



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:25 PM GMT

PDB ID : 1ANX
Title : THE CRYSTAL STRUCTURE OF A NEW HIGH-CALCIUM FORM OF ANNEXIN V
Authors : Sopkova, J.; Renouard, M.; Lewit-Bentley, A.
Deposited on : 1993-10-26
Resolution : 1.90 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

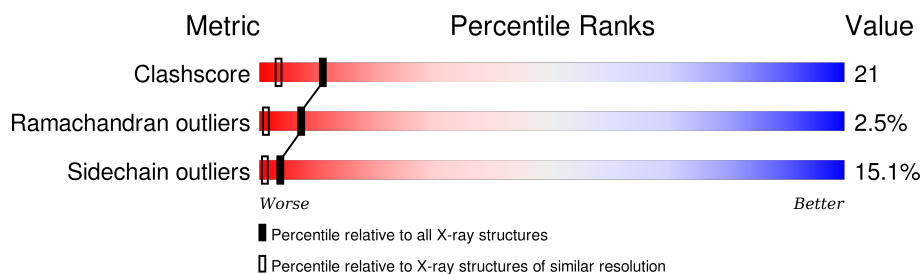
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	319	 49% 34% 13% • •
1	B	319	 53% 31% 11% • •
1	C	319	 55% 26% 13% 6% •

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7990 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 ANNEXIN V.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	316	Total	C	N	O	S	0	5	0
			2519	1587	428	496	8			
1	B	316	Total	C	N	O	S	0	4	0
			2513	1584	425	496	8			
1	C	316	Total	C	N	O	S	0	4	0
			2513	1584	425	496	8			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 4 is water.

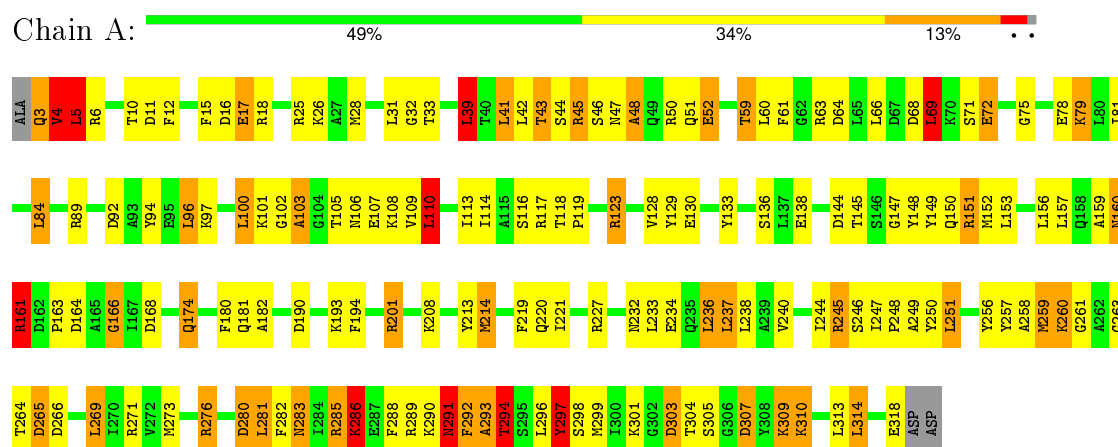
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	151	Total	O	0	0
			151	151		
4	B	133	Total	O	0	0
			133	133		
4	C	134	Total	O	0	0
			134	134		

3 Residue-property plots

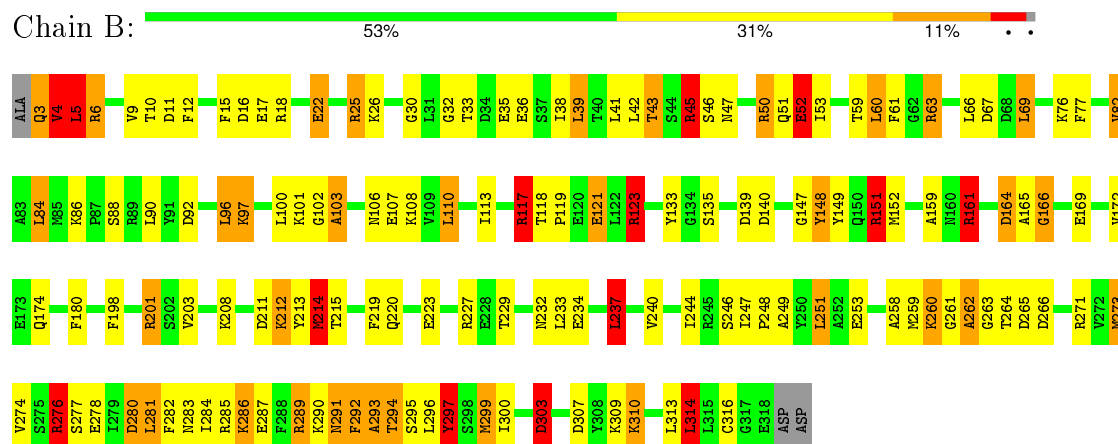
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS was not executed.

