



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:37 AM UTC

PDB ID : 2LAL / pdb_00002lal
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 : 1993-06-10
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

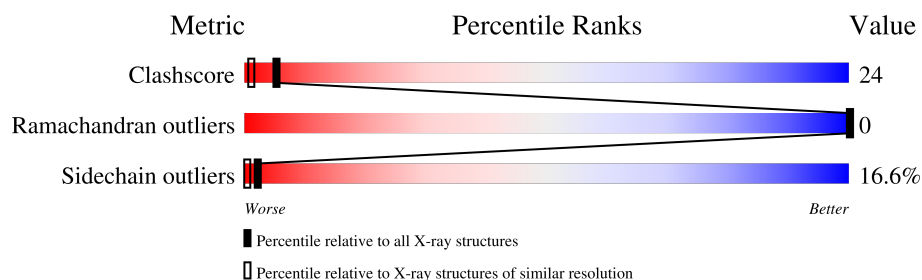
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	181	37% 43% 15% .
1	C	181	39% 43% 16% .
2	B	52	38% 33% 13% 6% 10%
2	D	52	31% 44% 15% 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.

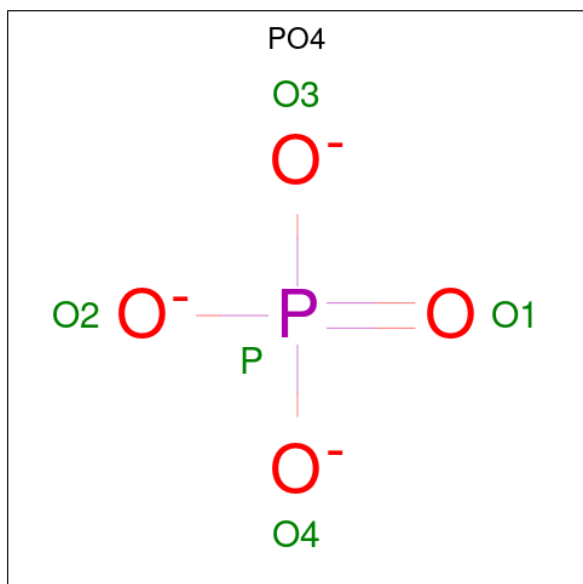
- Molecule 1 is a protein called LENTIL LECTIN (ALPHA CHAIN).

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 (CCD ID: PO4) (formula: O₄P).



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 (CCD ID: 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 (CCD ID: 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.

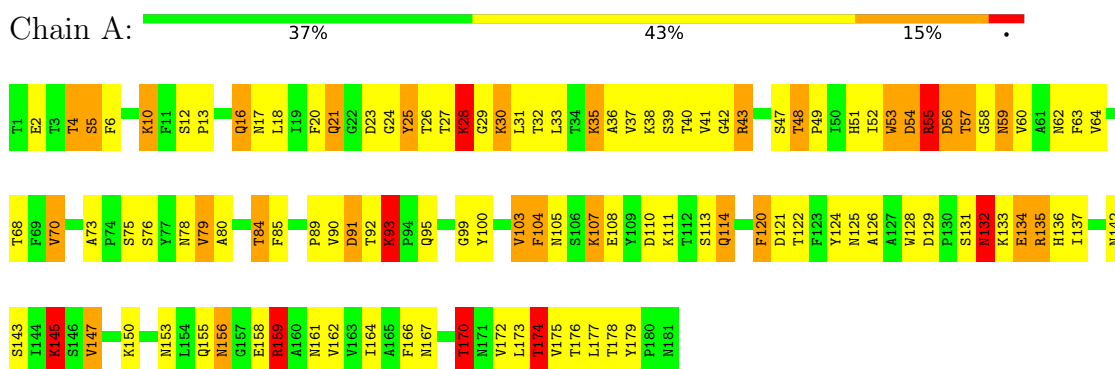
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	98	Total O 98 98	0	0
6	B	15	Total O 15 15	0	0
6	C	88	Total O 88 88	0	0
6	D	14	Total O 14 14	0	0

