



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:40 PM GMT

PDB ID : 1LFH  
Title : MOLECULAR REPLACEMENT SOLUTION OF THE STRUCTURE OF  
APOLACTOFERRIN, A PROTEIN DISPLAYING LARGE-SCALE CON-  
FORMATIONAL CHANGE  
Authors : Anderson, B.F.; Baker, E.N.; Norris, G.E.  
Deposited on : 1991-09-04  
Resolution : 2.80 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

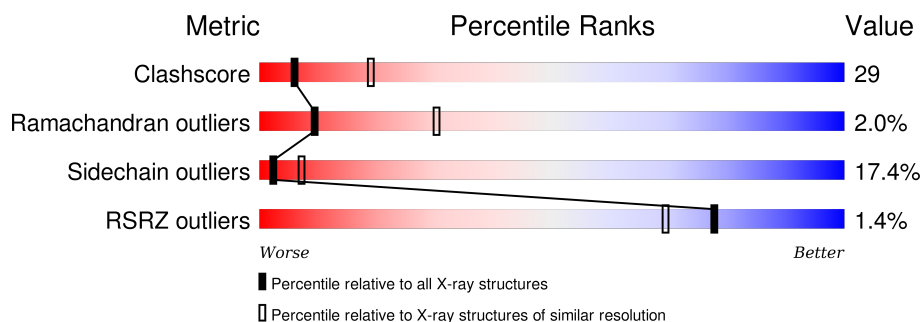
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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.

Mol	Chain	Length	Quality of chain
1	A	691	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5716 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 LACTOFERRIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	691	Total	C	N	O	S	0	0	0
			5342	3337	954	1014	37			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	ASN	GLN	CONFLICT	UNP P02788
A	200	LYS	ARG	CONFLICT	UNP P02788
A	512	GLU	GLN	CONFLICT	UNP P02788

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

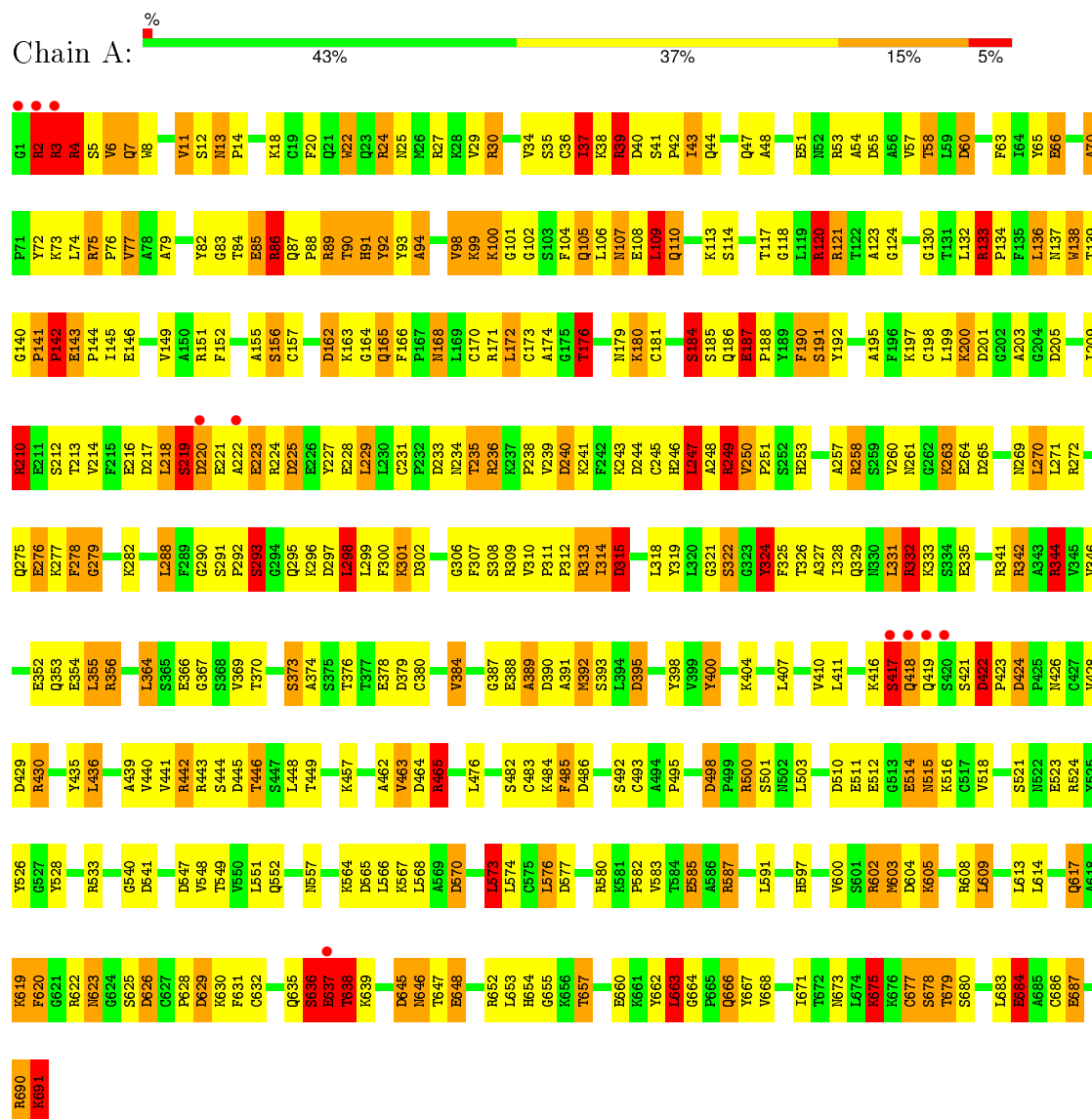
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	373	Total	O	0	0
			373	373		

### 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 errors 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: LACTOFERRIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	152.09 Å 94.58 Å 55.79 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.80 29.39 – 2.79	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-2.80) 86.2 (29.39-2.79)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.90 (at 2.80 Å)	Xtriage
Refinement program	TNT	Depositor
R, $R_{free}$	0.213 , (Not available) 0.190 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	41.8	Xtriage
Anisotropy	0.407	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 78.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 17783 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	5716	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.19% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: CL

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	0.93	0/5456	2.52	297/7378 (4.0%)

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	2

There are no bond length outliers.