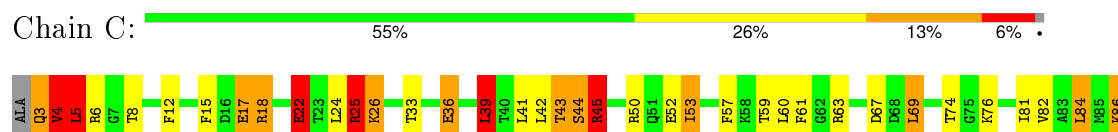
• Molecule 1: ANNEXIN V

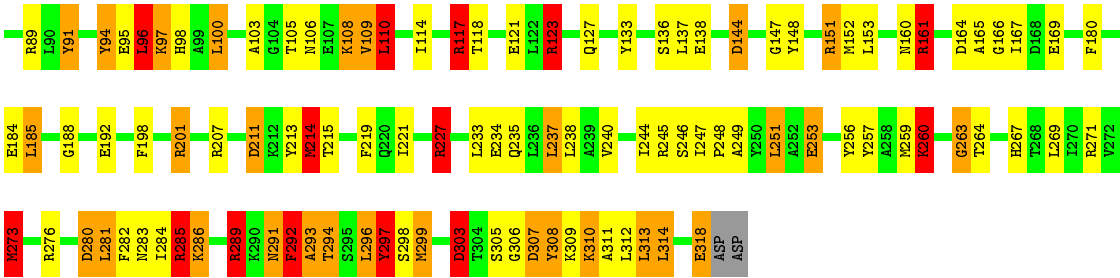


• Molecule 1: ANNEXIN V



• Molecule 1: ANNEXIN V





4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	91.20 Å 91.30 Å 36.20 Å 82.40° 82.40° 118.20°	Depositor
Resolution (Å)	12.00 – 1.90	Depositor
% Data completeness (in resolution range)	(Not available) (12.00-1.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.198 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7990	wwPDB-VP
Average B, all atoms (Å ²)	29.0	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, SO4

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	0.92	1/2579 (0.0%)	2.19	98/3468 (2.8%)
1	B	0.92	1/2568 (0.0%)	2.07	89/3454 (2.6%)
1	C	0.94	1/2568 (0.0%)	2.10	112/3454 (3.2%)
All	All	0.93	3/7715 (0.0%)	2.12	299/10376 (2.9%)

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	3
1	B	0	7
1	C	0	9
All	All	0	19

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	88	SER	C-N	-6.32	1.19	1.34
1	A	234	GLU	CD-OE1	-5.39	1.19	1.25
1	C	263	GLY	C-N	-5.09	1.22	1.34

