Full wwPDB X-ray Structure Validation Report (i)

Feb 10, 2024 – 11:51 AM EST

PDB ID	:	2LTN
Title	:	DESIGN, EXPRESSION, AND CRYSTALLIZATION OF RECOMBINANT LECTIN FROM THE GARDEN PEA (PISUM SATIVUM)
Authors	:	Suddath, F.L.; Phillips, S.R.; Einspahr, H.
Deposited on	:	1990-06-26
Resolution	:	1.70 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 (i) 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 (i)) were used in the production of this report:

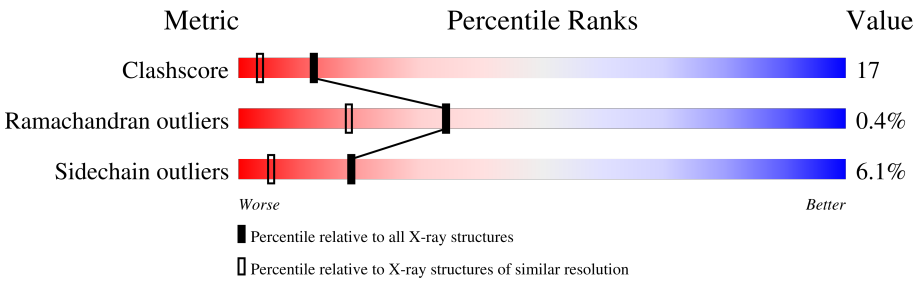
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	181	60% 30% 8% •
1	C	181	59% 33% 8% •
2	B	52	60% 29% • 8%
2	D	52	62% 27% • 8%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 3866 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, ALPHA CHAIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
1	A	181	1417	903	233	281	0	0	0
1	C	181	1417	903	233	281	0	0	0

- Molecule 2 is a protein called PEA LECTIN, BETA CHAIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	48	367	236	58	73	0	0	1
2	D	48	367	236	58	73	0	0	1

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	120	120	120	0	0
			Total	O		
5	B	27	27	27	0	0
			Total	O		
5	C	125	125	125	0	0
			Total	O		
5	D	22	22	22	0	0

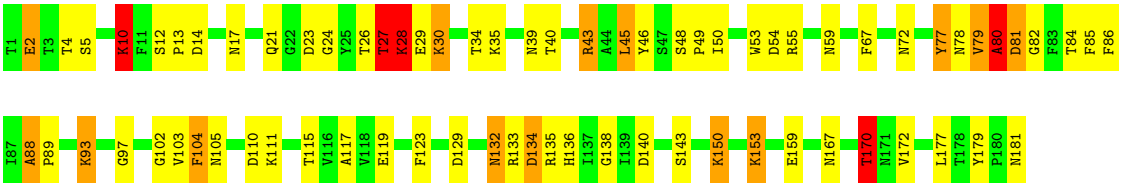
3 Residue-property plots (i)

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.

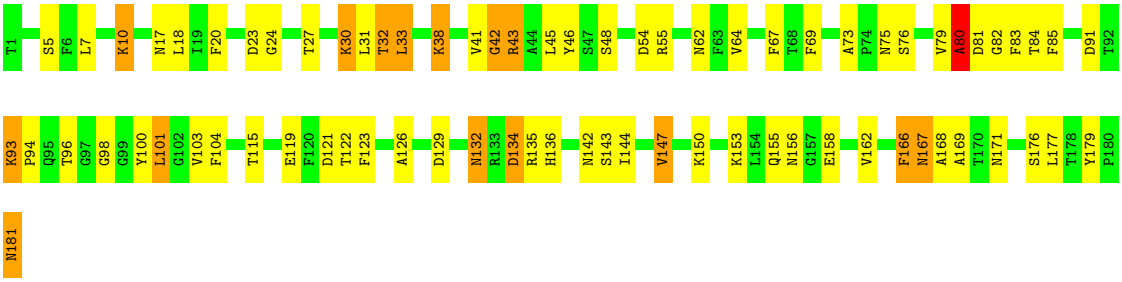
• Molecule 1: PEA LECTIN, ALPHA CHAIN

Chain A:



