



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 21, 2017 – 03:16 PM EST

PDB ID : 2LAL  
Title : CRYSTAL STRUCTURE DETERMINATION AND REFINEMENT AT 2.3  
ANGSTROMS RESOLUTION OF THE LENTIL LECTIN  
Authors : Loris, R.; Steyaert, J.; Maes, D.; Lisgarten, J.; Pickersgill, R.; Wyns, L.  
Deposited on : unknown  
Resolution : 1.80 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

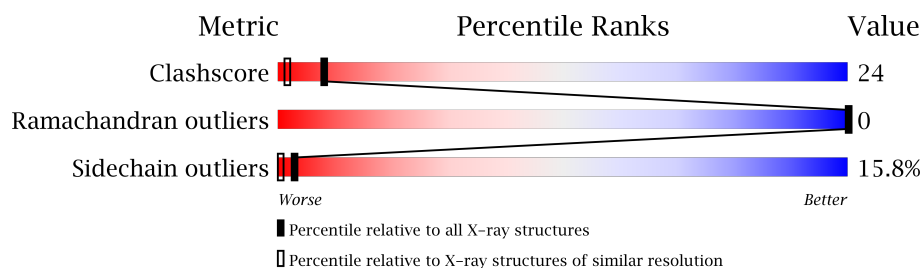
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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	112137	5742 (1.80-1.80)
Ramachandran outliers	110173	5676 (1.80-1.80)
Sidechain outliers	110143	5675 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	181	 50% 36% 12% •
1	C	181	 50% 40% 8% •
2	B	52	 48% 33% 8% • 10%
2	D	52	 48% 31% 12% 10%

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 3779 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 LENTIL LECTIN (ALPHA CHAIN).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	181	Total	C	N	O	0	0	0
			1409	898	232	279			
1	C	181	Total	C	N	O	0	0	0
			1409	898	232	279			

- Molecule 2 is a protein called LENTIL LECTIN (BETA CHAIN).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	47	Total	C	N	O	0	0	0
			366	236	59	71			
2	D	47	Total	C	N	O	0	0	0
			366	236	59	71			

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O P 5 4 1	0	0
3	C	1	Total O P 5 4 1	0	0

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 6 is water.

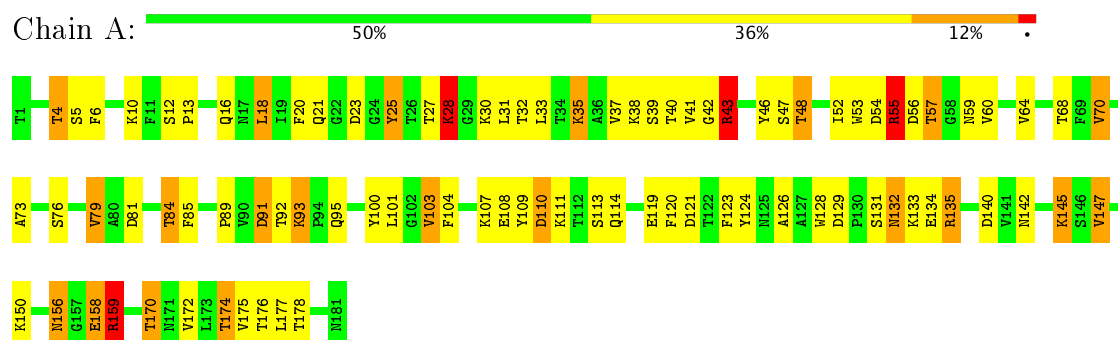
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	98	Total O 98 98	0	0
6	B	15	Total O 15 15	0	0
6	C	88	Total O 88 88	0	0
6	D	14	Total O 14 14	0	0

### 3 Residue-property plots

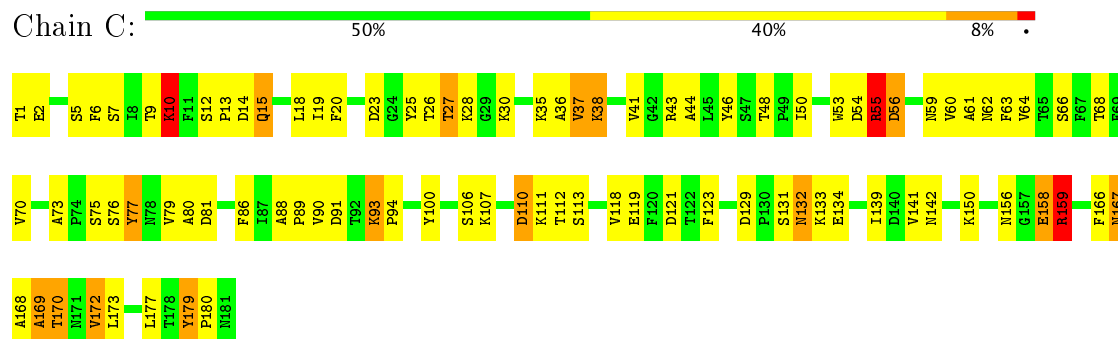
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