3 Residue-property plots

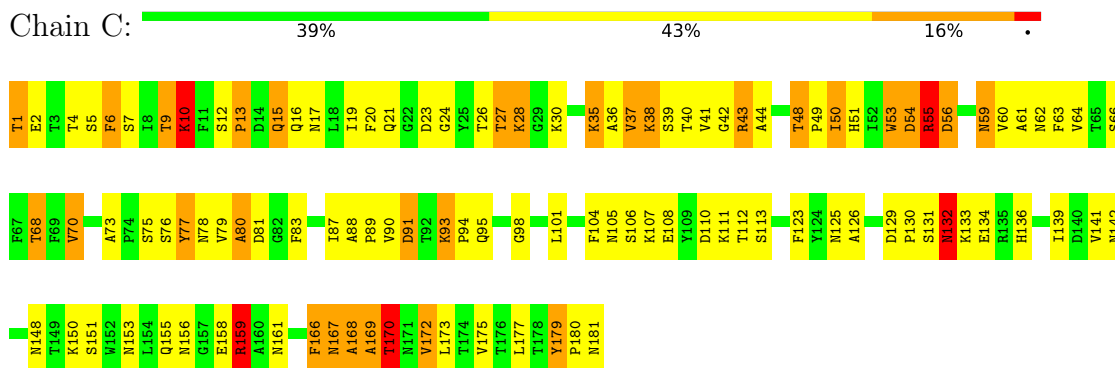
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

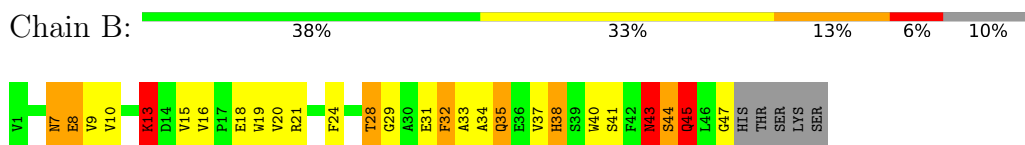
• Molecule 1: LENTIL LECTIN (ALPHA CHAIN)



• Molecule 1: LENTIL LECTIN (ALPHA CHAIN)



• Molecule 2: LENTIL LECTIN (BETA 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, α , β , γ	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 ²)	26.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, 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	1.48	14/1443 (1.0%)	2.35	95/1970 (4.8%)
1	C	1.45	15/1443 (1.0%)	2.37	102/1970 (5.2%)
2	B	1.56	6/376 (1.6%)	2.40	30/515 (5.8%)
2	D	1.62	7/376 (1.9%)	2.54	39/515 (7.6%)
All	All	1.49	42/3638 (1.2%)	2.39	266/4970 (5.4%)

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 (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	38	HIS	ND1-CE1	10.43	1.43	1.32
1	C	136	HIS	CE1-NE2	8.71	1.41	1.32
2	D	38	HIS	ND1-CE1	7.93	1.40	1.32
1	A	51	HIS	ND1-CE1	7.48	1.40	1.32
1	A	136	HIS	CE1-NE2	7.18	1.39	1.32
2	B	45	GLN	CD-OE1	7.16	1.37	1.23
2	D	45	GLN	CD-OE1	7.07	1.36	1.23
1	C	51	HIS	CE1-NE2	6.63	1.39	1.32
2	D	19	TRP	NE1-CE2	-6.30	1.30	1.37
2	D	29	GLY	N-CA	6.15	1.54	1.45
1	A	95	GLN	CD-OE1	6.13	1.35	1.23
2	D	43	ASN	CG-OD1	6.12	1.35	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	43	ASN	CG-OD1	6.11	1.35	1.23
1	A	21	GLN	CD-OE1	5.97	1.34	1.23
1	A	16	GLN	CD-OE1	5.88	1.34	1.23
1	A	155	GLN	CD-OE1	5.85	1.34	1.23
1	C	155	GLN	CD-OE1	5.78	1.34	1.23
1	A	51	HIS	CE1-NE2	5.75	1.38	1.32
1	C	16	GLN	CD-OE1	5.74	1.34	1.23
1	C	6	PHE	C-N	-5.69	1.26	1.33
1	C	51	HIS	ND1-CE1	5.68	1.38	1.32
1	C	136	HIS	ND1-CE1	5.65	1.38	1.32
2	B	19	TRP	NE1-CE2	-5.65	1.31	1.37
1	C	21	GLN	CD-OE1	5.63	1.34	1.23
1	C	4	THR	C-N	-5.61	1.25	1.33
1	A	132	ASN	CG-OD1	5.58	1.34	1.23
1	C	159	ARG	NE-CZ	5.58	1.39	1.33
1	C	53	TRP	NE1-CE2	-5.57	1.31	1.37
1	A	161	ASN	CG-OD1	5.48	1.33	1.23
2	D	7	ASN	CG-OD1	5.47	1.33	1.23
1	A	114	GLN	CD-OE1	5.37	1.33	1.23
1	C	95	GLN	CD-OE1	5.33	1.33	1.23
1	C	181	ASN	CG-OD1	5.33	1.33	1.23
2	B	7	ASN	CG-OD1	5.27	1.33	1.23
1	A	136	HIS	CG-CD2	5.25	1.41	1.35
1	A	105	ASN	CG-OD1	5.22	1.33	1.23
1	C	59	ASN	CG-OD1	5.21	1.33	1.23
1	C	161	ASN	CG-OD1	5.17	1.33	1.23
2	D	44	SER	C-N	-5.15	1.26	1.33
2	B	38	HIS	CG-CD2	5.10	1.41	1.35
1	A	136	HIS	ND1-CE1	5.09	1.37	1.32
1	A	29	GLY	N-CA	5.07	1.52	1.45