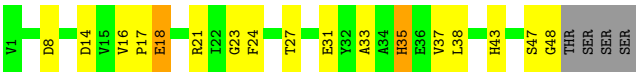
• Molecule 1: PEA LECTIN, ALPHA CHAIN

Chain C:



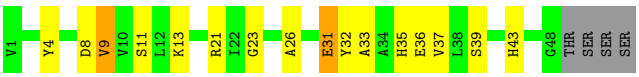
• Molecule 2: PEA LECTIN, BETA CHAIN

Chain B:



• Molecule 2: PEA LECTIN, BETA CHAIN

Chain D:



4 Data and refinement statistics (i)

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	50.73Å 61.16Å 136.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 1.70	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-1.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.177 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3866	wwPDB-VP
Average B, all atoms ($Å^2$)	16.0	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: 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	1.52	9/1451 (0.6%)	2.27	70/1981 (3.5%)
1	C	1.47	11/1451 (0.8%)	2.25	63/1981 (3.2%)
2	B	1.57	2/377 (0.5%)	2.16	17/517 (3.3%)
2	D	1.44	1/377 (0.3%)	2.00	15/517 (2.9%)
All	All	1.49	23/3656 (0.6%)	2.22	165/4996 (3.3%)

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	1	2
1	C	1	3
All	All	2	5

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	80	ALA	N-CA	-10.05	1.26	1.46
1	A	80	ALA	N-CA	-8.79	1.28	1.46
1	C	80	ALA	CA-CB	8.54	1.70	1.52
1	C	119	GLU	CD-OE2	-7.99	1.16	1.25
2	D	39	SER	CA-CB	7.22	1.63	1.52
1	C	43	ARG	CZ-NH2	6.39	1.41	1.33
1	A	181	ASN	C-OXT	6.35	1.35	1.23
2	B	24	PHE	CG-CD1	5.66	1.47	1.38
1	A	143	SER	CA-CB	5.62	1.61	1.52
1	A	102	GLY	C-O	5.51	1.32	1.23
1	C	143	SER	CA-CB	5.50	1.61	1.52
1	A	27	THR	N-CA	-5.48	1.35	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	119	GLU	CB-CG	5.37	1.62	1.52
1	C	121	ASP	CB-CG	5.34	1.62	1.51
1	A	115	THR	CB-OG1	5.32	1.53	1.43
2	B	21	ARG	CZ-NH2	5.18	1.39	1.33
1	C	18	LEU	N-CA	5.18	1.56	1.46
1	C	81	ASP	N-CA	-5.16	1.36	1.46
1	C	46	TYR	N-CA	5.16	1.56	1.46
1	A	82	GLY	CA-C	5.15	1.60	1.51
1	C	98	GLY	C-O	5.12	1.31	1.23
1	C	42	GLY	N-CA	5.06	1.53	1.46
1	A	138	GLY	N-CA	-5.04	1.38	1.46

