%)	7 (1%)	18	14

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	120	THR
1	C	121	HIS
1	A	121	HIS
1	B	204	SER
1	D	21	SER
1	B	203	ASP
1	C	21	SER

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%)	200 (98%)	3 (2%)	57	64
1	B	203/203 (100%)	201 (99%)	2 (1%)	68	75
1	C	203/203 (100%)	192 (95%)	11 (5%)	20	17
1	D	203/203 (100%)	195 (96%)	8 (4%)	28	28
All	All	812/812 (100%)	788 (97%)	24 (3%)	36	38

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	ILE
1	A	122	GLU
1	A	200	LYS
1	B	53	ILE
1	B	228	ARG
1	C	4	ILE
1	C	15	THR

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Mol	Chain	Res	Type
1	C	121	HIS
1	C	135	LYS
1	C	147	THR
1	C	161	SER
1	C	184	SER
1	C	192	GLU
1	C	203	ASP
1	C	223	SER
1	C	228	ARG
1	D	101	LYS
1	D	118	ASN
1	D	121	HIS
1	D	151	ASP
1	D	198	LEU
1	D	223	SER
1	D	226	THR
1	D	228	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	118	ASN
1	A	153	ASN
1	A	237	ASN
1	B	43	GLN
1	B	153	ASN
1	B	237	ASN
1	C	43	GLN
1	D	43	GLN
1	D	118	ASN
1	D	132	GLN
1	D	153	ASN
1	D	237	ASN

5.3.3 RNA ⓘ

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 13 ligands modelled in this entry, 9 are monoatomic - leaving 4 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	MMA	D	238	-	13,13,13	1.14	1 (7%)	18,18,18	1.36	3 (16%)
2	MMA	A	238	-	13,13,13	1.23	1 (7%)	18,18,18	1.02	1 (5%)
2	MMA	B	238	-	13,13,13	0.67	0	18,18,18	1.01	2 (11%)
2	MMA	C	238	-	13,13,13	1.23	1 (7%)	18,18,18	0.99	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	MMA	D	238	-	-	0/4/24/24	0/1/1/1
2	MMA	A	238	-	-	2/4/24/24	0/1/1/1
2	MMA	B	238	-	-	0/4/24/24	0/1/1/1
2	MMA	C	238	-	-	0/4/24/24	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	238	MMA	O1-C1	3.23	1.45	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	238	MMA	O1-C1	3.10	1.45	1.40
2	A	238	MMA	O1-C1	2.80	1.44	1.40

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	238	MMA	O4-C4-C3	-3.12	103.03	110.38
2	D	238	MMA	O1-C1-C2	2.72	111.28	108.14
2	D	238	MMA	C6-C5-C4	-2.43	107.05	113.02
2	B	238	MMA	O4-C4-C3	-2.38	104.76	110.38
2	A	238	MMA	O4-C4-C3	-2.25	105.07	110.38
2	B	238	MMA	C6-C5-C4	-2.21	107.60	113.02

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	238	MMA	O5-C5-C6-O6
2	A	238	MMA	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	238	MMA	1	0
2	B	238	MMA	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 ⓘ

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%)	-0.54	6 (2%) 58 58	12, 22, 61, 93	0
1	B	237/237 (100%)	-0.48	8 (3%) 48 47	11, 23, 60, 85	0
1	C	237/237 (100%)	0.03	5 (2%) 63 63	16, 39, 70, 99	0
1	D	237/237 (100%)	-0.49	6 (2%) 58 58	14, 26, 66, 97	0
All	All	948/948 (100%)	-0.37	25 (2%) 57 56	11, 27, 67, 99	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	120	THR	5.3
1	B	120	THR	5.1
1	B	204	SER	4.9
1	D	120	THR	3.7
1	B	119	SER	3.4
1	C	121	HIS	3.4
1	A	120	THR	3.4
1	A	119	SER	3.0
1	D	150	THR	2.8
1	D	121	HIS	2.8
1	A	121	HIS	2.7
1	B	185	SER	2.7
1	B	203	ASP	2.7
1	A	118	ASN	2.6
1	C	160	SER	2.6
1	B	121	HIS	2.5
1	A	1	ALA	2.3
1	B	1	ALA	2.3
1	B	118	ASN	2.3
1	D	204	SER	2.3
1	D	118	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	119	SER	2.2
1	D	119	SER	2.2
1	C	17	ILE	2.1
1	A	161	SER	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	MMA	C	238	13/13	0.83	0.10	45,51,57,59	0
4	CA	C	240	1/1	0.91	0.04	39,39,39,39	0
3	MN	C	239	1/1	0.92	0.06	41,41,41,41	0
5	CL	A	241	1/1	0.93	0.04	32,32,32,32	0
2	MMA	D	238	13/13	0.96	0.06	22,30,36,36	0
2	MMA	B	238	13/13	0.96	0.06	16,23,28,28	0
2	MMA	A	238	13/13	0.97	0.05	16,19,23,25	0
3	MN	D	239	1/1	0.97	0.06	26,26,26,26	0
3	MN	B	239	1/1	0.98	0.02	18,18,18,18	0
4	CA	A	240	1/1	0.99	0.01	14,14,14,14	0
4	CA	D	240	1/1	0.99	0.02	23,23,23,23	0
4	CA	B	240	1/1	0.99	0.04	19,19,19,19	0
3	MN	A	239	1/1	1.00	0.04	19,19,19,19	0

6.5 Other polymers [i](#)

There are no such residues in this entry.