All (297) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	258	ARG	NE-CZ-NH2	-32.77	103.91	120.30
1	A	442	ARG	CD-NE-CZ	28.96	164.15	123.60
1	A	524	ARG	NE-CZ-NH1	-25.53	107.54	120.30
1	A	210	ARG	CD-NE-CZ	23.89	157.05	123.60
1	A	142	PRO	C-N-CA	22.29	177.43	121.70
1	A	39	ARG	NE-CZ-NH1	22.15	131.38	120.30
1	A	602	ARG	NE-CZ-NH2	-17.55	111.52	120.30
1	A	332	ARG	NE-CZ-NH1	16.92	128.76	120.30
1	A	424	ASP	CB-CG-OD2	-16.34	103.59	118.30
1	A	210	ARG	NE-CZ-NH1	-15.00	112.80	120.30
1	A	533	ARG	NE-CZ-NH1	14.67	127.63	120.30
1	A	662	TYR	CB-CG-CD1	-13.63	112.82	121.00
1	A	662	TYR	CB-CG-CD2	13.23	128.94	121.00
1	A	293	SER	CA-C-N	12.90	142.00	116.20
1	A	258	ARG	NH1-CZ-NH2	12.84	133.53	119.40
1	A	652	ARG	NE-CZ-NH2	-12.73	113.93	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	602	ARG	NE-CZ-NH1	12.38	126.49	120.30
1	A	133	ARG	CD-NE-CZ	12.02	140.43	123.60
1	A	486	ASP	CB-CG-OD1	11.83	128.95	118.30
1	A	510	ASP	CB-CG-OD2	-11.75	107.72	118.30
1	A	500	ARG	NE-CZ-NH1	11.69	126.14	120.30
1	A	580	ARG	NE-CZ-NH1	11.61	126.10	120.30
1	A	344	ARG	NE-CZ-NH2	-11.47	114.56	120.30
1	A	390	ASP	CB-CG-OD1	-11.33	108.11	118.30
1	A	604	ASP	CB-CG-OD1	-11.29	108.14	118.30
1	A	319	TYR	CB-CG-CD2	11.27	127.76	121.00
1	A	314	ILE	C-N-CA	11.06	149.35	121.70
1	A	210	ARG	NE-CZ-NH2	11.05	125.82	120.30
1	A	356	ARG	CD-NE-CZ	10.99	138.99	123.60
1	A	465	ARG	NE-CZ-NH1	10.98	125.79	120.30
1	A	524	ARG	NE-CZ-NH2	10.87	125.74	120.30
1	A	498	ASP	CB-CG-OD1	10.79	128.01	118.30
1	A	249	ARG	N-CA-CB	10.75	129.95	110.60
1	A	400	TYR	CB-CG-CD1	-10.73	114.56	121.00
1	A	205	ASP	CB-CG-OD2	10.61	127.84	118.30
1	A	53	ARG	NE-CZ-NH2	-10.40	115.10	120.30
1	A	4	ARG	NE-CZ-NH1	10.38	125.49	120.30
1	A	608	ARG	NE-CZ-NH1	-10.34	115.13	120.30
1	A	587	ARG	NE-CZ-NH1	-10.33	115.14	120.30
1	A	435	TYR	CB-CG-CD2	-10.15	114.91	121.00
1	A	342	ARG	NE-CZ-NH1	-10.10	115.25	120.30
1	A	313	ARG	CG-CD-NE	10.06	132.93	111.80
1	A	442	ARG	NE-CZ-NH2	10.02	125.31	120.30
1	A	547	ASP	CB-CG-OD1	10.02	127.31	118.30
1	A	236	ARG	NE-CZ-NH2	-10.00	115.30	120.30
1	A	39	ARG	NH1-CZ-NH2	-9.99	108.42	119.40
1	A	443	ARG	NE-CZ-NH1	9.80	125.20	120.30
1	A	356	ARG	NE-CZ-NH1	9.66	125.13	120.30
1	A	30	ARG	NE-CZ-NH2	-9.61	115.50	120.30
1	A	619	LYS	CA-CB-CG	9.53	134.36	113.40
1	A	227	TYR	CB-CG-CD1	-9.48	115.31	121.00
1	A	75	ARG	NE-CZ-NH2	9.46	125.03	120.30
1	A	225	ASP	CB-CG-OD1	9.44	126.79	118.30
1	A	486	ASP	CB-CG-OD2	-9.36	109.87	118.30
1	A	223	GLU	CA-CB-CG	9.32	133.92	113.40
1	A	225	ASP	CA-CB-CG	9.32	133.91	113.40
1	A	142	PRO	O-C-N	-9.31	107.80	122.70
1	A	53	ARG	NE-CZ-NH1	9.29	124.94	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	315	ASP	N-CA-CB	-9.23	93.99	110.60
1	A	60	ASP	CB-CG-OD1	9.19	126.57	118.30
1	A	528	TYR	CB-CG-CD1	-9.19	115.49	121.00
1	A	577	ASP	CB-CG-OD1	9.14	126.53	118.30
1	A	570	ASP	CB-CG-OD2	-9.07	110.14	118.30
1	A	493	CYS	N-CA-CB	8.97	126.75	110.60
1	A	356	ARG	NE-CZ-NH2	-8.96	115.82	120.30
1	A	39	ARG	CD-NE-CZ	8.79	135.91	123.60
1	A	691	LYS	N-CA-CB	8.73	126.31	110.60
1	A	293	SER	CA-C-O	-8.70	101.83	120.10
1	A	395	ASP	CB-CG-OD1	8.66	126.09	118.30
1	A	629	ASP	CB-CG-OD2	-8.66	110.51	118.30
1	A	424	ASP	OD1-CG-OD2	8.63	139.69	123.30
1	A	395	ASP	CA-C-N	8.37	132.95	116.20
1	A	376	THR	O-C-N	8.35	136.06	122.70
1	A	187	GLU	CA-CB-CG	8.34	131.75	113.40
1	A	227	TYR	CA-CB-CG	-8.27	97.69	113.40
1	A	157	CYS	N-CA-CB	8.23	125.41	110.60
1	A	580	ARG	CD-NE-CZ	8.12	134.96	123.60
1	A	40	ASP	CB-CG-OD2	-8.02	111.08	118.30
1	A	319	TYR	CB-CG-CD1	-8.01	116.19	121.00
1	A	37	ILE	CB-CA-C	7.99	127.57	111.60
1	A	366	GLU	CA-CB-CG	7.97	130.94	113.40
1	A	514	GLU	OE1-CD-OE2	7.97	132.87	123.30
1	A	176	THR	CA-CB-CG2	7.94	123.52	112.40
1	A	309	ARG	NE-CZ-NH1	7.92	124.26	120.30
1	A	660	GLU	CA-CB-CG	7.91	130.81	113.40
1	A	332	ARG	CD-NE-CZ	7.90	134.66	123.60
1	A	541	ASP	CB-CG-OD2	7.80	125.32	118.30
1	A	398	TYR	CB-CG-CD1	7.80	125.68	121.00
1	A	512	GLU	OE1-CD-OE2	7.79	132.64	123.30
1	A	435	TYR	CB-CG-CD1	7.77	125.66	121.00
1	A	364	LEU	CA-CB-CG	7.68	132.97	115.30
1	A	133	ARG	NE-CZ-NH1	7.58	124.09	120.30
1	A	430	ARG	CD-NE-CZ	-7.57	113.00	123.60
1	A	65	TYR	CB-CG-CD1	-7.54	116.47	121.00
1	A	439	ALA	O-C-N	7.51	134.72	122.70
1	A	626	ASP	CB-CG-OD1	-7.47	111.58	118.30
1	A	184	SER	CB-CA-C	-7.46	95.92	110.10