All (165) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	79	VAL	O-C-N	23.56	160.40	122.70
1	C	80	ALA	N-CA-C	18.54	161.06	111.00
1	C	43	ARG	NE-CZ-NH1	17.10	128.85	120.30
1	C	79	VAL	O-C-N	16.46	149.04	122.70
1	A	79	VAL	CA-C-N	-14.62	85.04	117.20
1	C	79	VAL	CA-C-N	-14.17	86.02	117.20
1	C	80	ALA	O-C-N	-13.26	101.48	122.70
1	A	28	LYS	N-CA-CB	13.15	134.28	110.60
2	D	21	ARG	NE-CZ-NH1	12.97	126.78	120.30
2	B	21	ARG	NE-CZ-NH1	12.80	126.70	120.30
1	C	80	ALA	CA-C-N	12.46	144.61	117.20
1	C	80	ALA	CB-CA-C	-11.98	92.14	110.10
1	A	26	THR	C-N-CA	11.80	151.19	121.70
1	A	27	THR	C-N-CA	11.35	150.08	121.70
1	C	81	ASP	N-CA-CB	11.07	130.53	110.60
1	C	45	LEU	O-C-N	11.06	140.40	122.70
1	C	181	ASN	N-CA-CB	10.74	129.94	110.60
1	C	119	GLU	OE1-CD-OE2	10.41	135.79	123.30
1	A	80	ALA	CA-C-N	10.37	140.02	117.20
1	C	67	PHE	CB-CG-CD1	-10.23	113.64	120.80
1	A	80	ALA	O-C-N	-10.21	106.37	122.70
1	A	2	GLU	OE1-CD-OE2	9.92	135.20	123.30
1	C	100	TYR	O-C-N	9.49	137.89	122.70
1	A	170	THR	N-CA-CB	-9.41	92.43	110.30
1	A	54	ASP	CB-CG-OD1	9.37	126.73	118.30
1	C	147	VAL	CG1-CB-CG2	9.28	125.75	110.90
1	C	121	ASP	CB-CG-OD2	-9.27	109.96	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	27	THR	CA-C-O	9.16	139.33	120.10
1	C	54	ASP	CB-CG-OD2	-9.02	110.18	118.30
1	A	80	ALA	N-CA-C	8.99	135.28	111.00
2	B	35	HIS	O-C-N	8.96	137.04	122.70
2	B	21	ARG	NE-CZ-NH2	-8.89	115.85	120.30
1	C	91	ASP	CB-CG-OD1	8.82	126.24	118.30
2	B	8	ASP	CB-CG-OD2	-8.65	110.52	118.30
1	A	82	GLY	O-C-N	8.60	136.46	122.70
1	A	123	PHE	CB-CG-CD2	-8.56	114.81	120.80
1	A	2	GLU	CG-CD-OE2	-8.55	101.19	118.30
1	A	54	ASP	CB-CG-OD2	-8.55	110.60	118.30
2	B	23	GLY	O-C-N	8.38	136.10	122.70
1	A	170	THR	OG1-CB-CG2	8.36	129.23	110.00
1	A	129	ASP	CB-CG-OD1	-8.34	110.80	118.30
1	C	84	THR	O-C-N	8.30	135.98	122.70
1	A	27	THR	N-CA-C	8.23	133.22	111.00
1	A	27	THR	O-C-N	-8.22	109.55	122.70
1	C	121	ASP	OD1-CG-OD2	8.20	138.88	123.30
1	A	85	PHE	CB-CG-CD2	-8.19	115.07	120.80
2	B	27	THR	O-C-N	8.13	135.70	122.70
1	C	121	ASP	CB-CG-OD1	-7.95	111.15	118.30
2	D	8	ASP	CB-CG-OD1	-7.90	111.19	118.30
1	A	136	HIS	O-C-N	7.78	135.15	122.70
1	A	80	ALA	CA-C-O	-7.74	103.85	120.10
1	A	134	ASP	O-C-N	7.71	135.03	122.70
2	D	35	HIS	O-C-N	7.68	134.99	122.70
2	D	23	GLY	O-C-N	7.56	134.79	122.70
2	B	8	ASP	CB-CG-OD1	7.45	125.00	118.30