Note EDS was not executed.

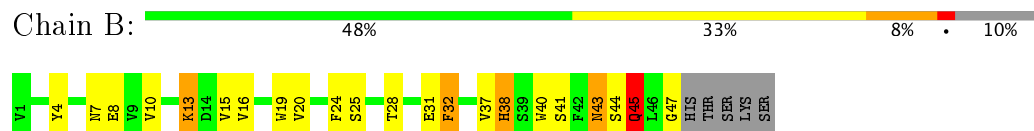
#### • Molecule 1: LENTIL LECTIN (ALPHA CHAIN)

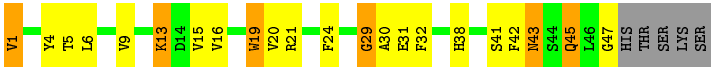


#### • Molecule 1: LENTIL LECTIN (ALPHA CHAIN)



#### • Molecule 2: LENTIL LECTIN (BETA CHAIN)





## 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, $\alpha$ , $\beta$ , $\gamma$	75.81Å 125.47Å 56.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 1.80	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-1.80)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	RESTRAIN	Depositor
R, $R_{free}$	0.189 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3779	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	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: CA, MN, PO4

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	1.19	1/1443 (0.1%)	1.90	40/1970 (2.0%)
1	C	1.15	0/1443	1.91	48/1970 (2.4%)
2	B	1.19	2/376 (0.5%)	1.96	13/515 (2.5%)
2	D	1.30	5/376 (1.3%)	2.12	17/515 (3.3%)
All	All	1.19	8/3638 (0.2%)	1.93	118/4970 (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	5
1	C	0	6
All	All	0	11

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	41	SER	CB-OG	-6.84	1.33	1.42
2	B	45	GLN	CD-OE1	6.00	1.37	1.24
2	D	45	GLN	CD-OE1	5.93	1.36	1.24
2	D	29	GLY	N-CA	5.49	1.54	1.46
2	D	19	TRP	NE1-CE2	-5.41	1.30	1.37
1	A	95	GLN	CD-OE1	5.11	1.35	1.24
2	D	43	ASN	CG-OD1	5.11	1.35	1.24
2	B	43	ASN	CG-OD1	5.09	1.35	1.24