All (299) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	151[A]	ARG	CD-NE-CZ	27.49	162.09	123.60
1	A	151[B]	ARG	CD-NE-CZ	27.49	162.09	123.60
1	B	45	ARG	NE-CZ-NH2	20.95	130.77	120.30
1	B	25	ARG	NE-CZ-NH2	19.00	129.80	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	201	ARG	NE-CZ-NH2	16.55	128.57	120.30
1	B	276	ARG	NE-CZ-NH1	14.36	127.48	120.30
1	B	45	ARG	NE-CZ-NH1	-13.97	113.31	120.30
1	A	194	PHE	CB-CG-CD1	-13.58	111.30	120.80
1	C	45	ARG	NE-CZ-NH2	-13.28	113.66	120.30
1	C	45	ARG	NE-CZ-NH1	13.17	126.88	120.30
1	A	161	ARG	NE-CZ-NH1	-12.51	114.05	120.30
1	C	280	ASP	CB-CG-OD1	12.48	129.53	118.30
1	B	280	ASP	CB-CG-OD1	12.43	129.48	118.30
1	B	213	TYR	CB-CG-CD1	-12.27	113.64	121.00
1	C	297	TYR	CB-CG-CD1	12.13	128.28	121.00
1	A	123	ARG	NE-CZ-NH1	11.65	126.13	120.30
1	B	50	ARG	NE-CZ-NH2	-11.41	114.59	120.30
1	A	271	ARG	NE-CZ-NH2	-10.90	114.85	120.30
1	B	271	ARG	NE-CZ-NH2	-10.81	114.89	120.30
1	C	213	TYR	CB-CG-CD1	-10.66	114.60	121.00
1	A	271	ARG	NE-CZ-NH1	10.35	125.47	120.30
1	B	117	ARG	NE-CZ-NH2	-10.12	115.24	120.30
1	A	194	PHE	CB-CG-CD2	10.02	127.81	120.80
1	C	50	ARG	NE-CZ-NH1	-9.70	115.45	120.30
1	A	129	TYR	CB-CG-CD1	9.64	126.78	121.00
1	A	266	ASP	CB-CG-OD2	-9.62	109.64	118.30
1	A	161	ARG	NH1-CZ-NH2	9.61	129.97	119.40
1	B	214	MET	CG-SD-CE	9.49	115.38	100.20
1	A	123	ARG	CD-NE-CZ	9.43	136.80	123.60
1	B	297	TYR	CB-CG-CD1	9.34	126.60	121.00
1	C	297	TYR	CB-CG-CD2	-9.28	115.44	121.00
1	B	123	ARG	NE-CZ-NH2	-9.19	115.70	120.30
1	C	201	ARG	NE-CZ-NH2	9.11	124.85	120.30
1	C	144	ASP	CB-CG-OD2	-9.03	110.17	118.30
1	A	280	ASP	CB-CG-OD1	8.94	126.34	118.30
1	B	271	ARG	CD-NE-CZ	8.79	135.90	123.60
1	B	271	ARG	NE-CZ-NH1	8.76	124.68	120.30
1	A	148	TYR	CB-CG-CD2	-8.71	115.78	121.00
1	A	161	ARG	NE-CZ-NH2	-8.62	115.99	120.30
1	A	117	ARG	NE-CZ-NH2	-8.61	115.99	120.30
1	C	25	ARG	NE-CZ-NH2	8.57	124.59	120.30
1	C	253	GLU	OE1-CD-OE2	8.45	133.44	123.30
1	B	82	VAL	CA-CB-CG2	8.42	123.53	110.90
1	B	16	ASP	CB-CG-OD1	8.36	125.82	118.30
1	C	123	ARG	NE-CZ-NH1	-8.35	116.13	120.30
1	B	25	ARG	NE-CZ-NH1	-8.32	116.14	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	161	ARG	NE-CZ-NH2	-8.32	116.14	120.30
1	B	201	ARG	CD-NE-CZ	8.31	135.24	123.60
1	A	250	TYR	CB-CG-CD2	-8.24	116.05	121.00
1	A	285	ARG	NE-CZ-NH2	8.21	124.41	120.30
1	A	18	ARG	NE-CZ-NH2	-8.20	116.20	120.30
1	A	297	TYR	CB-CG-CD1	8.15	125.89	121.00
1	C	303	ASP	CB-CG-OD2	8.13	125.62	118.30
1	C	213	TYR	CB-CG-CD2	8.11	125.87	121.00
1	B	61	PHE	CB-CG-CD2	-8.11	115.13	120.80
1	B	213	TYR	CB-CG-CD2	8.03	125.82	121.00
1	B	139	ASP	CB-CG-OD2	-7.91	111.18	118.30