1	C	83	PHE	N-CA-CB	-7.41	97.26	110.60
2	B	18	GLU	OE1-CD-OE2	7.35	132.12	123.30
1	A	45	LEU	CA-CB-CG	7.33	132.15	115.30
1	A	129	ASP	OD1-CG-OD2	7.32	137.20	123.30
1	A	26	THR	O-C-N	-7.31	111.00	122.70
1	C	17	ASN	O-C-N	7.22	134.25	122.70
1	A	26	THR	CA-C-O	7.13	135.07	120.10
1	A	140	ASP	CB-CG-OD2	7.13	124.72	118.30
1	A	129	ASP	CB-CG-OD2	-7.12	111.89	118.30
1	A	134	ASP	CB-CG-OD2	-7.11	111.90	118.30
1	A	133	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	C	43	ARG	NH1-CZ-NH2	-7.00	111.69	119.40
1	C	23	ASP	CB-CG-OD1	6.99	124.59	118.30
1	A	43	ARG	O-C-N	6.96	133.84	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	24	PHE	CB-CG-CD2	6.91	125.64	120.80
1	A	17	ASN	O-C-N	6.91	133.75	122.70
1	C	122	THR	O-C-N	6.91	133.75	122.70
1	C	46	TYR	CB-CG-CD2	-6.87	116.88	121.00
1	A	80	ALA	N-CA-CB	6.87	119.72	110.10
2	D	31	GLU	O-C-N	6.84	133.65	122.70
1	A	181	ASN	CA-C-O	6.75	134.28	120.10
1	A	24	GLY	O-C-N	6.70	133.41	122.70
1	C	80	ALA	CA-C-O	-6.68	106.08	120.10
1	A	84	THR	O-C-N	6.66	133.36	122.70
1	C	31	LEU	O-C-N	6.66	133.35	122.70
1	A	14	ASP	CB-CG-OD1	6.65	124.29	118.30
2	B	31	GLU	O-C-N	6.65	133.34	122.70
2	B	47	SER	CB-CA-C	6.65	122.74	110.10
1	A	81	ASP	N-CA-CB	6.62	122.52	110.60
1	C	85	PHE	CB-CG-CD1	-6.59	116.19	120.80
1	A	23	ASP	CB-CG-OD2	6.56	124.20	118.30
1	A	123	PHE	CB-CG-CD1	6.49	125.34	120.80
1	A	39	ASN	O-C-N	6.47	133.05	122.70
1	A	86	PHE	CB-CG-CD1	-6.46	116.28	120.80
1	C	64	VAL	CB-CA-C	-6.38	99.27	111.40
1	A	45	LEU	O-C-N	6.32	132.81	122.70
1	C	135	ARG	NE-CZ-NH1	-6.28	117.16	120.30
1	C	45	LEU	CB-CG-CD1	-6.25	100.37	111.00
2	B	33	ALA	O-C-N	6.25	132.69	122.70
2	D	37	VAL	O-C-N	6.23	132.66	122.70
1	C	129	ASP	CB-CG-OD1	-6.21	112.71	118.30
1	C	64	VAL	CA-CB-CG1	6.20	120.20	110.90
1	C	135	ARG	NE-CZ-NH2	6.16	123.38	120.30
1	C	181	ASN	CA-CB-CG	-6.14	99.90	113.40
1	A	40	THR	CA-CB-OG1	-6.11	96.17	109.00
2	D	21	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	A	105	ASN	OD1-CG-ND2	6.05	135.82	121.90
1	A	138	GLY	O-C-N	6.04	132.37	122.70
1	C	69	PHE	O-C-N	6.04	132.37	122.70
1	A	97	GLY	O-C-N	5.97	133.36	123.20
2	D	13	LYS	CA-CB-CG	5.95	126.50	113.40
1	C	41	VAL	O-C-N	5.94	133.29	123.20
1	A	159	GLU	OE1-CD-OE2	5.92	130.40	123.30
1	A	105	ASN	O-C-N	5.89	132.12	122.70
1	A	88	ALA	O-C-N	5.88	132.28	121.10