All (118) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	21	ARG	NE-CZ-NH1	14.34	127.47	120.30
2	D	21	ARG	NE-CZ-NH2	-12.88	113.86	120.30
1	A	46	TYR	CB-CG-CD2	-10.33	114.80	121.00
1	C	121	ASP	CB-CG-OD1	10.26	127.53	118.30
1	C	159	ARG	CD-NE-CZ	-10.10	109.46	123.60
1	C	123	PHE	CG-CD1-CE1	-9.89	109.92	120.80
1	A	100	TYR	CB-CG-CD2	-9.58	115.25	121.00
1	A	135	ARG	NE-CZ-NH2	9.42	125.01	120.30
2	D	20	VAL	CA-CB-CG2	9.04	124.47	110.90
1	A	119	GLU	OE1-CD-OE2	-9.00	112.50	123.30
1	C	79	VAL	CA-CB-CG2	8.94	124.31	110.90
1	A	109	TYR	CB-CG-CD2	-8.89	115.67	121.00
2	B	16	VAL	CA-CB-CG2	8.77	124.06	110.90
1	A	110	ASP	CB-CG-OD1	-8.72	110.45	118.30
2	D	4	TYR	CB-CG-CD2	-8.70	115.78	121.00
1	A	41	VAL	CA-CB-CG2	8.66	123.90	110.90
1	C	90	VAL	CA-CB-CG1	8.62	123.84	110.90
1	C	55	ARG	C-N-CA	8.41	142.72	121.70
1	C	25	TYR	CB-CG-CD2	-8.37	115.98	121.00
1	A	121	ASP	CB-CG-OD1	8.34	125.81	118.30
1	A	79	VAL	CA-CB-CG2	8.21	123.21	110.90
1	C	46	TYR	CB-CG-CD2	-8.20	116.08	121.00
1	A	55	ARG	NE-CZ-NH1	-7.89	116.35	120.30
1	A	43	ARG	NE-CZ-NH1	7.89	124.25	120.30
1	A	103	VAL	CA-CB-CG2	7.85	122.67	110.90
1	C	63	PHE	CB-CG-CD1	7.82	126.27	120.80
2	B	20	VAL	CA-CB-CG2	7.79	122.58	110.90
1	A	25	TYR	CB-CG-CD2	-7.74	116.36	121.00
2	D	4	TYR	CG-CD2-CE2	-7.69	115.15	121.30
1	A	100	TYR	CB-CG-CD1	7.63	125.58	121.00
1	A	18	LEU	CB-CG-CD1	7.59	123.91	111.00
2	B	10	VAL	CA-CB-CG2	7.55	122.22	110.90
1	A	108	GLU	OE1-CD-OE2	-7.29	114.56	123.30
2	B	19	TRP	CH2-CZ2-CE2	7.27	124.67	117.40
1	C	100	TYR	CB-CG-CD2	-7.21	116.67	121.00
1	C	37	VAL	CA-CB-CG2	7.20	121.70	110.90
1	A	147	VAL	CA-CB-CG2	7.15	121.62	110.90
1	A	28	LYS	C-N-CA	-7.04	107.52	122.30
2	B	31	GLU	OE1-CD-OE2	-7.00	114.90	123.30
1	A	123	PHE	CB-CG-CD2	-7.00	115.90	120.80
1	C	179	TYR	CB-CG-CD2	-6.99	116.81	121.00
1	A	37	VAL	CA-CB-CG1	6.90	121.25	110.90
1	C	18	LEU	CB-CG-CD1	6.87	122.68	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	175	VAL	CA-CB-CG2	6.87	121.20	110.90
2	D	1	VAL	CA-CB-CG1	6.87	121.20	110.90
2	B	4	TYR	CG-CD2-CE2	-6.81	115.85	121.30
1	C	23	ASP	CB-CG-OD2	6.73	124.35	118.30
1	C	25	TYR	CB-CG-CD1	6.73	125.03	121.00
2	D	24	PHE	CB-CG-CD2	-6.65	116.14	120.80
1	C	26	THR	C-N-CA	6.63	138.27	121.70
2	B	47	GLY	CA-C-O	6.56	132.40	120.60
1	A	123	PHE	CG-CD1-CE1	-6.51	113.64	120.80
1	C	123	PHE	CZ-CE2-CD2	-6.38	112.45	120.10
2	D	16	VAL	CA-CB-CG2	6.37	120.46	110.90
1	A	25	TYR	CB-CG-CD1	6.37	124.82	121.00
1	C	63	PHE	CB-CG-CD2	-6.30	116.39	120.80
1	C	129	ASP	CB-CG-OD1	-6.14	112.77	118.30
1	C	123	PHE	CD1-CE1-CZ	6.14	127.47	120.10