All (266) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	9	VAL	CA-C-O	-11.34	107.23	120.95
1	C	55	ARG	CA-C-N	11.09	142.72	121.54
1	C	55	ARG	C-N-CA	11.09	142.72	121.54
1	C	26	THR	CA-C-N	10.99	138.27	122.77
1	C	26	THR	C-N-CA	10.99	138.27	122.77
1	C	159	ARG	CD-NE-CZ	-10.67	109.46	124.40
1	A	55	ARG	CA-C-N	10.20	134.31	120.44
1	A	55	ARG	C-N-CA	10.20	134.31	120.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	7	ASN	CA-CB-CG	10.10	122.70	112.60
1	A	167	ASN	CA-C-N	9.81	133.42	120.28
1	A	167	ASN	C-N-CA	9.81	133.42	120.28
1	A	80	ALA	CA-C-O	-9.80	110.74	121.23
1	A	28	LYS	CA-C-N	-9.55	107.52	122.51
1	A	28	LYS	C-N-CA	-9.55	107.52	122.51
2	D	7	ASN	OD1-CG-ND2	-9.44	113.16	122.60
2	B	35	GLN	OE1-CD-NE2	-9.40	113.20	122.60
2	B	38	HIS	CA-CB-CG	-9.36	104.44	113.80
1	C	80	ALA	CA-C-O	-9.32	111.25	121.23
1	A	78	ASN	OD1-CG-ND2	-9.30	113.30	122.60
1	A	56	ASP	CA-CB-CG	-9.19	103.41	112.60
1	A	175	VAL	O-C-N	-9.06	113.47	123.26
1	C	63	PHE	CA-CB-CG	8.98	122.78	113.80
1	C	77	TYR	CA-C-O	8.85	128.98	119.34
1	A	95	GLN	OE1-CD-NE2	-8.82	113.78	122.60
1	C	37	VAL	CA-C-N	-8.73	107.42	123.05
1	C	37	VAL	C-N-CA	-8.73	107.42	123.05
1	A	85	PHE	CA-CB-CG	-8.60	105.20	113.80
1	C	15	GLN	CB-CG-CD	8.59	127.19	112.60
1	C	24	GLY	CA-C-O	-8.46	113.96	121.41
2	D	20	VAL	CA-CB-CG2	8.27	124.47	110.40
1	C	79	VAL	CA-CB-CG2	8.18	124.31	110.40
2	B	38	HIS	CB-CG-CD2	-8.16	120.59	131.20
1	C	179	TYR	CA-C-N	8.13	128.08	119.05
1	C	179	TYR	C-N-CA	8.13	128.08	119.05
1	A	129	ASP	CA-CB-CG	-8.12	104.48	112.60
2	B	16	VAL	CA-CB-CG2	8.03	124.06	110.40
2	D	43	ASN	OD1-CG-ND2	-7.98	114.62	122.60
1	A	166	PHE	CA-C-O	-7.97	111.78	120.30
1	A	62	ASN	OD1-CG-ND2	-7.94	114.66	122.60
1	A	41	VAL	CA-CB-CG2	7.94	123.90	110.40
1	C	90	VAL	CA-CB-CG1	7.90	123.84	110.40
1	A	59	ASN	CA-CB-CG	-7.85	104.75	112.60
1	C	15	GLN	OE1-CD-NE2	-7.83	114.77	122.60
2	B	32	PHE	CA-CB-CG	-7.83	105.97	113.80
1	A	29	GLY	N-CA-C	-7.72	104.89	114.92
1	C	141	VAL	CA-C-N	7.65	135.05	123.05
1	C	141	VAL	C-N-CA	7.65	135.05	123.05
1	A	120	PHE	CA-CB-CG	-7.64	106.16	113.80
1	A	137	ILE	CA-C-O	-7.60	112.12	120.71
1	A	5	SER	O-C-N	-7.57	114.85	123.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	161	ASN	CA-C-O	-7.57	112.26	120.36
2	D	6	LEU	CA-C-N	7.55	134.26	122.94
2	D	6	LEU	C-N-CA	7.55	134.26	122.94
1	A	79	VAL	CA-CB-CG2	7.53	123.21	110.40
1	A	26	THR	CA-C-N	7.50	133.72	121.58
1	A	26	THR	C-N-CA	7.50	133.72	121.58
1	C	139	ILE	CB-CG1-CD1	7.48	129.51	113.80
2	D	21	ARG	CA-C-N	7.37	134.50	122.64
2	D	21	ARG	C-N-CA	7.37	134.50	122.64
2	D	42	PHE	CA-C-N	7.34	134.62	122.73
2	D	42	PHE	C-N-CA	7.34	134.62	122.73
1	A	164	ILE	CA-C-O	-7.34	112.69	120.39
2	D	46	LEU	CA-C-O	-7.28	112.97	120.54
1	A	179	TYR	CA-C-N	7.23	126.49	118.97
1	A	179	TYR	C-N-CA	7.23	126.49	118.97