1	A	342	ARG	CD-NE-CZ	-7.41	113.23	123.60
1	A	660	GLU	OE1-CD-OE2	-7.36	114.47	123.30
1	A	249	ARG	NE-CZ-NH1	7.34	123.97	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	249	ARG	CA-CB-CG	7.34	129.54	113.40
1	A	687	GLU	CB-CG-CD	7.32	133.95	114.20
1	A	313	ARG	NE-CZ-NH2	-7.23	116.68	120.30
1	A	398	TYR	CB-CG-CD2	-7.20	116.68	121.00
1	A	314	ILE	O-C-N	-7.19	111.20	122.70
1	A	374	ALA	CB-CA-C	7.18	120.87	110.10
1	A	617	GLN	CG-CD-OE1	-7.16	107.27	121.60
1	A	36	CYS	O-C-N	7.16	134.16	122.70
1	A	379	ASP	CB-CG-OD1	7.16	124.74	118.30
1	A	442	ARG	NE-CZ-NH1	-7.15	116.72	120.30
1	A	429	ASP	CB-CG-OD2	7.14	124.73	118.30
1	A	422	ASP	CB-CG-OD1	7.14	124.72	118.30
1	A	143	GLU	N-CA-CB	7.13	123.43	110.60
1	A	580	ARG	NE-CZ-NH2	-7.11	116.75	120.30
1	A	315	ASP	CA-C-N	7.08	132.77	117.20
1	A	272	ARG	NE-CZ-NH2	-7.05	116.77	120.30
1	A	133	ARG	CA-CB-CG	7.02	128.85	113.40
1	A	104	PHE	N-CA-CB	6.97	123.15	110.60
1	A	63	PHE	CB-CG-CD2	6.90	125.63	120.80
1	A	315	ASP	O-C-N	-6.89	111.67	122.70
1	A	570	ASP	OD1-CG-OD2	6.86	136.33	123.30
1	A	332	ARG	NH1-CZ-NH2	-6.75	111.97	119.40
1	A	587	ARG	CD-NE-CZ	-6.74	114.17	123.60
1	A	65	TYR	CB-CG-CD2	6.72	125.03	121.00
1	A	278	PHE	CB-CG-CD1	-6.72	116.10	120.80
1	A	146	GLU	CG-CD-OE1	6.71	131.72	118.30
1	A	493	CYS	N-CA-C	-6.68	92.97	111.00
1	A	102	GLY	N-CA-C	-6.66	96.45	113.10
1	A	524	ARG	NH1-CZ-NH2	6.61	126.68	119.40
1	A	296	LYS	C-N-CA	6.61	138.21	121.70
1	A	92	TYR	CB-CA-C	6.60	123.60	110.40
1	A	146	GLU	OE1-CD-OE2	-6.58	115.40	123.30
1	A	465	ARG	NH1-CZ-NH2	-6.58	112.16	119.40
1	A	210	ARG	N-CA-CB	6.57	122.43	110.60
1	A	482	SER	CA-C-O	6.56	133.88	120.10
1	A	41	SER	O-C-N	6.55	133.54	121.10
1	A	464	ASP	CB-CG-OD1	6.54	124.19	118.30
1	A	523	GLU	O-C-N	-6.51	112.28	122.70
1	A	223	GLU	N-CA-CB	6.51	122.32	110.60
1	A	109	LEU	CB-CA-C	6.50	122.56	110.20
1	A	70	ALA	N-CA-CB	6.50	119.19	110.10
1	A	603	MET	CA-CB-CG	-6.48	102.28	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	623	ASN	CB-CA-C	6.48	123.36	110.40
1	A	89	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	A	190	PHE	C-N-CA	6.48	137.90	121.70
1	A	51	GLU	OE1-CD-OE2	6.42	131.00	123.30
1	A	66	GLU	OE1-CD-OE2	-6.41	115.60	123.30
1	A	3	ARG	NE-CZ-NH2	-6.41	117.10	120.30
1	A	354	GLU	N-CA-CB	6.39	122.10	110.60
1	A	315	ASP	CB-CG-OD2	-6.39	112.55	118.30
1	A	660	GLU	O-C-N	-6.37	112.51	122.70
1	A	636	SER	N-CA-CB	6.34	120.02	110.50
1	A	526	TYR	C-N-CA	6.33	135.60	122.30
1	A	133	ARG	CG-CD-NE	6.33	125.09	111.80
1	A	250	VAL	CB-CA-C	6.31	123.40	111.40
1	A	57	VAL	CA-CB-CG1	6.30	120.35	110.90
1	A	675	LYS	CB-CA-C	6.30	122.99	110.40
1	A	400	TYR	CB-CG-CD2	6.29	124.78	121.00
1	A	387	GLY	O-C-N	-6.25	112.69	122.70
1	A	585	GLU	CG-CD-OE1	-6.24	105.83	118.30
1	A	684	GLU	CG-CD-OE2	-6.22	105.86	118.30
1	A	533	ARG	CD-NE-CZ	-6.20	114.92	123.60
1	A	424	ASP	N-CA-CB	-6.19	99.47	110.60
1	A	205	ASP	CB-CG-OD1	-6.14	112.78	118.30
1	A	151	ARG	N-CA-CB	6.14	121.65	110.60
1	A	547	ASP	CB-CG-OD2	-6.13	112.79	118.30
1	A	631	PHE	CB-CG-CD2	-6.12	116.52	120.80
1	A	149	VAL	CB-CA-C	6.11	123.00	111.40
1	A	626	ASP	O-C-N	6.10	132.47	122.70
1	A	3	ARG	NE-CZ-NH1	6.09	123.34	120.30
1	A	38	LYS	CB-CG-CD	6.09	127.43	111.60
1	A	216	GLU	CA-CB-CG	6.09	126.80	113.40
1	A	240	ASP	CB-CG-OD1	6.09	123.78	118.30
1	A	652	ARG	NH1-CZ-NH2	6.08	126.09	119.40
1	A	666	GLN	CA-CB-CG	6.07	126.76	113.40
1	A	39	ARG	CG-CD-NE	-6.07	99.06	111.80
1	A	258	ARG	CG-CD-NE	-6.06	99.07	111.80
1	A	120	ARG	NE-CZ-NH2	-6.05	117.27	120.30
1	A	92	TYR	CB-CG-CD1	-6.02	117.39	121.00
1	A	36	CYS	CA-CB-SG	-6.02	103.17	114.00
1	A	225	ASP	CB-CA-C	6.01	122.42	110.40
1	A	123	ALA	CA-C-N	6.00	128.19	116.20
1	A	654	HIS	CA-CB-CG	-6.00	103.41	113.60
1	A	523	GLU	CA-C-N	5.96	130.32	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	24	ARG	CD-NE-CZ	-5.96	115.25	123.60
1	A	648	GLU	OE1-CD-OE2	5.96	130.45	123.30
1	A	428	VAL	CA-C-O	-5.95	107.60	120.10
1	A	411	LEU	O-C-N	5.92	132.17	122.70
1	A	162	ASP	CB-CG-OD1	-5.88	113.01	118.30
1	A	249	ARG	O-C-N	5.87	132.09	122.70
1	A	533	ARG	NH1-CZ-NH2	-5.87	112.94	119.40
1	A	677	CYS	CB-CA-C	-5.86	98.68	110.40
1	A	573	LEU	CA-CB-CG	5.83	128.72	115.30
1	A	549	THR	O-C-N	5.80	131.99	122.70
1	A	82	TYR	CB-CG-CD1	-5.80	117.52	121.00
1	A	645	ASP	CB-CG-OD1	5.79	123.52	118.30
1	A	605	LYS	CG-CD-CE	5.79	129.27	111.90