2	D	9	VAL	CA-C-O	-6.13	107.23	120.10
2	B	4	TYR	CB-CG-CD2	-6.12	117.33	121.00
1	C	159	ARG	NE-CZ-NH1	-6.11	117.24	120.30
1	C	64	VAL	CA-CB-CG1	6.10	120.05	110.90
1	C	14	ASP	CB-CG-OD1	6.09	123.78	118.30
2	D	47	GLY	CA-C-O	6.05	131.50	120.60
1	C	46	TYR	CG-CD2-CE2	-6.02	116.48	121.30
1	A	85	PHE	CB-CG-CD2	-6.01	116.59	120.80
2	D	15	VAL	CA-CB-CG2	6.00	119.90	110.90
1	C	15	GLN	CB-CG-CD	6.00	127.19	111.60
1	C	123	PHE	CB-CG-CD2	-6.00	116.60	120.80
1	A	123	PHE	CD1-CG-CD2	5.95	126.04	118.30
1	C	123	PHE	CD1-CG-CD2	5.92	125.99	118.30
1	C	129	ASP	CB-CG-OD2	5.91	123.62	118.30
1	C	41	VAL	CA-CB-CG2	5.88	119.73	110.90
1	C	119	GLU	OE1-CD-OE2	-5.87	116.25	123.30
1	A	175	VAL	O-C-N	-5.77	113.47	122.70
1	C	77	TYR	CB-CG-CD1	-5.77	117.54	121.00
2	B	40	TRP	CB-CG-CD2	-5.75	119.12	126.60
2	B	32	PHE	CB-CG-CD1	-5.74	116.78	120.80
1	A	140	ASP	CB-CG-OD2	-5.72	113.15	118.30
1	C	37	VAL	C-N-CA	-5.71	107.42	121.70
1	C	46	TYR	CD1-CG-CD2	5.68	124.15	117.90
1	A	159	ARG	CD-NE-CZ	-5.63	115.72	123.60
1	A	55	ARG	NE-CZ-NH2	5.60	123.10	120.30
1	C	158	GLU	OE1-CD-OE2	-5.60	116.58	123.30
2	D	4	TYR	CD1-CG-CD2	5.58	124.04	117.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	139	ILE	CB-CG1-CD1	5.58	129.51	113.90
1	A	110	ASP	CB-CG-OD2	5.55	123.30	118.30
1	A	121	ASP	OD1-CG-OD2	-5.54	112.77	123.30
1	C	118	VAL	CG1-CB-CG2	-5.53	102.05	110.90
1	C	10	LYS	O-C-N	5.51	131.52	122.70
2	B	40	TRP	CH2-CZ2-CE2	5.49	122.89	117.40
1	A	101	LEU	CB-CG-CD2	5.48	120.32	111.00
1	A	64	VAL	CA-CB-CG2	5.48	119.12	110.90
2	D	4	TYR	CD1-CE1-CZ	-5.48	114.87	119.80
1	A	159	ARG	CA-CB-CG	-5.46	101.38	113.40
1	C	81	ASP	CB-CG-OD2	5.42	123.18	118.30
1	C	86	PHE	CG-CD2-CE2	5.42	126.76	120.80
2	B	38	HIS	CA-CB-CG	-5.39	104.44	113.60
1	C	25	TYR	CZ-CE2-CD2	5.38	124.64	119.80
1	A	70	VAL	CA-CB-CG1	5.36	118.94	110.90
1	C	77	TYR	CB-CG-CD2	5.34	124.21	121.00
1	C	100	TYR	CG-CD1-CE1	-5.34	117.03	121.30
1	C	141	VAL	C-N-CA	5.34	135.05	121.70
1	C	60	VAL	CG1-CB-CG2	-5.30	102.42	110.90
1	A	129	ASP	CB-CG-OD2	5.28	123.06	118.30
1	C	20	PHE	CB-CG-CD2	-5.22	117.14	120.80
1	A	108	GLU	CG-CD-OE1	5.20	128.69	118.30
1	C	179	TYR	CG-CD2-CE2	-5.17	117.16	121.30
2	D	42	PHE	C-N-CA	5.17	134.62	121.70
1	A	158	GLU	OE1-CD-OE2	-5.17	117.10	123.30
1	A	55	ARG	CD-NE-CZ	-5.16	116.38	123.60
1	C	110	ASP	CB-CG-OD2	5.13	122.92	118.30
2	D	29	GLY	N-CA-C	-5.13	100.28	113.10
2	D	21	ARG	C-N-CA	5.12	134.50	121.70
1	C	36	ALA	C-N-CA	5.12	134.49	121.70
2	B	15	VAL	CA-CB-CG2	5.05	118.48	110.90
1	A	55	ARG	C-N-CA	5.04	134.31	121.70
2	D	6	LEU	C-N-CA	5.02	134.26	121.70