1	A	52	GLU	CG-CD-OE2	7.88	134.06	118.30
1	A	52	GLU	CG-CD-OE1	-7.87	102.55	118.30
1	C	94	TYR	CB-CG-CD1	-7.83	116.30	121.00
1	A	117	ARG	NE-CZ-NH1	7.76	124.18	120.30
1	B	280	ASP	OD1-CG-OD2	-7.76	108.55	123.30
1	C	273	MET	CA-CB-CG	-7.76	100.11	113.30
1	A	214	MET	CG-SD-CE	-7.75	87.80	100.20
1	B	166	GLY	CA-C-O	7.68	134.42	120.60
1	C	52	GLU	CG-CD-OE1	-7.62	103.06	118.30
1	B	22	GLU	OE1-CD-OE2	7.62	132.44	123.30
1	C	271	ARG	NE-CZ-NH2	-7.56	116.52	120.30
1	A	3	GLN	O-C-N	7.55	134.78	122.70
1	A	16	ASP	CB-CG-OD1	7.54	125.08	118.30
1	B	50	ARG	NH1-CZ-NH2	7.52	127.67	119.40
1	C	161	ARG	NE-CZ-NH1	-7.51	116.54	120.30
1	B	161	ARG	NE-CZ-NH1	-7.51	116.55	120.30
1	B	276	ARG	NH1-CZ-NH2	-7.51	111.14	119.40
1	A	69	LEU	CA-CB-CG	7.46	132.46	115.30
1	A	6[A]	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	A	6[B]	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	A	250	TYR	CB-CG-CD1	7.46	125.48	121.00
1	C	45	ARG	CD-NE-CZ	-7.40	113.24	123.60
1	A	168	ASP	CB-CG-OD1	7.39	124.95	118.30
1	A	285	ARG	NE-CZ-NH1	-7.34	116.63	120.30
1	C	164	ASP	CB-CG-OD2	7.33	124.90	118.30
1	B	25	ARG	CD-NE-CZ	-7.32	113.36	123.60
1	C	280	ASP	OD1-CG-OD2	-7.31	109.41	123.30
1	B	198	PHE	CB-CG-CD2	-7.27	115.71	120.80
1	B	4	VAL	O-C-N	7.19	134.20	122.70
1	C	161	ARG	NH1-CZ-NH2	7.17	127.28	119.40
1	A	68	ASP	CB-CG-OD2	-7.14	111.87	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	94	TYR	CB-CG-CD2	7.09	125.25	121.00
1	B	273	MET	CA-CB-CG	-7.04	101.33	113.30
1	B	123	ARG	NE-CZ-NH1	7.01	123.81	120.30
1	C	52	GLU	OE1-CD-OE2	7.01	131.71	123.30
1	C	151[A]	ARG	CD-NE-CZ	-6.99	113.82	123.60
1	C	151[B]	ARG	CD-NE-CZ	-6.99	113.82	123.60
1	C	245	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	B	278	GLU	OE1-CD-OE2	6.95	131.63	123.30
1	B	296	LEU	CB-CA-C	6.93	123.36	110.20
1	A	265	ASP	O-C-N	6.93	133.78	122.70
1	A	201	ARG	CD-NE-CZ	6.84	133.18	123.60
1	B	314	LEU	CA-CB-CG	6.83	131.00	115.30
1	A	276	ARG	NE-CZ-NH1	6.81	123.71	120.30
1	C	289	ARG	CG-CD-NE	6.81	126.10	111.80
1	B	3	GLN	O-C-N	6.80	133.58	122.70
1	C	165	ALA	C-N-CA	-6.77	108.08	122.30
1	A	148	TYR	CB-CG-CD1	6.75	125.05	121.00
1	A	166	GLY	CA-C-O	6.74	132.73	120.60
1	C	4	VAL	O-C-N	6.72	133.46	122.70
1	A	174	GLN	CA-CB-CG	6.67	128.08	113.40
1	B	227	ARG	NE-CZ-NH1	6.67	123.64	120.30
1	C	273	MET	CG-SD-CE	6.63	110.81	100.20
1	B	52	GLU	OE1-CD-OE2	6.63	131.25	123.30
1	A	213	TYR	CB-CG-CD1	-6.62	117.03	121.00
1	A	18	ARG	NE-CZ-NH1	6.60	123.60	120.30
1	C	308	TYR	CB-CG-CD1	6.60	124.96	121.00
1	C	285	ARG	NE-CZ-NH1	-6.59	117.01	120.30
1	A	297	TYR	CA-CB-CG	6.56	125.87	113.40