1	A	225	ASP	CB-CG-OD2	-5.78	113.10	118.30
1	A	565	ASP	CB-CG-OD2	-5.76	113.11	118.30
1	A	248	ALA	CA-C-O	-5.76	108.01	120.10
1	A	327	ALA	CB-CA-C	5.75	118.73	110.10
1	A	625	SER	CA-CB-OG	5.75	126.72	111.20
1	A	636	SER	N-CA-C	-5.74	95.51	111.00
1	A	313	ARG	NE-CZ-NH1	5.73	123.17	120.30
1	A	620	PHE	CB-CG-CD2	-5.73	116.79	120.80
1	A	430	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	A	485	PHE	CB-CG-CD1	-5.71	116.80	120.80
1	A	609	LEU	CA-C-O	-5.71	108.12	120.10
1	A	390	ASP	CB-CG-OD2	5.70	123.43	118.30
1	A	11	VAL	N-CA-CB	-5.68	98.99	111.50
1	A	551	LEU	CB-CG-CD2	-5.68	101.35	111.00
1	A	637	GLU	CA-CB-CG	5.67	125.88	113.40
1	A	482	SER	O-C-N	-5.63	113.69	122.70
1	A	199	LEU	CA-C-O	5.60	131.87	120.10
1	A	677	CYS	O-C-N	5.60	131.66	122.70
1	A	684	GLU	OE1-CD-OE2	5.59	130.01	123.30
1	A	500	ARG	NH1-CZ-NH2	-5.59	113.25	119.40
1	A	389	ALA	N-CA-CB	5.58	117.92	110.10
1	A	580	ARG	N-CA-CB	5.58	120.64	110.60
1	A	264	GLU	CA-CB-CG	5.57	125.66	113.40
1	A	313	ARG	CD-NE-CZ	-5.57	115.80	123.60
1	A	551	LEU	CB-CG-CD1	5.55	120.44	111.00
1	A	369	VAL	CA-CB-CG2	5.55	119.23	110.90
1	A	614	LEU	CA-C-N	-5.55	104.99	117.20
1	A	168	ASN	O-C-N	5.55	131.57	122.70
1	A	393	SER	CA-C-O	-5.54	108.46	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	98	VAL	CA-CB-CG1	5.53	119.19	110.90
1	A	250	VAL	CA-C-O	5.52	131.69	120.10
1	A	498	ASP	CB-CG-OD2	-5.52	113.33	118.30
1	A	7	GLN	O-C-N	5.50	131.50	122.70
1	A	201	ASP	CB-CG-OD1	5.49	123.24	118.30
1	A	342	ARG	NH1-CZ-NH2	5.49	125.44	119.40
1	A	306	GLY	O-C-N	5.47	131.46	122.70
1	A	657	THR	N-CA-CB	-5.46	99.94	110.30
1	A	138	TRP	CB-CA-C	-5.45	99.50	110.40
1	A	6	VAL	CA-C-N	5.45	129.19	117.20
1	A	457	LYS	CA-CB-CG	-5.45	101.42	113.40
1	A	557	ASN	CA-CB-CG	-5.45	101.42	113.40
1	A	37	ILE	N-CA-CB	-5.44	98.28	110.80
1	A	463	VAL	CB-CA-C	5.43	121.72	111.40
1	A	666	GLN	N-CA-CB	5.42	120.36	110.60
1	A	653	LEU	N-CA-CB	-5.42	99.57	110.40
1	A	515	ASN	O-C-N	5.41	131.35	122.70
1	A	457	LYS	CD-CE-NZ	-5.40	99.27	111.70
1	A	94	ALA	N-CA-CB	5.40	117.66	110.10
1	A	258	ARG	O-C-N	5.39	131.32	122.70
1	A	324	TYR	CA-CB-CG	5.38	123.63	113.40
1	A	246	HIS	O-C-N	5.38	131.31	122.70
1	A	388	GLU	CA-CB-CG	5.37	125.21	113.40
1	A	2	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	A	51	GLU	CG-CD-OE1	-5.36	107.59	118.30
1	A	298	LEU	O-C-N	5.35	131.26	122.70
1	A	626	ASP	CA-C-O	-5.34	108.88	120.10
1	A	258	ARG	N-CA-CB	5.34	120.22	110.60
1	A	600	VAL	O-C-N	5.33	131.24	122.70
1	A	27	ARG	CD-NE-CZ	5.33	131.06	123.60
1	A	570	ASP	CB-CG-OD1	-5.32	113.51	118.30
1	A	335	GLU	CG-CD-OE1	5.32	128.94	118.30
1	A	585	GLU	CG-CD-OE2	5.30	128.89	118.30
1	A	355	LEU	CB-CG-CD2	-5.29	102.02	111.00
1	A	366	GLU	CG-CD-OE2	5.29	128.87	118.30
1	A	647	THR	CA-CB-CG2	5.26	119.76	112.40
1	A	22	TRP	CA-CB-CG	5.25	123.67	113.70
1	A	648	GLU	CA-C-O	5.25	131.12	120.10
1	A	25	ASN	OD1-CG-ND2	5.22	133.90	121.90
1	A	99	LYS	N-CA-CB	5.20	119.96	110.60
1	A	136	LEU	CA-C-N	5.20	128.65	117.20
1	A	449	THR	CA-CB-OG1	-5.20	98.08	109.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	637	GLU	CA-C-O	5.20	131.01	120.10
1	A	136	LEU	CB-CG-CD1	-5.19	102.17	111.00
1	A	335	GLU	CA-CB-CG	5.18	124.80	113.40
1	A	445	ASP	C-N-CA	5.17	134.63	121.70
1	A	133	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	A	485	PHE	CB-CG-CD2	5.17	124.42	120.80
1	A	108	GLU	OE1-CD-OE2	5.15	129.48	123.30
1	A	511	GLU	O-C-N	5.14	130.93	122.70
1	A	30	ARG	C-N-CA	5.14	133.09	122.30
1	A	603	MET	CB-CG-SD	-5.14	96.98	112.40
1	A	245	CYS	N-CA-CB	-5.13	101.37	110.60
1	A	217	ASP	CB-CG-OD2	5.11	122.90	118.30
1	A	25	ASN	CA-C-O	-5.11	109.37	120.10
1	A	691	LYS	CB-CA-C	-5.10	100.21	110.40
1	A	247	LEU	CA-CB-CG	5.09	127.02	115.30
1	A	258	ARG	CB-CG-CD	-5.09	98.36	111.60
1	A	446	THR	CA-CB-CG2	5.09	119.52	112.40
1	A	392	MET	CA-CB-CG	-5.08	104.66	113.30
1	A	344	ARG	NH1-CZ-NH2	5.07	124.98	119.40
1	A	373	SER	CA-C-N	-5.07	106.05	117.20
1	A	580	ARG	O-C-N	5.06	130.79	122.70
1	A	391	ALA	N-CA-CB	-5.05	103.03	110.10
1	A	146	GLU	CA-CB-CG	5.04	124.49	113.40
1	A	384	VAL	CA-CB-CG2	5.04	118.46	110.90
1	A	258	ARG	CD-NE-CZ	-5.03	116.55	123.60
1	A	663	LEU	CA-CB-CG	5.03	126.86	115.30
1	A	652	ARG	CB-CG-CD	5.02	124.66	111.60
1	A	604	ASP	OD1-CG-OD2	5.02	132.84	123.30
1	A	482	SER	N-CA-CB	-5.01	102.99	110.50