1	A	93	LYS	CA-C-O	-7.22	113.22	120.66
1	A	103	VAL	CA-CB-CG2	7.22	122.67	110.40
1	C	21	GLN	OE1-CD-NE2	-7.19	115.41	122.60
1	A	104	PHE	CA-C-O	-7.18	113.25	121.58
2	B	29	GLY	CA-C-N	7.18	130.23	120.54
2	B	29	GLY	C-N-CA	7.18	130.23	120.54
2	B	20	VAL	CA-CB-CG2	7.17	122.58	110.40
2	D	11	PRO	CA-C-N	7.10	130.12	120.54
2	D	11	PRO	C-N-CA	7.10	130.12	120.54
1	C	36	ALA	CA-C-N	7.04	134.49	122.67
1	C	36	ALA	C-N-CA	7.04	134.49	122.67
1	C	59	ASN	CA-CB-CG	-7.03	105.57	112.60
1	C	132	ASN	OD1-CG-ND2	-7.01	115.59	122.60
1	C	78	ASN	OD1-CG-ND2	-6.99	115.61	122.60
1	C	153	ASN	CA-CB-CG	-6.97	105.63	112.60
2	B	10	VAL	CA-CB-CG2	6.96	122.22	110.40
1	C	148	ASN	OD1-CG-ND2	-6.95	115.65	122.60
1	A	49	PRO	CA-C-O	-6.87	113.06	121.31
1	A	36	ALA	CA-C-N	6.84	133.57	122.69
1	A	36	ALA	C-N-CA	6.84	133.57	122.69
1	C	78	ASN	CA-CB-CG	6.82	119.42	112.60
1	C	23	ASP	CA-CB-CG	-6.81	105.79	112.60
1	C	68	THR	CA-C-O	-6.80	113.01	120.36
2	D	44	SER	CA-C-N	6.79	132.73	122.95
2	D	44	SER	C-N-CA	6.79	132.73	122.95
1	C	10	LYS	O-C-N	6.71	131.52	122.59
1	A	173	LEU	O-C-N	-6.70	115.42	123.13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	43	ARG	CA-C-N	6.68	132.13	122.44
1	C	43	ARG	C-N-CA	6.68	132.13	122.44
1	C	37	VAL	CA-CB-CG2	6.64	121.70	110.40
1	C	91	ASP	CA-CB-CG	-6.63	105.97	112.60
1	A	132	ASN	OD1-CG-ND2	-6.61	115.99	122.60
1	A	147	VAL	CA-CB-CG2	6.60	121.62	110.40
2	B	8	GLU	O-C-N	-6.55	116.01	123.48
2	D	35	GLN	OE1-CD-NE2	-6.55	116.05	122.60
1	A	145	LYS	CA-C-O	-6.52	113.23	120.60
1	A	54	ASP	CA-C-N	6.46	129.81	120.38
1	A	54	ASP	C-N-CA	6.46	129.81	120.38
1	A	63	PHE	CA-C-O	-6.46	114.36	121.33
1	A	135	ARG	NE-CZ-NH2	6.46	125.01	119.20
1	C	4	THR	CA-C-O	-6.45	111.50	120.21
1	C	129	ASP	CA-C-O	-6.42	113.69	120.88
1	A	167	ASN	OD1-CG-ND2	-6.40	116.20	122.60
1	A	37	VAL	CA-CB-CG1	6.38	121.25	110.40
1	C	9	THR	CA-C-N	-6.38	109.35	121.54
1	C	9	THR	C-N-CA	-6.38	109.35	121.54
1	A	159	ARG	CA-CB-CG	-6.36	101.38	114.10
1	A	175	VAL	CA-CB-CG2	6.35	121.20	110.40
2	D	1	VAL	CA-CB-CG1	6.35	121.20	110.40
1	C	123	PHE	CG-CD1-CE1	-6.34	109.92	120.70
1	C	155	GLN	OE1-CD-NE2	-6.33	116.27	122.60
1	C	161	ASN	CA-CB-CG	-6.33	106.27	112.60
1	A	153	ASN	CA-CB-CG	-6.33	106.27	112.60
1	A	159	ARG	CA-C-O	-6.28	113.40	120.43
1	A	161	ASN	O-C-N	6.27	130.37	123.22
1	C	98	GLY	CA-C-O	-6.23	113.94	121.67
1	A	159	ARG	CD-NE-CZ	-6.20	115.72	124.40
1	A	143	SER	CA-C-O	-6.20	114.07	120.89
2	D	38	HIS	CA-CB-CG	-6.20	107.60	113.80
1	A	16	GLN	CA-C-O	-6.19	111.00	119.05
1	A	156	ASN	OD1-CG-ND2	-6.17	116.43	122.60
1	C	6	PHE	CA-C-N	6.15	131.49	122.39
1	C	6	PHE	C-N-CA	6.15	131.49	122.39
1	C	36	ALA	CA-C-O	-6.15	114.20	122.44
2	B	15	VAL	CA-C-O	-6.14	114.75	120.34
1	C	15	GLN	CA-C-O	-6.12	115.21	122.13
1	C	175	VAL	O-C-N	-6.11	116.67	123.26