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	120	PHE	Mainchain
1	A	135	ARG	Sidechain
1	A	159	ARG	Sidechain
1	A	43	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	84	THR	Peptide
1	C	159	ARG	Sidechain
1	C	169	ALA	Peptide
1	C	27	THR	Peptide
1	C	43	ARG	Sidechain
1	C	55	ARG	Sidechain
1	C	61	ALA	Peptide

## 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	1363	70	0
1	C	1409	0	1361	78	0
2	B	366	0	350	21	0
2	D	366	0	350	20	0
3	A	5	0	0	0	0
3	C	5	0	0	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	98	0	0	4	0
6	B	15	0	0	0	0
6	C	88	0	0	4	0
6	D	14	0	0	0	0
All	All	3779	0	3424	165	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 24.

All (165) 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:73:ALA:H	1:C:156:ASN:HD21	0.98	0.97
2:B:13:LYS:NZ	2:B:13:LYS:HB2	1.77	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:167:ASN:HD21	1:C:169:ALA:HB3	1.26	0.96
1:C:27:THR:HG22	1:C:28:LYS:HB2	1.50	0.94
1:A:73:ALA:H	1:A:156:ASN:HD21	1.15	0.93
1:C:10:LYS:HG3	1:C:10:LYS:O	1.67	0.93
1:A:170:THR:HG23	1:A:172:VAL:HG23	1.50	0.92
1:C:35:LYS:HB2	1:C:37:VAL:HG23	1.50	0.92
1:C:53:TRP:CE3	2:D:13:LYS:HD3	2.07	0.89
2:B:13:LYS:HZ2	2:B:13:LYS:HB2	1.34	0.88
1:C:38:LYS:HE2	2:D:30:ALA:HA	1.54	0.87
1:C:27:THR:CG2	1:C:28:LYS:HD2	2.05	0.86
1:C:170:THR:HG23	1:C:172:VAL:HB	1.59	0.83
2:B:13:LYS:NZ	2:B:13:LYS:CB	2.41	0.82
1:A:132:ASN:HD22	1:A:134:GLU:H	1.26	0.79
1:A:132:ASN:ND2	1:A:134:GLU:HG2	1.99	0.78
1:C:132:ASN:ND2	1:C:134:GLU:H	1.82	0.77
1:C:132:ASN:HD22	1:C:134:GLU:H	1.32	0.77
1:A:91:ASP:HB2	6:A:240:HOH:O	1.85	0.75
1:A:128:TRP:HB2	1:A:145:LYS:HG2	1.70	0.73
1:A:21:GLN:HE22	1:A:43:ARG:HH21	1.36	0.73
1:A:35:LYS:HB3	1:A:35:LYS:NZ	2.04	0.72
1:C:27:THR:HG22	1:C:28:LYS:HD2	1.71	0.72
1:C:167:ASN:HD22	1:C:167:ASN:C	1.92	0.72
1:C:38:LYS:HB2	2:D:29:GLY:O	1.90	0.72
1:C:59:ASN:OD1	1:C:59:ASN:N	2.22	0.71
1:A:73:ALA:H	1:A:156:ASN:ND2	1.91	0.69
1:A:27:THR:O	1:A:27:THR:HG23	1.94	0.68
2:B:13:LYS:CB	2:B:13:LYS:HZ3	2.05	0.68
1:A:28:LYS:HB2	1:A:28:LYS:NZ	2.04	0.68
1:C:38:LYS:HB3	2:D:32:PHE:CD2	2.29	0.68
1:A:60:VAL:CG2	2:B:13:LYS:HE3	2.24	0.67
1:C:38:LYS:HE2	2:D:30:ALA:CA	2.23	0.67
1:A:170:THR:HG23	1:A:172:VAL:CG2	2.22	0.66
1:C:62:ASN:ND2	1:C:168:ALA:H	1.94	0.66
1:C:132:ASN:CG	1:C:134:GLU:HG3	2.16	0.65
1:A:27:THR:O	1:A:27:THR:CG2	2.45	0.65
1:C:170:THR:CG2	1:C:172:VAL:HB	2.27	0.65
1:C:167:ASN:ND2	1:C:169:ALA:HB3	2.05	0.64
1:A:177:LEU:C	1:A:177:LEU:HD23	2.19	0.64
1:C:38:LYS:HB3	2:D:32:PHE:HD2	1.63	0.64
1:A:132:ASN:ND2	1:A:134:GLU:H	1.93	0.63
1:A:35:LYS:HG3	6:A:223:HOH:O	1.96	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:80:ALA:HB3	2:D:31:GLU:O	1.99	0.63
1:C:73:ALA:H	1:C:156:ASN:ND2	1.83	0.62
2:B:38:HIS:CD2	2:B:38:HIS:N	2.66	0.62