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	258	ARG	Sidechain
1	A	465	ARG	Sidechain

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5342	0	5205	301	0
2	A	1	0	0	0	0
3	A	373	0	0	33	0
All	All	5716	0	5205	301	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 29.

All (301) 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:37:ILE:HD11	1:A:39:ARG:NH2	1.50	1.23
1:A:37:ILE:HD11	1:A:39:ARG:HH21	1.02	1.10
1:A:105:GLN:HA	1:A:105:GLN:HE21	1.24	1.02
1:A:679:THR:HG23	1:A:680:SER:H	1.22	1.00
1:A:622:ARG:NH1	1:A:635:GLN:HE21	1.57	0.99
1:A:622:ARG:HH12	1:A:635:GLN:NE2	1.59	0.98
1:A:37:ILE:CD1	1:A:39:ARG:HH21	1.79	0.95
1:A:85:GLU:O	1:A:86:ARG:HB2	1.66	0.95
1:A:87:GLN:N	1:A:88:PRO:HD3	1.82	0.95
1:A:269:ASN:HB3	3:A:783:HOH:O	1.66	0.94
1:A:155:ALA:HB1	1:A:172:LEU:HD21	1.50	0.93
1:A:4:ARG:HB2	1:A:4:ARG:HH11	1.32	0.92
1:A:87:GLN:N	1:A:88:PRO:CD	2.36	0.88
1:A:636:SER:HB2	1:A:639:LYS:CB	2.02	0.88
1:A:679:THR:CG2	1:A:680:SER:H	1.87	0.88
1:A:311:PRO:HD2	1:A:314:ILE:HD12	1.56	0.87
1:A:344:ARG:CD	1:A:370:THR:HG21	2.06	0.85
1:A:626:ASP:HB3	1:A:630:LYS:HG3	1.60	0.84
1:A:218:LEU:HD23	1:A:224:ARG:HG2	1.59	0.84
1:A:636:SER:HB2	1:A:639:LYS:HB3	1.59	0.82
1:A:155:ALA:CB	1:A:172:LEU:HD21	2.09	0.82
1:A:8:TRP:O	1:A:37:ILE:HG22	1.81	0.81
1:A:121:ARG:HH12	1:A:191:SER:HB2	1.46	0.80
1:A:276:GLU:O	1:A:282:LYS:HD2	1.82	0.79
1:A:344:ARG:HD2	1:A:370:THR:HG21	1.66	0.78
1:A:515:ASN:O	1:A:518:VAL:HG22	1.84	0.78
1:A:346:VAL:HG22	1:A:370:THR:CG2	2.15	0.76
1:A:100:LYS:HD2	1:A:100:LYS:C	2.05	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:ARG:CB	1:A:4:ARG:HH11	1.99	0.75
1:A:13:ASN:N	1:A:14:PRO:CD	2.49	0.75
1:A:105:GLN:HA	1:A:105:GLN:NE2	1.99	0.74
1:A:77:VAL:HG11	1:A:257:ALA:HB3	1.69	0.74
1:A:344:ARG:HD3	1:A:370:THR:CG2	2.17	0.74
1:A:3:ARG:C	1:A:5:SER:H	1.90	0.74
1:A:86:ARG:H	1:A:88:PRO:HD3	1.53	0.74
1:A:143:GLU:HG3	1:A:144:PRO:CD	2.18	0.74
1:A:646:ASN:HD22	1:A:646:ASN:H	1.31	0.74
1:A:293:SER:HB2	3:A:977:HOH:O	1.87	0.74
1:A:105:GLN:HE22	1:A:236:ARG:HG3	1.53	0.73
1:A:110:GLN:HG2	1:A:152:PHE:CE2	2.22	0.73
1:A:3:ARG:O	1:A:5:SER:N	2.22	0.72
1:A:679:THR:CG2	1:A:680:SER:N	2.52	0.72
1:A:344:ARG:HD3	1:A:370:THR:HG21	1.72	0.72
1:A:162:ASP:OD1	1:A:165:GLN:HB2	1.89	0.72
1:A:3:ARG:HB3	1:A:3:ARG:NH1	2.05	0.72
1:A:418:GLN:NE2	1:A:587:ARG:NH1	2.37	0.71
1:A:344:ARG:O	1:A:605:LYS:NZ	2.19	0.71
1:A:686:CYS:O	1:A:690:ARG:HG3	1.91	0.71
1:A:570:ASP:OD2	3:A:1041:HOH:O	2.08	0.70
1:A:133:ARG:NH1	1:A:333:LYS:O	2.23	0.70
1:A:663:LEU:HG	1:A:667:TYR:HD2	1.54	0.70
1:A:2:ARG:HG2	1:A:2:ARG:HH11	1.56	0.70
1:A:87:GLN:HG3	3:A:706:HOH:O	1.92	0.70
1:A:180:LYS:HG2	3:A:952:HOH:O	1.92	0.70
1:A:636:SER:HB2	1:A:639:LYS:HB2	1.73	0.69
1:A:86:ARG:N	1:A:88:PRO:HD3	2.08	0.69
1:A:14:PRO:HB3	1:A:295:GLN:OE1	1.93	0.68
1:A:613:LEU:O	1:A:617:GLN:HB2	1.93	0.68
1:A:138:TRP:CH2	1:A:141:PRO:HD3	2.28	0.68
1:A:240:ASP:HB3	3:A:962:HOH:O	1.94	0.68
1:A:249:ARG:HG3	1:A:249:ARG:NH1	2.07	0.68
1:A:174:ALA:HB3	1:A:188:PRO:HG2	1.76	0.68
1:A:143:GLU:HG3	1:A:144:PRO:HD2	1.75	0.68
1:A:70:ALA:HB2	1:A:73:LYS:HE2	1.76	0.68
1:A:315:ASP:HB3	1:A:318:LEU:H	1.57	0.67
1:A:2:ARG:NH1	1:A:2:ARG:HG2	2.09	0.67
1:A:155:ALA:HB1	1:A:172:LEU:CD2	2.23	0.66
1:A:346:VAL:HG22	1:A:370:THR:HG23	1.76	0.66
1:A:638:THR:N	1:A:645:ASP:OD2	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:ARG:HD3	3:A:806:HOH:O	1.96	0.66
1:A:691:LYS:HG2	1:A:691:LYS:O	1.94	0.66
1:A:241:LYS:HA	3:A:963:HOH:O	1.97	0.65
1:A:105:GLN:HB2	1:A:107:ASN:HD21	1.60	0.65
1:A:646:ASN:ND2	1:A:646:ASN:H	1.95	0.65
1:A:133:ARG:N	1:A:134:PRO:HD2	2.12	0.65
1:A:42:PRO:HG3	3:A:927:HOH:O	1.97	0.65
1:A:114:SER:O	1:A:156:SER:HA	1.96	0.65
1:A:107:ASN:HD22	1:A:107:ASN:H	1.45	0.64
1:A:22:TRP:CZ2	1:A:270:LEU:HD21	2.32	0.64
1:A:241:LYS:HE3	1:A:244:ASP:HB2	1.80	0.63
1:A:184:SER:HB2	1:A:186:GLN:H	1.63	0.63
1:A:344:ARG:CD	1:A:370:THR:CG2	2.75	0.62
1:A:418:GLN:HE22	1:A:587:ARG:HD3	1.64	0.62
1:A:105:GLN:HB2	1:A:107:ASN:ND2	2.15	0.61
1:A:3:ARG:HB3	1:A:3:ARG:HH11	1.63	0.61
1:A:93:TYR:OH	1:A:243:LYS:HE2	2.00	0.61
1:A:100:LYS:HD2	1:A:101:GLY:N	2.16	0.61
1:A:675:LYS:HE2	3:A:1024:HOH:O	2.01	0.61
1:A:39:ARG:HB3	1:A:44:GLN:HB3	1.83	0.61
1:A:384:VAL:HG22	1:A:407:LEU:HD11	1.81	0.61
1:A:87:GLN:H	1:A:88:PRO:HD3	1.65	0.61
1:A:4:ARG:HB2	1:A:4:ARG:NH1	2.10	0.60
1:A:637:GLU:C	1:A:639:LYS:H	2.03	0.60
1:A:573:LEU:HD22	1:A:583:VAL:HA	1.83	0.60
1:A:424:ASP:OD1	1:A:426:ASN:N	2.32	0.60