1	A	81	ASP	CB-CG-OD1	5.87	123.58	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	110	ASP	CB-CG-OD2	-5.87	113.02	118.30
1	A	133	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	C	80	ALA	C-N-CA	5.85	136.33	121.70
1	C	134	ASP	O-C-N	5.85	132.06	122.70
2	D	39	SER	CA-CB-OG	-5.84	95.43	111.20
1	A	133	ARG	CD-NE-CZ	5.83	131.76	123.60
1	C	176	SER	N-CA-CB	5.82	119.24	110.50
1	C	82	GLY	O-C-N	5.81	132.00	122.70
2	D	39	SER	N-CA-CB	-5.76	101.86	110.50
1	C	136	HIS	O-C-N	5.73	131.86	122.70
1	A	10	LYS	CA-CB-CG	5.72	125.99	113.40
1	C	147	VAL	N-CA-CB	-5.72	98.92	111.50
1	A	117	ALA	O-C-N	5.60	131.66	122.70
1	C	64	VAL	CG1-CB-CG2	5.60	119.87	110.90
2	B	37	VAL	O-C-N	5.60	131.65	122.70
1	C	104	PHE	O-C-N	5.59	131.64	122.70
1	C	96	THR	CA-CB-CG2	-5.58	104.58	112.40
2	D	33	ALA	O-C-N	5.54	131.57	122.70
2	D	36	GLU	CG-CD-OE1	5.53	129.35	118.30
1	A	27	THR	CA-CB-CG2	5.49	120.08	112.40
1	A	115	THR	O-C-N	5.48	131.47	122.70
1	A	67	PHE	CB-CG-CD1	-5.48	116.97	120.80
1	A	93	LYS	CA-CB-CG	5.47	125.43	113.40
2	D	9	VAL	CG1-CB-CG2	5.43	119.59	110.90
1	C	126	ALA	CB-CA-C	5.43	118.24	110.10
1	C	166	PHE	CB-CG-CD2	-5.36	117.05	120.80
1	C	24	GLY	O-C-N	5.36	131.27	122.70
1	C	45	LEU	C-N-CA	-5.32	108.39	121.70
1	C	162	VAL	CG1-CB-CG2	5.26	119.31	110.90
1	C	80	ALA	N-CA-CB	-5.25	102.74	110.10
1	A	170	THR	CA-CB-CG2	5.20	119.69	112.40
2	B	24	PHE	CB-CG-CD1	-5.20	117.16	120.80
2	B	14	ASP	CB-CG-OD1	5.19	122.97	118.30
1	C	123	PHE	CB-CG-CD2	-5.19	117.17	120.80
1	A	80	ALA	CB-CA-C	-5.19	102.32	110.10
1	A	35	LYS	O-C-N	5.17	130.98	122.70
2	B	18	GLU	CG-CD-OE2	-5.17	107.96	118.30
1	A	179	TYR	CB-CG-CD2	5.17	124.10	121.00
1	C	20	PHE	CB-CG-CD1	-5.17	117.18	120.80
1	C	82	GLY	CA-C-N	-5.17	105.83	117.20
2	B	21	ARG	O-C-N	5.12	130.89	122.70
1	A	78	ASN	O-C-N	5.10	130.87	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	46	TYR	CB-CG-CD2	-5.09	117.95	121.00
2	D	26	ALA	N-CA-CB	5.09	117.22	110.10
1	C	64	VAL	CA-CB-CG2	5.08	118.53	110.90
1	C	48	SER	O-C-N	5.08	130.76	121.10
1	C	23	ASP	CB-CG-OD2	-5.08	113.73	118.30
1	A	104	PHE	CB-CG-CD2	-5.07	117.25	120.80
1	A	135	ARG	NE-CZ-NH2	-5.07	117.76	120.30
1	C	179	TYR	CB-CG-CD1	5.07	124.04	121.00
1	C	158	GLU	OE1-CD-OE2	5.05	129.36	123.30
1	C	75	ASN	CA-CB-CG	-5.04	102.31	113.40
2	D	11	SER	N-CA-CB	5.04	118.07	110.50
1	C	43	ARG	O-C-N	5.01	130.71	122.70