1	C	48	THR	CA-C-O	-6.08	115.08	120.19
1	C	40	THR	O-C-N	-6.08	115.25	123.15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	21	ARG	NE-CZ-NH1	5.97	127.47	121.50
1	A	36	ALA	CA-C-O	-5.96	115.20	122.41
1	C	87	ILE	CA-C-O	-5.95	114.05	120.36
1	C	126	ALA	CA-C-O	-5.94	113.39	120.10
2	D	21	ARG	NE-CZ-NH2	-5.93	113.86	119.20
1	C	54	ASP	CA-CB-CG	-5.92	106.68	112.60
2	D	16	VAL	CA-CB-CG2	5.92	120.46	110.40
1	A	162	VAL	CA-C-O	5.89	126.73	120.48
2	D	27	THR	CA-C-N	5.89	132.71	122.81
2	D	27	THR	C-N-CA	5.89	132.71	122.81
1	A	10	LYS	CA-C-O	-5.87	112.81	119.98
1	C	55	ARG	CA-C-O	-5.87	114.32	120.55
1	C	10	LYS	CA-C-N	5.85	130.21	121.72
1	C	10	LYS	C-N-CA	5.85	130.21	121.72
1	A	10	LYS	CA-C-N	5.84	130.42	122.19
1	A	10	LYS	C-N-CA	5.84	130.42	122.19
1	A	2	GLU	CA-C-N	-5.83	113.02	122.82
1	A	2	GLU	C-N-CA	-5.83	113.02	122.82
2	B	21	ARG	CA-C-O	-5.83	114.53	120.71
1	A	155	GLN	CA-C-N	5.83	129.04	120.82
1	A	155	GLN	C-N-CA	5.83	129.04	120.82
1	C	125	ASN	CA-CB-CG	-5.80	106.80	112.60
1	A	122	THR	CA-C-N	5.79	130.97	122.39
1	A	122	THR	C-N-CA	5.79	130.97	122.39
1	C	50	ILE	CB-CG1-CD1	5.78	125.93	113.80
1	A	55	ARG	CD-NE-CZ	-5.73	116.38	124.40
1	C	83	PHE	CA-C-O	-5.73	113.73	120.60
1	C	16	GLN	CG-CD-NE2	5.71	124.96	116.40
2	B	38	HIS	CB-CG-ND1	5.71	131.26	122.70
1	A	162	VAL	CA-C-N	-5.68	115.22	123.06
1	A	162	VAL	C-N-CA	-5.68	115.22	123.06
2	D	33	ALA	CA-C-O	-5.68	114.86	121.10
1	C	64	VAL	CA-CB-CG1	5.67	120.05	110.40
1	C	132	ASN	CA-C-O	-5.67	111.68	119.05
1	C	132	ASN	CB-CG-ND2	5.67	124.90	116.40
1	A	25	TYR	O-C-N	-5.65	117.32	123.26
1	C	70	VAL	CA-C-N	-5.62	115.85	122.93
1	C	70	VAL	C-N-CA	-5.62	115.85	122.93
1	C	53	TRP	CA-C-N	-5.61	114.86	122.77
1	C	53	TRP	C-N-CA	-5.61	114.86	122.77
2	D	15	VAL	CA-CB-CG2	5.59	119.90	110.40
1	C	9	THR	CA-C-O	5.58	125.88	119.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	125	ASN	O-C-N	5.57	129.68	123.05
1	C	4	THR	CA-C-N	5.55	131.45	122.29
1	C	4	THR	C-N-CA	5.55	131.45	122.29
1	C	81	ASP	CA-CB-CG	-5.54	107.06	112.60
2	B	47	GLY	CA-C-O	5.53	132.40	120.80
1	C	104	PHE	CA-C-O	-5.52	115.33	121.51
2	D	7	ASN	CA-C-O	5.52	126.66	120.70
2	B	9	VAL	CA-C-O	-5.52	114.28	120.95
2	B	19	TRP	CH2-CZ2-CE2	5.51	124.67	117.50
1	C	20	PHE	CA-CB-CG	-5.51	108.29	113.80
1	C	108	GLU	O-C-N	5.50	129.22	123.06
1	A	58	GLY	CA-C-O	5.50	126.28	119.25
2	B	28	THR	O-C-N	-5.49	115.76	123.11
1	C	41	VAL	CA-CB-CG2	5.49	119.73	110.40
2	B	40	TRP	CB-CG-CD2	-5.49	119.12	126.80
2	D	27	THR	CA-C-O	-5.48	115.21	121.40
2	D	29	GLY	N-CA-C	-5.44	100.28	113.18
1	C	23	ASP	CA-C-O	-5.44	112.70	119.28
1	C	79	VAL	CA-C-N	5.43	131.56	121.62
1	C	79	VAL	C-N-CA	5.43	131.56	121.62
2	B	43	ASN	OD1-CG-ND2	-5.42	117.18	122.60
2	B	34	ALA	CA-C-O	5.42	126.86	120.69
2	B	31	GLU	O-C-N	-5.41	116.85	122.96