1:A:324:TYR:CE1	1:A:328:ILE:HD11	2.37	0.59
1:A:302:ASP:HA	3:A:696:HOH:O	2.02	0.59
1:A:106:LEU:HD12	1:A:109:LEU:CD2	2.32	0.59
1:A:4:ARG:HH11	1:A:4:ARG:CG	2.15	0.59
1:A:680:SER:O	1:A:684:GLU:HB2	2.03	0.59
1:A:663:LEU:HG	1:A:667:TYR:CD2	2.37	0.59
1:A:29:VAL:HG11	1:A:277:LYS:HD3	1.85	0.59
1:A:587:ARG:HG2	3:A:881:HOH:O	2.02	0.59
1:A:91:HIS:C	1:A:91:HIS:CD2	2.76	0.58
1:A:664:GLY:O	1:A:668:VAL:HG23	2.03	0.58
1:A:192:TYR:CE1	1:A:210:ARG:HG3	2.37	0.58
1:A:442:ARG:NH1	1:A:540:GLY:O	2.36	0.58
1:A:24:ARG:NH1	3:A:919:HOH:O	2.37	0.58
1:A:279:GLY:HA3	1:A:282:LYS:HG3	1.86	0.58
1:A:120:ARG:HB2	3:A:944:HOH:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:TRP:HZ2	1:A:58:THR:HG22	1.68	0.58
1:A:18:LYS:NZ	1:A:288:LEU:O	2.33	0.57
1:A:218:LEU:HB3	1:A:224:ARG:HG3	1.85	0.57
1:A:691:LYS:HB3	1:A:691:LYS:NZ	2.20	0.57
1:A:92:TYR:CE2	1:A:250:VAL:HG22	2.40	0.57
1:A:130:GLY:HA2	1:A:331:LEU:HD13	1.87	0.57
1:A:139:THR:HG22	1:A:140:GLY:N	2.19	0.57
1:A:192:TYR:CD1	1:A:210:ARG:HG3	2.40	0.57
1:A:691:LYS:CB	1:A:691:LYS:NZ	2.67	0.57
1:A:210:ARG:HD3	1:A:212:SER:OG	2.05	0.57
1:A:86:ARG:C	1:A:88:PRO:HD3	2.24	0.57
1:A:329:GLN:O	1:A:333:LYS:HG3	2.04	0.57
1:A:568:LEU:HD11	1:A:583:VAL:HB	1.86	0.56
1:A:20:PHE:HB3	1:A:24:ARG:HH21	1.69	0.56
1:A:400:TYR:CZ	1:A:404:LYS:HE3	2.40	0.56
1:A:275:GLN:HE22	1:A:307:PHE:H	1.52	0.56
1:A:132:LEU:C	1:A:134:PRO:HD2	2.26	0.56
1:A:197:LYS:HA	1:A:200:LYS:HB2	1.87	0.56
1:A:416:LYS:HE3	1:A:648:GLU:HG3	1.88	0.55
1:A:191:SER:OG	1:A:192:TYR:N	2.40	0.55
1:A:312:PRO:HG2	3:A:981:HOH:O	2.05	0.55
1:A:462:ALA:HB3	1:A:465:ARG:HD3	1.88	0.55
1:A:637:GLU:O	1:A:639:LYS:N	2.39	0.55
1:A:378:GLU:HG3	3:A:737:HOH:O	2.06	0.55
1:A:2:ARG:O	1:A:3:ARG:O	2.25	0.55
1:A:58:THR:HG23	3:A:693:HOH:O	2.06	0.54
1:A:4:ARG:O	1:A:4:ARG:CG	2.55	0.54
1:A:424:ASP:C	1:A:424:ASP:OD1	2.41	0.54
1:A:233:ASP:HB3	1:A:603:MET:HB3	1.88	0.54
1:A:162:ASP:OD1	1:A:165:GLN:N	2.40	0.54
1:A:441:VAL:HG11	1:A:448:LEU:HD23	1.89	0.54
1:A:18:LYS:NZ	3:A:695:HOH:O	2.39	0.54
1:A:421:SER:OG	1:A:422:ASP:N	2.38	0.54
1:A:79:ALA:O	1:A:307:PHE:HA	2.07	0.54
1:A:13:ASN:ND2	3:A:781:HOH:O	2.41	0.53
1:A:77:VAL:CG1	1:A:257:ALA:HB3	2.38	0.53
1:A:118:GLY:O	1:A:121:ARG:HG3	2.09	0.53
1:A:297:ASP:HB3	1:A:301:LYS:HA	1.90	0.53
1:A:133:ARG:HD3	1:A:133:ARG:O	2.09	0.53
1:A:498:ASP:O	1:A:501:SER:OG	2.25	0.52
1:A:3:ARG:C	1:A:5:SER:N	2.60	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:GLN:HG2	3:A:819:HOH:O	2.09	0.52
1:A:516:LYS:CD	3:A:1035:HOH:O	2.57	0.52
1:A:107:ASN:ND2	1:A:107:ASN:H	2.08	0.52
1:A:94:ALA:O	1:A:247:LEU:HB2	2.10	0.52
1:A:622:ARG:HH12	1:A:635:GLN:HE21	0.75	0.52
1:A:136:LEU:O	1:A:137:ASN:HB2	2.09	0.52
1:A:353:GLN:NE2	1:A:521:SER:HB3	2.24	0.52
1:A:180:LYS:O	1:A:181:CYS:CB	2.57	0.51
1:A:270:LEU:C	1:A:270:LEU:CD2	2.79	0.51
1:A:4:ARG:HG3	1:A:4:ARG:O	2.11	0.51
1:A:2:ARG:CG	1:A:2:ARG:HH11	2.23	0.51
1:A:279:GLY:CA	1:A:282:LYS:HG3	2.40	0.51
1:A:291:SER:HB3	1:A:295:GLN:O	2.11	0.51
1:A:288:LEU:HD22	1:A:300:PHE:CE2	2.46	0.51
1:A:404:LYS:O	1:A:690:ARG:HD2	2.11	0.51
1:A:234:ASN:N	1:A:234:ASN:ND2	2.57	0.51
1:A:389:ALA:O	1:A:602:ARG:NH1	2.44	0.51
1:A:671:ILE:HG22	1:A:675:LYS:HG3	1.92	0.51
1:A:106:LEU:HD12	1:A:109:LEU:HD21	1.92	0.51
1:A:7:GLN:O	1:A:55:ASP:N	2.32	0.51
1:A:675:LYS:HA	1:A:678:SER:O	2.11	0.50
1:A:98:VAL:HG22	1:A:228:GLU:O	2.11	0.50
1:A:622:ARG:HG2	1:A:648:GLU:O	2.12	0.50
1:A:12:SER:HB2	1:A:14:PRO:HD2	1.93	0.50
1:A:417:SER:O	1:A:418:GLN:HB2	2.12	0.50
1:A:418:GLN:NE2	1:A:587:ARG:HH11	2.06	0.50
1:A:436:LEU:HD21	1:A:587:ARG:HD2	1.92	0.50
1:A:55:ASP:OD2	1:A:263:LYS:NZ	2.43	0.50
1:A:13:ASN:N	1:A:14:PRO:HD3	2.26	0.49
1:A:249:ARG:HG3	1:A:249:ARG:HH11	1.77	0.49
1:A:14:PRO:CB	1:A:295:GLN:OE1	2.61	0.49
1:A:229:LEU:HD22	1:A:239:VAL:HA	1.93	0.49
1:A:628:PRO:HA	1:A:632:CYS:SG	2.52	0.49
1:A:655:GLY:C	1:A:657:THR:HG23	2.33	0.49
1:A:222:ALA:C	1:A:224:ARG:H	2.16	0.49
1:A:290:GLY:N	3:A:696:HOH:O	2.45	0.49
1:A:218:LEU:HB3	1:A:224:ARG:CG	2.42	0.48
1:A:133:ARG:HD3	1:A:133:ARG:C	2.33	0.48
1:A:55:ASP:OD2	1:A:263:LYS:CE	2.61	0.48
1:A:422:ASP:HB3	1:A:423:PRO:HD2	1.94	0.48
1:A:6:VAL:HG11	1:A:270:LEU:HD12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:ALA:O	1:A:198:CYS:HB3	2.14	0.48
1:A:250:VAL:HA	1:A:251:PRO:HD3	1.55	0.48
1:A:142:PRO:HD2	3:A:800:HOH:O	2.12	0.48
1:A:214:VAL:O	1:A:218:LEU:HB2	2.13	0.48
1:A:138:TRP:CE2	1:A:140:GLY:HA2	2.49	0.48
1:A:637:GLU:C	1:A:639:LYS:N	2.67	0.48
1:A:12:SER:CB	1:A:14:PRO:HD2	2.44	0.48