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	27	THR	CA
1	C	80	ALA	CA

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	80	ALA	Peptide,Mainchain
1	C	43	ARG	Sidechain
1	C	80	ALA	Peptide,Mainchain

5.2 Too-close contacts (i)

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	1417	0	1364	70	0
1	C	1417	0	1366	47	0
2	B	367	0	349	10	0
2	D	367	0	349	9	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
4	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	1	0	0	0	0
5	A	120	0	0	5	0
5	B	27	0	0	0	0
5	C	125	0	0	0	0
5	D	22	0	0	0	0
All	All	3866	0	3428	118	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 17.

All (118) 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:A:153:LYS:HZ3	1:A:153:LYS:CB	1.33	1.32
1:A:153:LYS:HB2	1:A:153:LYS:NZ	1.18	1.25
1:A:27:THR:HG23	1:A:29:GLU:N	1.62	1.11
1:A:28:LYS:HE3	1:A:30:LYS:HE2	1.33	1.09
1:A:27:THR:CG2	1:A:29:GLU:H	1.74	1.01
1:A:27:THR:HG23	1:A:29:GLU:H	0.85	0.99
1:A:29:GLU:HB2	1:A:30:LYS:HZ1	1.29	0.95
1:A:29:GLU:C	1:A:30:LYS:NZ	2.22	0.93
1:C:73:ALA:H	1:C:156:ASN:HD21	1.19	0.90
1:A:28:LYS:CE	1:A:30:LYS:HE2	2.03	0.89
1:A:29:GLU:HB2	1:A:30:LYS:NZ	1.92	0.84
1:A:27:THR:CG2	1:A:28:LYS:N	2.44	0.81
1:C:38:LYS:HE3	2:D:32:TYR:CE1	2.17	0.80
1:A:30:LYS:N	1:A:30:LYS:HZ3	1.80	0.79
1:A:21:GLN:HE22	1:A:43:ARG:HH11	1.32	0.78
1:A:30:LYS:NZ	1:A:30:LYS:N	2.32	0.78
1:A:170:THR:HG23	1:A:172:VAL:HG23	1.66	0.77
1:A:153:LYS:CB	1:A:153:LYS:NZ	2.04	0.77
1:C:5:SER:OG	2:D:43:HIS:HD2	1.67	0.77
1:A:28:LYS:HE3	1:A:30:LYS:CE	2.15	0.76
1:C:167:ASN:HD22	1:C:167:ASN:C	1.92	0.73
1:C:55:ARG:HB3	1:C:55:ARG:CZ	2.18	0.73
1:A:132:ASN:HD22	1:A:134:ASP:H	1.36	0.73
1:A:77:TYR:HE1	5:A:624:HOH:O	1.73	0.71
1:C:38:LYS:HZ2	1:C:38:LYS:H	1.38	0.71
1:C:153:LYS:HE2	2:D:4:TYR:OH	1.90	0.71
1:C:38:LYS:H	1:C:38:LYS:NZ	1.89	0.71
1:A:27:THR:HG23	1:A:28:LYS:N	2.06	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:132:ASN:HD22	1:C:134:ASP:H	1.39	0.70
1:C:55:ARG:HG2	1:C:55:ARG:HH21	1.57	0.69
1:C:27:THR:O	1:C:30:LYS:HG2	1.92	0.69
1:A:21:GLN:NE2	1:A:43:ARG:HE	1.93	0.66
1:A:29:GLU:C	1:A:30:LYS:HZ3	1.94	0.66
1:C:27:THR:HG22	1:C:32:THR:CG2	2.28	0.64
1:A:28:LYS:NZ	1:A:29:GLU:OE2	2.31	0.63
1:C:27:THR:HG22	1:C:32:THR:HG23	1.81	0.62
1:C:167:ASN:ND2	1:C:169:ALA:H	1.98	0.62
1:C:155:GLN:HE22	1:C:181:ASN:C	2.03	0.62
1:A:53:TRP:O	2:B:18:GLU:HG3	2.00	0.61
1:A:29:GLU:CB	1:A:30:LYS:HZ1	2.09	0.61
1:A:28:LYS:O	1:A:30:LYS:NZ	2.35	0.60
1:C:132:ASN:ND2	1:C:134:ASP:H	1.98	0.60
1:A:4:THR:HG21	1:A:50:ILE:CD1	2.32	0.60
1:C:167:ASN:HD22	1:C:169:ALA:H	1.50	0.60
1:A:79:VAL:O	5:A:407:HOH:O	2.17	0.59
1:A:10:LYS:C	1:A:10:LYS:HD3	2.21	0.59
1:A:170:THR:HG23	1:A:172:VAL:CG2	2.32	0.59
1:A:21:GLN:HE21	1:A:43:ARG:HE	1.52	0.57
1:A:77:TYR:CD1	1:A:77:TYR:N	2.71	0.57
1:C:167:ASN:HD21	1:C:169:ALA:HB3	1.68	0.57
1:C:80:ALA:HB3	2:D:31:GLU:HB2	1.87	0.57
1:C:103:VAL:CG1	1:C:115:THR:HG21	2.35	0.56
1:A:5:SER:OG	2:B:43:HIS:HD2	1.90	0.54
1:A:28:LYS:HE3	1:A:28:LYS:O	2.08	0.54