1	C	130	PRO	CA-C-N	5.41	128.53	120.31
1	C	130	PRO	C-N-CA	5.41	128.53	120.31
1	C	161	ASN	CA-C-O	-5.40	114.54	120.43
2	B	21	ARG	CA-C-N	5.40	131.34	122.64
2	B	21	ARG	C-N-CA	5.40	131.34	122.64
1	A	132	ASN	CB-CG-ND2	5.39	124.48	116.40
2	D	26	ALA	CA-C-O	-5.39	114.81	121.06
1	C	151	SER	CA-C-O	5.38	126.83	120.96
1	A	95	GLN	CG-CD-NE2	5.37	124.46	116.40
2	D	9	VAL	O-C-N	5.37	128.84	122.66
1	C	168	ALA	O-C-N	5.36	128.87	122.27
1	C	170	THR	CA-C-O	5.36	124.58	118.47
2	D	28	THR	O-C-N	-5.34	115.95	123.11
1	C	60	VAL	CA-C-N	5.32	128.26	120.71
1	C	60	VAL	C-N-CA	5.32	128.26	120.71
2	D	32	PHE	CA-CB-CG	-5.31	108.49	113.80
1	A	125	ASN	CA-CB-CG	-5.31	107.29	112.60
1	C	101	LEU	CA-C-O	-5.31	112.63	119.59
1	C	42	GLY	CA-C-O	-5.31	116.95	121.57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	24	GLY	N-CA-C	-5.30	105.15	111.36
2	D	2	THR	CA-C-O	-5.29	114.70	120.36
1	A	53	TRP	CA-C-O	-5.29	115.43	121.40
2	B	33	ALA	O-C-N	5.27	129.59	122.59
1	C	13	PRO	N-CA-CB	-5.26	98.47	103.41
1	C	49	PRO	O-C-N	5.25	128.98	123.10
1	A	108	GLU	CA-C-N	5.24	129.60	121.26
1	A	108	GLU	C-N-CA	5.24	129.60	121.26
1	C	1	THR	CA-C-O	5.22	129.68	120.80
1	A	166	PHE	CA-C-N	5.22	129.36	122.42
1	A	166	PHE	C-N-CA	5.22	129.36	122.42
2	D	12	LEU	CA-C-N	5.22	128.00	120.38
2	D	12	LEU	C-N-CA	5.22	128.00	120.38
1	A	17	ASN	CA-CB-CG	-5.21	107.39	112.60
1	A	120	PHE	CA-C-N	-5.21	115.84	122.77
1	A	120	PHE	C-N-CA	-5.21	115.84	122.77
1	C	15	GLN	O-C-N	5.21	128.44	122.55
1	A	75	SER	CA-C-N	5.20	128.93	120.60
1	A	75	SER	C-N-CA	5.20	128.93	120.60
1	A	107	LYS	CA-C-O	5.20	125.36	119.18
1	C	51	HIS	CA-C-O	5.18	126.31	120.92
2	D	20	VAL	CA-C-O	-5.16	116.53	121.63
1	C	17	ASN	O-C-N	-5.15	115.74	122.39
2	B	44	SER	CA-C-N	5.15	130.01	122.39
2	B	44	SER	C-N-CA	5.15	130.01	122.39
1	A	55	ARG	NE-CZ-NH1	-5.15	116.35	121.50
1	A	24	GLY	O-C-N	-5.14	116.02	122.70
1	C	130	PRO	CA-C-O	5.13	127.19	121.34
1	A	30	LYS	CA-CB-CG	5.13	124.35	114.10
1	A	64	VAL	CA-CB-CG2	5.13	119.12	110.40
1	A	174	THR	CA-CB-OG1	5.12	117.29	109.60
1	C	166	PHE	CA-C-O	-5.12	114.83	120.30
1	A	99	GLY	N-CA-C	-5.10	107.62	115.73
1	A	121	ASP	CA-C-O	-5.09	114.91	120.36
2	D	47	GLY	CA-C-O	5.09	131.50	120.80
2	B	20	VAL	CA-C-O	-5.08	116.60	121.63
1	C	77	TYR	O-C-N	-5.07	115.81	122.20
1	C	105	ASN	CA-CB-CG	-5.07	107.53	112.60
2	B	13	LYS	CA-C-O	5.06	125.62	119.49
1	C	39	SER	CA-C-O	-5.06	116.40	122.27
2	D	7	ASN	O-C-N	-5.05	116.66	123.23
2	D	40	TRP	CA-C-O	-5.04	113.40	120.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	100	TYR	CA-C-N	5.04	130.97	123.05
1	A	100	TYR	C-N-CA	5.04	130.97	123.05
1	A	155	GLN	CG-CD-NE2	5.03	123.94	116.40
1	A	70	VAL	CA-CB-CG1	5.03	118.94	110.40
1	A	170	THR	CA-C-O	5.02	124.27	118.55
2	B	18	GLU	CB-CG-CD	-5.01	104.09	112.60