1:C:93:LYS:HG2	6:C:248:HOH:O	1.99	0.62
1:A:53:TRP:CD2	2:B:13:LYS:HG2	2.35	0.61
1:C:73:ALA:N	1:C:156:ASN:HD21	1.83	0.61
1:C:53:TRP:CZ3	2:D:13:LYS:HD3	2.35	0.61
1:C:62:ASN:HD22	1:C:168:ALA:H	1.49	0.60
1:A:70:VAL:CG2	1:A:159:ARG:HG2	2.32	0.59
2:D:1:VAL:O	2:D:1:VAL:HG23	2.02	0.59
1:A:55:ARG:HH11	1:A:55:ARG:CG	2.15	0.59
1:A:4:THR:HG22	1:A:4:THR:O	2.01	0.58
1:C:93:LYS:HB2	1:C:94:PRO:CD	2.34	0.58
1:A:35:LYS:CB	1:A:35:LYS:NZ	2.63	0.58
1:A:73:ALA:HB2	1:A:79:VAL:HG13	1.84	0.58
1:A:113:SER:HB3	1:A:142:ASN:HD22	1.69	0.58
1:A:147:VAL:HG23	2:B:8:GLU:HG2	1.85	0.58
1:A:174:THR:HG23	6:A:256:HOH:O	2.04	0.57
1:A:35:LYS:HB3	1:A:35:LYS:HZ3	1.68	0.57
1:A:103:VAL:HG23	1:A:104:PHE:CD2	2.40	0.57
1:A:55:ARG:NH1	1:A:55:ARG:CG	2.64	0.57
1:C:167:ASN:HD21	1:C:169:ALA:CB	2.09	0.56
2:B:38:HIS:HD2	2:B:38:HIS:N	2.03	0.56
1:C:172:VAL:HG12	1:C:172:VAL:O	2.06	0.56
2:B:37:VAL:C	2:B:38:HIS:HD2	2.09	0.55
1:C:12:SER:HB3	1:C:13:PRO:HD2	1.88	0.55
1:C:55:ARG:HH11	1:C:56:ASP:HA	1.72	0.55
1:A:60:VAL:HG22	2:B:13:LYS:HE3	1.88	0.55
1:A:110:ASP:OD1	1:A:110:ASP:C	2.42	0.55
1:A:54:ASP:HB3	1:A:57:THR:OG1	2.06	0.55
1:A:57:THR:HB	1:A:59:ASN:OD1	2.08	0.54
1:A:32:THR:HG23	6:A:264:HOH:O	2.06	0.54
1:C:38:LYS:HE2	2:D:30:ALA:O	2.08	0.54
1:C:48:THR:O	1:C:50:ILE:HD12	2.08	0.54
1:C:93:LYS:HB2	1:C:94:PRO:HD2	1.89	0.54
1:C:70:VAL:HG11	6:C:192:HOH:O	2.08	0.53
1:C:10:LYS:CG	1:C:10:LYS:O	2.43	0.53
1:A:114:GLN:N	1:A:142:ASN:HD21	2.07	0.53
1:A:35:LYS:HB3	1:A:35:LYS:HZ2	1.74	0.53
1:C:54:ASP:OD1	1:C:56:ASP:HB2	2.09	0.53
1:C:132:ASN:ND2	1:C:134:GLU:HG3	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:LEU:O	1:A:42:GLY:HA3	2.09	0.52
2:B:13:LYS:HZ3	2:B:13:LYS:HB2	1.62	0.51
1:A:89:PRO:HD3	1:A:114:GLN:O	2.11	0.51
1:A:170:THR:CG2	1:A:172:VAL:H	2.24	0.51
1:C:167:ASN:C	1:C:167:ASN:ND2	2.62	0.50
2:B:44:SER:C	2:B:45:GLN:HG3	2.31	0.50
1:C:6:PHE:C	1:C:6:PHE:CD1	2.85	0.50
1:A:68:THR:HG21	1:A:159:ARG:HE	1.77	0.50
1:C:68:THR:HG21	1:C:159:ARG:NH2	2.27	0.50
1:C:70:VAL:CG2	1:C:159:ARG:HG3	2.41	0.50
1:C:55:ARG:HG2	1:C:56:ASP:N	2.27	0.49
1:C:38:LYS:CE	2:D:30:ALA:HA	2.35	0.49
1:C:38:LYS:HE2	2:D:30:ALA:C	2.33	0.49
1:C:179:TYR:HB3	1:C:180:PRO:HD2	1.95	0.49
1:C:9:THR:O	1:C:10:LYS:CB	2.58	0.49
1:C:88:ALA:HB1	1:C:89:PRO:CD	2.43	0.49
1:A:35:LYS:CB	1:A:35:LYS:HZ2	2.26	0.49
2:B:28:THR:HB	2:B:32:PHE:HB3	1.95	0.49
1:A:55:ARG:HG2	1:A:55:ARG:HH11	1.78	0.48
2:D:13:LYS:HG3	2:D:13:LYS:HZ2	1.52	0.48
1:C:179:TYR:O	2:D:1:VAL:HA	2.12	0.48
1:A:113:SER:HB3	1:A:142:ASN:ND2	2.27	0.48
1:C:70:VAL:HG22	1:C:159:ARG:HA	1.94	0.48
1:C:27:THR:HG22	1:C:28:LYS:CB	2.34	0.48
1:A:91:ASP:O	1:A:93:LYS:HD3	2.14	0.47
1:A:38:LYS:HG3	2:B:32:PHE:CD2	2.49	0.47
1:A:48:THR:HG23	6:C:212:HOH:O	2.15	0.47
1:C:132:ASN:HD22	1:C:133:LYS:N	2.12	0.47