1:A:380:CYS:HB3	1:A:392:MET:SD	2.54	0.48
1:A:133:ARG:N	1:A:134:PRO:CD	2.77	0.47
1:A:192:TYR:CE1	1:A:210:ARG:CG	2.98	0.47
1:A:241:LYS:HD2	3:A:963:HOH:O	2.14	0.47
1:A:176:THR:O	1:A:179:ASN:HB2	2.14	0.47
1:A:417:SER:O	1:A:418:GLN:CB	2.62	0.47
1:A:325:PHE:O	1:A:329:GLN:HG3	2.15	0.47
1:A:233:ASP:C	1:A:233:ASP:OD1	2.50	0.47
1:A:410:VAL:HG21	1:A:609:LEU:HD23	1.95	0.47
1:A:170:CYS:O	1:A:173:CYS:HB2	2.15	0.47
1:A:66:GLU:OE2	1:A:332:ARG:NH2	2.48	0.47
1:A:209:ILE:HD12	1:A:213:THR:CG2	2.45	0.47
1:A:91:HIS:HB2	1:A:250:VAL:O	2.15	0.47
1:A:13:ASN:N	1:A:14:PRO:HD2	2.30	0.46
1:A:43:ILE:HG13	3:A:699:HOH:O	2.16	0.46
1:A:83:GLY:N	3:A:937:HOH:O	2.45	0.46
1:A:37:ILE:HG21	1:A:54:ALA:HB2	1.96	0.46
1:A:298:LEU:O	1:A:299:LEU:HB2	2.14	0.46
1:A:22:TRP:CZ2	1:A:270:LEU:CD2	2.99	0.46
1:A:691:LYS:CG	1:A:691:LYS:O	2.64	0.46
1:A:105:GLN:NE2	3:A:718:HOH:O	2.48	0.45
1:A:100:LYS:CD	1:A:101:GLY:N	2.78	0.45
1:A:113:LYS:HA	1:A:155:ALA:O	2.15	0.45
1:A:613:LEU:O	1:A:617:GLN:N	2.44	0.45
1:A:187:GLU:HA	1:A:188:PRO:HD2	1.78	0.45
1:A:121:ARG:HE	1:A:121:ARG:HB3	1.63	0.45
1:A:105:GLN:NE2	1:A:236:ARG:HG3	2.26	0.45
1:A:322:SER:O	1:A:326:THR:HG23	2.17	0.45
1:A:548:VAL:O	1:A:552:GLN:HG3	2.16	0.45
1:A:43:ILE:O	1:A:47:GLN:HG3	2.17	0.45
1:A:515:ASN:HB3	1:A:518:VAL:HG21	1.99	0.45
1:A:92:TYR:CZ	1:A:250:VAL:HG22	2.52	0.45
1:A:367:GLY:HA2	3:A:733:HOH:O	2.17	0.45
1:A:113:LYS:HE2	1:A:203:ALA:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:ARG:NH1	1:A:4:ARG:CG	2.76	0.44
1:A:400:TYR:OH	1:A:404:LYS:HE3	2.17	0.44
1:A:171:ARG:HD2	1:A:171:ARG:HH11	1.54	0.44
1:A:500:ARG:CD	3:A:1033:HOH:O	2.65	0.44
1:A:187:GLU:O	1:A:190:PHE:HB3	2.17	0.44
1:A:29:VAL:O	1:A:30:ARG:C	2.56	0.44
1:A:442:ARG:HD3	3:A:870:HOH:O	2.17	0.44
1:A:141:PRO:HG2	1:A:332:ARG:O	2.16	0.44
1:A:270:LEU:C	1:A:270:LEU:HD23	2.37	0.44
1:A:235:THR:HG22	1:A:236:ARG:H	1.83	0.44
1:A:89:ARG:HH21	1:A:92:TYR:HB3	1.81	0.44
1:A:87:GLN:O	1:A:87:GLN:HG3	2.18	0.44
1:A:222:ALA:C	1:A:224:ARG:N	2.71	0.44
1:A:384:VAL:HG22	1:A:407:LEU:CD1	2.46	0.44
1:A:341:ARG:HH12	1:A:605:LYS:HZ2	1.65	0.44
1:A:91:HIS:C	1:A:91:HIS:HD2	2.20	0.44
1:A:321:GLY:O	1:A:325:PHE:HB2	2.17	0.43
1:A:619:LYS:HD3	1:A:620:PHE:CZ	2.53	0.43
1:A:162:ASP:C	1:A:164:GLY:H	2.22	0.43
1:A:166:PHE:HD1	3:A:804:HOH:O	2.00	0.43
1:A:117:THR:OG1	1:A:124:GLY:HA3	2.18	0.43
1:A:573:LEU:HD13	1:A:583:VAL:HG22	2.01	0.43
1:A:238:PRO:O	1:A:241:LYS:HB2	2.17	0.43
1:A:679:THR:HG23	1:A:680:SER:N	2.05	0.43
1:A:430:ARG:HD3	1:A:430:ARG:HH11	1.49	0.43
1:A:515:ASN:HB3	1:A:518:VAL:CG2	2.48	0.43
1:A:603:MET:HE3	3:A:742:HOH:O	2.19	0.43
1:A:622:ARG:HH22	1:A:635:GLN:NE2	2.16	0.43
1:A:219:SER:O	1:A:220:ASP:O	2.37	0.43
1:A:622:ARG:HH22	1:A:635:GLN:HE22	1.67	0.42
1:A:341:ARG:NH1	1:A:605:LYS:HZ2	2.18	0.42
1:A:483:CYS:HB3	1:A:677:CYS:HB3	1.90	0.42
1:A:691:LYS:HB3	1:A:691:LYS:HZ2	1.84	0.42
1:A:311:PRO:HD2	1:A:314:ILE:CD1	2.40	0.42
1:A:47:GLN:O	1:A:48:ALA:C	2.54	0.42
1:A:352:GLU:O	1:A:356:ARG:HD3	2.19	0.42
1:A:143:GLU:HG3	1:A:144:PRO:N	2.35	0.42
1:A:192:TYR:HB3	1:A:213:THR:OG1	2.20	0.42
1:A:47:GLN:HG2	1:A:72:TYR:CE1	2.54	0.42
1:A:355:LEU:HD22	1:A:373:SER:OG	2.19	0.42
1:A:90:THR:O	1:A:91:HIS:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:ASP:HA	1:A:597:HIS:CD2	2.55	0.42
1:A:233:ASP:N	1:A:233:ASP:OD1	2.53	0.42
1:A:587:ARG:HH11	1:A:587:ARG:HD3	1.43	0.42
1:A:639:LYS:HA	1:A:639:LYS:HD3	1.77	0.41
1:A:291:SER:HA	1:A:292:PRO:HD3	1.78	0.41
1:A:582:PRO:HD2	1:A:585:GLU:OE2	2.21	0.41
1:A:485:PHE:CD2	3:A:1027:HOH:O	2.57	0.41
1:A:34:VAL:HG22	1:A:35:SER:O	2.19	0.41
1:A:168:ASN:OD1	1:A:171:ARG:NE	2.53	0.41
1:A:655:GLY:O	1:A:657:THR:HG23	2.20	0.41
1:A:492:SER:HB2	1:A:503:LEU:HA	2.02	0.41
1:A:622:ARG:NH2	1:A:645:ASP:O	2.54	0.41
1:A:84:THR:OG1	1:A:87:GLN:HB3	2.21	0.41
1:A:155:ALA:HB3	1:A:172:LEU:HD21	1.97	0.41
1:A:278:PHE:O	1:A:279:GLY:O	2.37	0.41
1:A:74:LEU:HB3	1:A:257:ALA:O	2.20	0.41
1:A:275:GLN:NE2	1:A:307:PHE:H	2.18	0.41
1:A:60:ASP:HA	1:A:253:HIS:CD2	2.56	0.41
1:A:75:ARG:HA	1:A:76:PRO:HD3	1.80	0.41
1:A:229:LEU:CD2	1:A:239:VAL:HA	2.51	0.41
1:A:91:HIS:HD2	1:A:91:HIS:O	2.05	0.40
1:A:43:ILE:H	1:A:43:ILE:HG13	1.68	0.40
1:A:270:LEU:O	1:A:270:LEU:HD23	2.22	0.40
1:A:566:LEU:HA	1:A:566:LEU:HD23	1.75	0.40
1:A:418:GLN:NE2	1:A:587:ARG:HD3	2.33	0.40
1:A:6:VAL:CG1	1:A:270:LEU:HD12	2.51	0.40
1:A:576:LEU:HD13	1:A:591:LEU:HD23	2.03	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	689/691 (100%)	624 (91%)	51 (7%)	14 (2%)	9 30