1	C	152	MET	CG-SD-CE	6.56	110.70	100.20
1	C	50	ARG	NH1-CZ-NH2	6.55	126.61	119.40
1	A	17	GLU	CG-CD-OE2	-6.54	105.21	118.30
1	C	307	ASP	CB-CG-OD1	-6.54	112.41	118.30
1	B	295	SER	CA-C-N	-6.52	102.85	117.20
1	A	72	GLU	OE1-CD-OE2	6.52	131.12	123.30
1	B	123	ARG	CD-NE-CZ	6.51	132.72	123.60
1	C	57	PHE	O-C-N	6.47	133.04	122.70
1	B	82	VAL	CG1-CB-CG2	-6.46	100.56	110.90
1	B	234	GLU	OE1-CD-OE2	6.44	131.03	123.30
1	B	52	GLU	CA-CB-CG	6.44	127.56	113.40
1	C	17	GLU	CG-CD-OE2	-6.38	105.55	118.30
1	C	151[A]	ARG	NE-CZ-NH2	-6.37	117.12	120.30
1	C	151[B]	ARG	NE-CZ-NH2	-6.37	117.12	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	211	ASP	CB-CG-OD2	-6.33	112.60	118.30
1	C	245	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	C	67	ASP	CB-CG-OD1	6.32	123.98	118.30
1	A	4	VAL	O-C-N	6.27	132.73	122.70
1	A	164	ASP	CB-CG-OD2	6.26	123.93	118.30
1	A	94	TYR	CB-CG-CD2	6.25	124.75	121.00
1	B	303	ASP	CB-CG-OD1	6.24	123.91	118.30
1	A	59	THR	CA-CB-CG2	6.22	121.10	112.40
1	C	227	ARG	NE-CZ-NH1	6.21	123.41	120.30
1	A	259	MET	CA-CB-CG	-6.20	102.77	113.30
1	B	165	ALA	C-N-CA	-6.19	109.30	122.30
1	C	22	GLU	OE1-CD-OE2	6.19	130.72	123.30
1	B	148	TYR	CB-CG-CD2	-6.18	117.29	121.00
1	A	32	GLY	CA-C-O	6.16	131.69	120.60
1	C	17	GLU	CG-CD-OE1	6.15	130.60	118.30
1	B	17	GLU	CG-CD-OE2	-6.14	106.02	118.30
1	C	84	LEU	CA-CB-CG	6.12	129.38	115.30
1	C	291	ASN	CB-CA-C	6.11	122.63	110.40
1	B	107	GLU	CG-CD-OE2	-6.09	106.11	118.30
1	A	61	PHE	CB-CG-CD2	-6.08	116.55	120.80
1	C	238	LEU	O-C-N	6.06	132.39	122.70
1	C	198	PHE	CB-CG-CD2	-6.05	116.56	120.80
1	C	39	LEU	CA-CB-CG	6.05	129.21	115.30
1	B	63	ARG	NE-CZ-NH1	6.01	123.31	120.30
1	A	17	GLU	CG-CD-OE1	6.01	130.32	118.30
1	C	303	ASP	CB-CG-OD1	-6.00	112.90	118.30
1	C	117	ARG	NE-CZ-NH2	-5.99	117.31	120.30
1	C	214	MET	CG-SD-CE	5.98	109.78	100.20
1	B	152	MET	CG-SD-CE	5.98	109.77	100.20
1	B	180	PHE	CB-CG-CD2	-5.98	116.62	120.80
1	A	245	ARG	CG-CD-NE	5.97	124.34	111.80
1	A	314	LEU	CB-CA-C	5.97	121.54	110.20
1	A	94	TYR	CB-CG-CD1	-5.96	117.42	121.00
1	A	5	LEU	O-C-N	-5.96	113.16	122.70
1	C	74	THR	C-N-CA	5.95	134.78	122.30
1	C	26	LYS	CB-CG-CD	5.93	127.03	111.60
1	C	180	PHE	CB-CG-CD2	-5.93	116.65	120.80
1	A	129	TYR	CB-CG-CD2	-5.93	117.44	121.00
1	A	107	GLU	CG-CD-OE1	5.92	130.15	118.30
1	C	18	ARG	CD-NE-CZ	5.92	131.89	123.60
1	C	44	SER	CA-C-O	5.91	132.51	120.10
1	B	92	ASP	CB-CG-OD2	5.89	123.60	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	52	GLU	CG-CD-OE1	-5.89	106.53	118.30
1	C	41	LEU	O-C-N	5.88	132.10	122.70
1	C	207	ARG	NE-CZ-NH1	-5.87	117.37	120.30
1	C	221	ILE	O-C-N	-5.87	113.31	122.70