1:A:28:LYS:O	1:A:28:LYS:HG2	2.05	0.54
1:A:59:ASN:HD22	2:B:48:GLY:N	2.06	0.53
1:A:28:LYS:O	1:A:28:LYS:CG	2.57	0.53
1:A:34:THR:OG1	2:B:35:HIS:HD2	1.92	0.53
1:C:38:LYS:CE	2:D:32:TYR:CE1	2.91	0.53
1:C:155:GLN:NE2	1:C:181:ASN:OXT	2.35	0.52
1:A:30:LYS:HZ2	1:A:30:LYS:CA	2.23	0.51
1:C:155:GLN:OE1	1:C:181:ASN:O	2.29	0.51
1:C:55:ARG:HH21	1:C:55:ARG:CG	2.22	0.51
1:C:55:ARG:HG2	1:C:55:ARG:NH2	2.25	0.50
1:C:10:LYS:O	1:C:10:LYS:HG3	2.10	0.50
1:A:30:LYS:HG3	2:B:38:LEU:HD22	1.94	0.50
2:B:16:VAL:HB	2:B:17:PRO:HD2	1.93	0.49
1:A:30:LYS:CG	2:B:38:LEU:CD2	2.90	0.49
1:A:80:ALA:HB1	1:A:81:ASP:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:55:ARG:CG	1:C:55:ARG:NH2	2.75	0.49
1:C:166:PHE:HZ	1:C:171:ASN:HD22	1.59	0.49
1:C:177:LEU:C	1:C:177:LEU:HD23	2.33	0.49
1:A:28:LYS:CE	1:A:28:LYS:O	2.62	0.47
1:C:101:LEU:HD22	1:C:144:ILE:HD11	1.96	0.47
1:A:88:ALA:HB1	1:A:89:PRO:CD	2.44	0.47
1:C:167:ASN:C	1:C:167:ASN:ND2	2.64	0.47
1:A:28:LYS:O	1:A:30:LYS:CE	2.62	0.47
1:A:30:LYS:CG	2:B:38:LEU:HD22	2.43	0.47
1:C:62:ASN:ND2	1:C:168:ALA:H	2.12	0.47
1:A:29:GLU:C	1:A:30:LYS:HZ2	2.15	0.47
1:A:132:ASN:ND2	1:A:134:ASP:H	2.06	0.47
1:C:167:ASN:HD21	1:C:169:ALA:CB	2.28	0.47
1:A:21:GLN:HE22	1:A:43:ARG:NH1	2.06	0.46
1:C:38:LYS:HE3	2:D:32:TYR:CD1	2.50	0.46
1:A:29:GLU:CB	1:A:30:LYS:NZ	2.72	0.46
1:A:55:ARG:HD3	5:A:683:HOH:O	2.15	0.46
1:A:10:LYS:HD3	1:A:10:LYS:O	2.16	0.46
1:A:30:LYS:HG2	2:B:38:LEU:CD2	2.46	0.46
1:A:27:THR:HG23	1:A:28:LYS:CA	2.45	0.45
1:A:30:LYS:N	1:A:30:LYS:HZ2	2.14	0.45
1:A:88:ALA:HB1	1:A:89:PRO:HD2	1.99	0.44
1:A:167:ASN:HB3	1:A:170:THR:HG22	1.99	0.44
1:C:132:ASN:HD22	1:C:132:ASN:C	2.21	0.44
1:A:29:GLU:O	1:A:30:LYS:NZ	2.50	0.44
1:C:115:THR:H	1:C:142:ASN:ND2	2.14	0.44
1:A:2:GLU:HA	1:C:7:LEU:O	2.18	0.44
1:A:28:LYS:O	1:A:29:GLU:HB2	2.19	0.43
1:C:153:LYS:HE2	1:C:153:LYS:HB2	1.73	0.43
5:A:538:HOH:O	1:C:10:LYS:HE3	2.18	0.42
1:A:153:LYS:NZ	1:A:153:LYS:CA	2.80	0.42
1:C:93:LYS:HG2	1:C:94:PRO:N	2.35	0.42
1:C:167:ASN:ND2	1:C:169:ALA:HB3	2.34	0.42
1:A:30:LYS:HG3	2:B:38:LEU:CD2	2.50	0.42
1:C:33:LEU:O	1:C:42:GLY:HA3	2.20	0.42
1:C:5:SER:OG	2:D:43:HIS:CD2	2.58	0.41
1:C:153:LYS:CE	2:D:4:TYR:OH	2.66	0.41
1:A:48:SER:HA	1:A:49:PRO:HD3	1.92	0.41
1:A:153:LYS:HD2	5:A:548:HOH:O	2.19	0.41
1:A:150:LYS:HB2	1:A:150:LYS:HE3	1.62	0.41
2:D:31:GLU:OE2	2:D:31:GLU:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:SER:HA	1:A:13:PRO:HD3	1.84	0.41
1:C:103:VAL:HG13	1:C:115:THR:HG21	2.01	0.41
1:C:93:LYS:HG2	1:C:94:PRO:HD2	2.03	0.40
1:A:30:LYS:NZ	1:A:30:LYS:CA	2.84	0.40
1:A:177:LEU:C	1:A:177:LEU:HD23	2.42	0.40
1:C:27:THR:CG2	1:C:32:THR:CG2	2.98	0.40
1:A:28:LYS:O	1:A:30:LYS:HE2	2.22	0.40
1:A:103:VAL:HG23	1:A:104:PHE:CD2	2.57	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%)	172 (96%)	5 (3%)	2 (1%)	14	3
1	C	179/181 (99%)	176 (98%)	3 (2%)	0	100	100
2	B	46/52 (88%)	46 (100%)	0	0	100	100
2	D	46/52 (88%)	46 (100%)	0	0	100	100
All	All	450/466 (97%)	440 (98%)	8 (2%)	2 (0%)	34	18