1:A:16:GLN:NE2	2:D:19:TRP:CD1	2.83	0.47
1:A:40:THR:HG22	2:B:28:THR:OG1	2.15	0.47
1:A:20:PHE:HE1	1:A:31:LEU:CD1	2.28	0.47
1:A:6:PHE:CD1	1:A:6:PHE:C	2.88	0.47
1:A:177:LEU:HD23	1:A:178:THR:N	2.30	0.46
1:A:38:LYS:HG3	2:B:32:PHE:CE2	2.50	0.46
1:A:170:THR:HG22	1:A:172:VAL:H	1.80	0.46
1:A:28:LYS:HE3	1:A:28:LYS:CA	2.39	0.46
1:C:19:ILE:O	1:C:44:ALA:HA	2.15	0.46
1:A:12:SER:HB3	1:A:13:PRO:HD2	1.97	0.46
1:A:21:GLN:NE2	1:A:43:ARG:HE	2.14	0.46
1:C:172:VAL:HG12	6:C:223:HOH:O	2.16	0.46
1:C:1:THR:HG22	1:C:2:GLU:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:TRP:HB2	1:A:145:LYS:CG	2.42	0.46
1:A:21:GLN:HE21	1:A:43:ARG:HE	1.63	0.45
1:C:1:THR:CG2	1:C:2:GLU:N	2.80	0.45
2:D:1:VAL:O	2:D:1:VAL:CG2	2.65	0.45
1:C:132:ASN:ND2	1:C:134:GLU:CG	2.79	0.45
1:A:124:TYR:CZ	1:A:126:ALA:HA	2.52	0.44
1:A:35:LYS:HG3	1:A:35:LYS:H	1.42	0.44
1:C:68:THR:HG21	1:C:159:ARG:HH21	1.82	0.44
1:C:55:ARG:HH11	1:C:56:ASP:CA	2.29	0.44
1:C:77:TYR:CD1	1:C:77:TYR:C	2.90	0.44
1:C:110:ASP:O	1:C:142:ASN:HB3	2.17	0.44
1:C:170:THR:HG23	1:C:172:VAL:H	1.83	0.44
1:C:170:THR:CG2	1:C:172:VAL:H	2.30	0.44
1:C:166:PHE:HB2	1:C:173:LEU:HD12	1.99	0.44
2:D:32:PHE:C	2:D:32:PHE:CD1	2.91	0.43
1:C:177:LEU:C	1:C:177:LEU:HD23	2.38	0.43
1:A:70:VAL:HG22	1:A:159:ARG:HA	2.01	0.43
1:A:84:THR:O	2:B:24:PHE:HA	2.19	0.43
1:C:132:ASN:C	1:C:132:ASN:HD22	2.21	0.43
2:B:43:ASN:ND2	2:B:43:ASN:C	2.72	0.43
1:C:9:THR:O	1:C:10:LYS:HB3	2.18	0.43
1:C:159:ARG:HD2	1:C:159:ARG:HH11	1.49	0.42
1:C:93:LYS:HG2	1:C:93:LYS:H	1.79	0.42
1:A:23:ASP:O	1:A:25:TYR:HD1	2.02	0.42
1:A:28:LYS:HB2	1:A:28:LYS:HZ1	1.83	0.42
1:A:114:GLN:N	1:A:142:ASN:ND2	2.67	0.42
1:A:53:TRP:CE3	2:B:13:LYS:HG2	2.54	0.42
2:D:13:LYS:CB	2:D:13:LYS:HZ3	2.32	0.42
1:C:159:ARG:NH1	2:D:38:HIS:ND1	2.68	0.42
1:A:92:THR:O	1:A:93:LYS:HD2	2.20	0.41
1:C:167:ASN:ND2	1:C:169:ALA:H	2.19	0.41
1:A:131:SER:O	1:A:133:LYS:HG3	2.20	0.41
1:C:167:ASN:HD22	1:C:169:ALA:N	2.17	0.41
1:A:170:THR:CG2	1:A:172:VAL:HB	2.51	0.41
1:C:70:VAL:CG2	1:C:159:ARG:CG	2.99	0.41
1:C:179:TYR:HA	1:C:180:PRO:HD3	1.66	0.41
1:C:62:ASN:ND2	1:C:168:ALA:HB3	2.35	0.41
1:A:28:LYS:HE3	1:A:28:LYS:N	2.36	0.40
2:B:13:LYS:HZ3	2:B:13:LYS:HB3	1.86	0.40
1:C:80:ALA:HB3	2:D:31:GLU:C	2.42	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	179/181 (99%)	174 (97%)	5 (3%)	0	100	100
1	C	179/181 (99%)	173 (97%)	6 (3%)	0	100	100
2	B	45/52 (86%)	43 (96%)	2 (4%)	0	100	100
2	D	45/52 (86%)	44 (98%)	1 (2%)	0	100	100
All	All	448/466 (96%)	434 (97%)	14 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	156/156 (100%)	128 (82%)	28 (18%)	2	0
1	C	156/156 (100%)	131 (84%)	25 (16%)	3	0
2	B	40/45 (89%)	35 (88%)	5 (12%)	5	1
2	D	40/45 (89%)	36 (90%)	4 (10%)	9	2
All	All	392/402 (98%)	330 (84%)	62 (16%)	3	0