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
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 [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	1409	0	1363	73	0
1	C	1409	0	1363	81	0
2	B	366	0	350	20	0
2	D	366	0	350	21	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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	3426	170	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 (170) 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)
2:B:13:LYS:HZ2	2:B:13:LYS:HB2	1.16	1.08
1:C:73:ALA:H	1:C:156:ASN:HD21	0.98	0.97
2:B:13:LYS:HB2	2:B:13:LYS:NZ	1.77	0.96
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:O	1:C:10:LYS:HG3	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
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:C:167:ASN:HD22	1:C:167:ASN:C	1.92	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:NZ	1:A:35:LYS:HB3	2.04	0.72
1:C:27:THR:HG22	1:C:28:LYS:HD2	1.71	0.72
1:C:38:LYS:HB2	2:D:29:GLY:O	1.90	0.72
1:C:59:ASN:N	1:C:59:ASN:OD1	2.22	0.71
1:C:132:ASN:CG	1:C:134:GLU:HG3	2.16	0.70
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:LYS:NZ	1:A:28:LYS:HB2	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:A:177:LEU:C	1:A:177:LEU:HD23	2.19	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: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: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
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:N	2:B:38:HIS:CD2	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
2:B:37:VAL:C	2:B:38:HIS:HD2	2.09	0.60
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:HG23	2:D:1:VAL:O	2.02	0.59
1:A:55:ARG:HH11	1:A:55:ARG:CG	2.15	0.59
1:A:110:ASP:C	1:A:110:ASP:OD1	2.42	0.59
1:A:4:THR:O	1:A:4:THR:HG22	2.01	0.58
1:C:93:LYS:HB2	1:C:94:PRO:CD	2.34	0.58
1:A:35:LYS:NZ	1:A:35:LYS:CB	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:55:ARG:CG	1:A:55:ARG:NH1	2.64	0.57
1:A:103:VAL:HG23	1:A:104:PHE:CD2	2.40	0.57
1:C:167:ASN:HD21	1:C:169:ALA:CB	2.09	0.56
2:B:38:HIS:N	2:B:38:HIS:HD2	2.03	0.56
1:C:172:VAL:HG12	1:C:172:VAL:O	2.06	0.56
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:VAL:HG22	2:B:13:LYS:HE3	1.88	0.55
1:C:6:PHE:C	1:C:6:PHE:CD1	2.85	0.55
2:B:44:SER:C	2:B:45:GLN:HG3	2.31	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:C:38:LYS:HE2	2:D:30:ALA:C	2.33	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:O	1:C:10:LYS:CG	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
1:A:28:LYS:HB2	1:A:28:LYS:HZ2	1.73	0.52
1:A:33:LEU:O	1:A:42:GLY:HA3	2.09	0.52
1:A:6:PHE:C	1:A:6:PHE:CD1	2.88	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
2:B:13:LYS:CB	2:B:13:LYS:HZ3	2.24	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: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:77:TYR:C	1:C:77:TYR:CD1	2.90	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:C:132:ASN:HD22	1:C:132:ASN:C	2.21	0.49
1:A:55:ARG:HH11	1:A:55:ARG:HG2	1.78	0.48
2:D:13:LYS:HZ2	2:D:13:LYS:HG3	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:177:LEU:C	1:C:177:LEU:HD23	2.38	0.48
2:D:32:PHE:C	2:D:32:PHE:CD1	2.91	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:27:THR:HG22	1:C:28:LYS:CB	2.34	0.48
2:B:43:ASN:C	2:B:43:ASN:ND2	2.72	0.47
1:A:38:LYS:HG3	2:B:32:PHE:CD2	2.49	0.47
1:A:91:ASP:O	1:A:93:LYS:HD3	2.14	0.47
1:A:16:GLN:NE2	2:D:19:TRP:CD1	2.83	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:40:THR:HG22	2:B:28:THR:OG1	2.15	0.47
1:A:16:GLN:HE21	2:D:19:TRP:CD1	2.32	0.47
1:A:20:PHE:HE1	1:A:31:LEU:CD1	2.28	0.47
1:A:38:LYS:HG3	2:B:32:PHE:CE2	2.50	0.46
1:A:177:LEU:HD23	1:A:178:THR:N	2.30	0.46
1:A:28:LYS:CA	1:A:28:LYS:HE3	2.39	0.46
1:A:170:THR:HG22	1:A:172:VAL:H	1.80	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:1:THR:HG22	1:C:2:GLU:N	2.31	0.46
1:C:172:VAL:HG12	6:C:223:HOH:O	2.16	0.46
1:A:128:TRP:HB2	1:A:145:LYS:CG	2.42	0.46
1:C:167:ASN:C	1:C:167:ASN:ND2	2.62	0.45
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:80:ALA:HB3	2:D:31:GLU:C	2.42	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:55:ARG:HH11	1:C:56:ASP:CA	2.29	0.44
1:C:68:THR:HG21	1:C:159:ARG:HH21	1.82	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
1:A:177:LEU:C	1:A:177:LEU:CD2	2.87	0.43
1:C:54:ASP:CG	1:C:56:ASP:HB2	2.43	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:9:THR:O	1:C:10:LYS:HB3	2.18	0.43
1:C:93:LYS:HG2	1:C:93:LYS:H	1.79	0.42
1:C:159:ARG:HH11	1:C:159:ARG:HD2	1.49	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:ASP:O	1:A:25:TYR:HD1	2.02	0.42
1:A:12:SER:O	1:A:13:PRO:C	2.63	0.42
1:C:10:LYS:CD	1:C:10:LYS:C	2.88	0.42
1:A:53:TRP:CE3	2:B:13:LYS:HG2	2.54	0.42
1:A:114:GLN:N	1:A:142:ASN:ND2	2.67	0.42
1:C:159:ARG:NH1	2:D:38:HIS:ND1	2.68	0.42
2:D:13:LYS:CB	2:D:13:LYS:HZ3	2.32	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:10:LYS:C	1:C:10:LYS:HD2	2.45	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:32:PHE:CD1	2:B:32:PHE:C	2.99	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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 ⓘ