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	28	LYS
1	A	27	THR

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%)	145 (93%)	11 (7%)	14 3
1	C	156/156 (100%)	144 (92%)	12 (8%)	13 3
2	B	41/45 (91%)	41 (100%)	0	100 100
2	D	41/45 (91%)	40 (98%)	1 (2%)	49 31
All	All	394/402 (98%)	370 (94%)	24 (6%)	18 5

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

Mol	Chain	Res	Type
1	A	10	LYS
1	A	30	LYS
1	A	45	LEU
1	A	72	ASN
1	A	77	TYR
1	A	93	LYS
1	A	111	LYS
1	A	132	ASN
1	A	150	LYS
1	A	153	LYS
1	A	170	THR
1	C	10	LYS
1	C	30	LYS
1	C	32	THR
1	C	33	LEU
1	C	38	LYS
1	C	76	SER
1	C	93	LYS
1	C	101	LEU
1	C	132	ASN
1	C	147	VAL
1	C	150	LYS
1	C	167	ASN
2	D	9	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	21	GLN
1	A	59	ASN
1	A	72	ASN
1	A	132	ASN
1	A	142	ASN
1	A	155	GLN
1	A	171	ASN
2	B	35	HIS
2	B	43	HIS
1	C	39	ASN
1	C	62	ASN
1	C	132	ASN
1	C	142	ASN
1	C	155	GLN
1	C	156	ASN
1	C	167	ASN
1	C	171	ASN
2	D	43	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

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 (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)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.