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	THR
1	A	5	SER

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Mol	Chain	Res	Type
1	A	10	LYS
1	A	18	LEU
1	A	28	LYS
1	A	30	LYS
1	A	35	LYS
1	A	39	SER
1	A	47	SER
1	A	48	THR
1	A	52	ILE
1	A	55	ARG
1	A	56	ASP
1	A	57	THR
1	A	76	SER
1	A	81	ASP
1	A	91	ASP
1	A	93	LYS
1	A	107	LYS
1	A	111	LYS
1	A	132	ASN
1	A	145	LYS
1	A	150	LYS
1	A	156	ASN
1	A	158	GLU
1	A	170	THR
1	A	174	THR
1	A	176	THR
2	B	7	ASN
2	B	13	LYS
2	B	25	SER
2	B	41	SER
2	B	45	GLN
1	C	5	SER
1	C	7	SER
1	C	10	LYS
1	C	15	GLN
1	C	30	LYS
1	C	38	LYS
1	C	55	ARG
1	C	56	ASP
1	C	66	SER
1	C	75	SER
1	C	76	SER

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Mol	Chain	Res	Type
1	C	91	ASP
1	C	93	LYS
1	C	106	SER
1	C	107	LYS
1	C	111	LYS
1	C	112	THR
1	C	113	SER
1	C	131	SER
1	C	132	ASN
1	C	150	LYS
1	C	158	GLU
1	C	167	ASN
1	C	170	THR
1	C	172	VAL
2	D	5	THR
2	D	13	LYS
2	D	43	ASN
2	D	45	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	21	GLN
1	A	105	ASN
1	A	132	ASN
1	A	142	ASN
1	A	156	ASN
1	A	171	ASN
2	B	35	GLN
2	B	38	HIS
2	B	43	ASN
2	B	45	GLN
1	C	62	ASN
1	C	105	ASN
1	C	132	ASN
1	C	142	ASN
1	C	156	ASN
1	C	161	ASN
1	C	167	ASN
2	D	35	GLN
2	D	43	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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	PO4	A	182	-	4,4,4	0.81	0	6,6,6	0.70	0
3	PO4	C	182	-	4,4,4	1.64	1 (25%)	6,6,6	0.61	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
3	PO4	A	182	-	-	0/0/0/0	0/0/0/0
3	PO4	C	182	-	-	0/0/0/0	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	182	PO4	P-O1	2.90	1.56	1.50

There are no bond angle outliers.

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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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.