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%)	129 (83%)	27 (17%)	2	0
2	B	40/45 (89%)	34 (85%)	6 (15%)	3	0
2	D	40/45 (89%)	36 (90%)	4 (10%)	7	2
All	All	392/402 (98%)	327 (83%)	65 (17%)	2	0

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	THR
1	A	5	SER
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	90	VAL
1	A	91	ASP
1	A	93	LYS
1	A	107	LYS
1	A	111	LYS
1	A	132	ASN
1	A	134	GLU
1	A	145	LYS
1	A	150	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	35	GLN
2	B	41	SER
2	B	43	ASN
2	B	45	GLN
1	C	5	SER
1	C	7	SER
1	C	10	LYS
1	C	15	GLN
1	C	28	LYS
1	C	30	LYS
1	C	35	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
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	78	ASN
1	A	132	ASN
1	A	142	ASN
1	A	156	ASN
1	A	171	ASN
2	B	38	HIS
2	B	45	GLN
1	C	62	ASN
1	C	105	ASN
1	C	132	ASN
1	C	142	ASN
1	C	148	ASN
1	C	153	ASN
1	C	156	ASN
1	C	161	ASN
1	C	167	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	PO4	C	182	-	4,4,4	1.63	1 (25%)	6,6,6	0.72	0
3	PO4	A	182	-	4,4,4	0.91	0	6,6,6	0.84	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	2.62	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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.