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	4	ARG
1	A	220	ASP
1	A	279	GLY
1	A	417	SER
1	A	418	GLN
1	A	86	ARG
1	A	219	SER
1	A	638	THR
1	A	293	SER
1	A	637	GLU
1	A	141	PRO
1	A	180	LYS
1	A	142	PRO

### 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	574/574 (100%)	474 (83%)	100 (17%)	2 7

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	3	ARG
1	A	4	ARG
1	A	11	VAL
1	A	13	ASN
1	A	37	ILE
1	A	39	ARG

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Mol	Chain	Res	Type
1	A	43	ILE
1	A	58	THR
1	A	77	VAL
1	A	85	GLU
1	A	86	ARG
1	A	90	THR
1	A	91	HIS
1	A	99	LYS
1	A	100	LYS
1	A	105	GLN
1	A	107	ASN
1	A	109	LEU
1	A	110	GLN
1	A	120	ARG
1	A	121	ARG
1	A	133	ARG
1	A	142	PRO
1	A	145	ILE
1	A	156	SER
1	A	163	LYS
1	A	165	GLN
1	A	172	LEU
1	A	176	THR
1	A	184	SER
1	A	185	SER
1	A	187	GLU
1	A	191	SER
1	A	200	LYS
1	A	210	ARG
1	A	218	LEU
1	A	219	SER
1	A	221	GLU
1	A	223	GLU
1	A	225	ASP
1	A	229	LEU
1	A	231	CYS
1	A	235	THR
1	A	247	LEU
1	A	249	ARG
1	A	260	VAL
1	A	261	ASN
1	A	263	LYS

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Mol	Chain	Res	Type
1	A	265	ASP
1	A	270	LEU
1	A	271	LEU
1	A	276	GLU
1	A	288	LEU
1	A	298	LEU
1	A	301	LYS
1	A	308	SER
1	A	310	VAL
1	A	313	ARG
1	A	315	ASP
1	A	322	SER
1	A	324	TYR
1	A	331	LEU
1	A	332	ARG
1	A	342	ARG
1	A	344	ARG
1	A	364	LEU
1	A	417	SER
1	A	419	GLN
1	A	422	ASP
1	A	436	LEU
1	A	440	VAL
1	A	444	SER
1	A	446	THR
1	A	463	VAL
1	A	476	LEU
1	A	484	LYS
1	A	495	PRO
1	A	514	GLU
1	A	564	LYS
1	A	567	LYS
1	A	573	LEU
1	A	574	LEU
1	A	576	LEU
1	A	623	ASN
1	A	629	ASP
1	A	636	SER
1	A	638	THR
1	A	646	ASN
1	A	663	LEU
1	A	666	GLN

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Mol	Chain	Res	Type
1	A	673	ASN
1	A	675	LYS
1	A	678	SER
1	A	679	THR
1	A	683	LEU
1	A	684	GLU
1	A	687	GLU
1	A	690	ARG
1	A	691	LYS

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

Mol	Chain	Res	Type
1	A	21	GLN
1	A	47	GLN
1	A	91	HIS
1	A	105	GLN
1	A	107	ASN
1	A	110	GLN
1	A	165	GLN
1	A	234	ASN
1	A	275	GLN
1	A	353	GLN
1	A	418	GLN
1	A	419	GLN
1	A	502	ASN
1	A	552	GLN
1	A	597	HIS
1	A	635	GLN
1	A	644	ASN
1	A	646	ASN
1	A	673	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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is 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](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	691/691 (100%)	-0.30	10 (1%) 78 69	18, 35, 62, 95	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	GLY	7.0
1	A	420	SER	6.0
1	A	637	GLU	5.2
1	A	2	ARG	3.9
1	A	3	ARG	3.8
1	A	418	GLN	3.8
1	A	419	GLN	3.6
1	A	222	ALA	3.5
1	A	417	SER	3.0
1	A	220	ASP	2.1

### 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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CL	A	692	1/1	0.98	0.16	-1.63	31,31,31,31	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.