1	C	251	LEU	CA-CB-CG	5.84	128.72	115.30
1	A	92	ASP	CB-CG-OD2	5.83	123.55	118.30
1	C	53	ILE	CA-C-O	5.82	132.33	120.10
1	A	4	VAL	CB-CA-C	-5.82	100.34	111.40
1	C	18	ARG	NE-CZ-NH2	-5.81	117.39	120.30
1	C	61	PHE	CA-C-O	-5.81	107.90	120.10
1	B	164	ASP	CB-CG-OD1	5.81	123.53	118.30
1	B	69	LEU	CA-CB-CG	5.81	128.66	115.30
1	A	296	LEU	CB-CA-C	5.81	121.23	110.20
1	B	307	ASP	CB-CG-OD1	-5.78	113.10	118.30
1	A	160	ASN	CA-CB-CG	5.78	126.11	113.40
1	A	307	ASP	CB-CG-OD1	-5.77	113.11	118.30
1	B	61	PHE	CB-CG-CD1	5.76	124.83	120.80
1	A	258	ALA	N-CA-CB	5.75	118.15	110.10
1	C	4	VAL	CB-CA-C	-5.75	100.48	111.40
1	C	69	LEU	CA-CB-CG	5.74	128.50	115.30
1	C	251	LEU	CB-CG-CD2	-5.73	101.26	111.00
1	C	69	LEU	CB-CA-C	5.72	121.07	110.20
1	A	292	PHE	CB-CG-CD1	-5.71	116.80	120.80
1	C	148	TYR	CB-CG-CD2	-5.71	117.57	121.00
1	C	184	GLU	OE1-CD-OE2	-5.71	116.45	123.30
1	C	260	LYS	N-CA-CB	5.70	120.86	110.60
1	C	198	PHE	CB-CG-CD1	5.67	124.77	120.80
1	C	18	ARG	NE-CZ-NH1	5.65	123.13	120.30
1	B	297	TYR	CB-CG-CD2	-5.65	117.61	121.00
1	A	266	ASP	O-C-N	5.64	131.72	122.70
1	B	174	GLN	CA-CB-CG	5.63	125.78	113.40
1	A	138	GLU	OE1-CD-OE2	5.62	130.05	123.30
1	B	88	SER	C-N-CA	5.62	135.75	121.70
1	C	234	GLU	OE1-CD-OE2	5.61	130.04	123.30
1	B	229	THR	CA-CB-CG2	5.60	120.24	112.40
1	C	292	PHE	CA-C-O	-5.60	108.34	120.10
1	B	4	VAL	CA-C-N	-5.58	104.92	117.20
1	C	188	GLY	N-CA-C	-5.58	99.15	113.10
1	B	67	ASP	CB-CG-OD1	5.58	123.32	118.30
1	B	294	THR	N-CA-CB	5.57	120.89	110.30
1	B	9	VAL	CA-C-O	5.57	131.79	120.10
1	B	135	SER	O-C-N	5.57	131.60	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	306	GLY	N-CA-C	5.56	127.00	113.10
1	B	110	LEU	N-CA-CB	-5.54	99.32	110.40
1	B	151[A]	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	B	151[B]	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	B	69	LEU	CB-CA-C	5.52	120.68	110.20
1	B	161	ARG	CA-CB-CG	5.52	125.53	113.40
1	C	96	LEU	CA-CB-CG	5.51	127.98	115.30
1	C	138	GLU	CG-CD-OE2	-5.50	107.30	118.30
1	A	148	TYR	O-C-N	5.49	131.49	122.70
1	C	91	TYR	O-C-N	-5.49	113.91	122.70
1	A	181	GLN	O-C-N	-5.49	113.92	122.70
1	B	287	GLU	N-CA-CB	5.48	120.47	110.60
1	C	296	LEU	CB-CA-C	5.48	120.61	110.20
1	B	161	ARG	CB-CA-C	5.47	121.35	110.40
1	C	318	GLU	CA-CB-CG	5.47	125.43	113.40
1	B	63	ARG	CD-NE-CZ	5.46	131.24	123.60
1	C	110	LEU	CA-CB-CG	5.46	127.85	115.30
1	A	110	LEU	CA-CB-CG	5.45	127.84	115.30
1	C	292	PHE	CA-CB-CG	-5.45	100.81	113.90
1	B	12	PHE	CB-CG-CD1	-5.44	116.99	120.80
1	A	174	GLN	N-CA-CB	-5.44	100.81	110.60
1	C	308	TYR	CB-CG-CD2	-5.44	117.74	121.00
1	B	164	ASP	CB-CA-C	5.44	121.28	110.40
1	A	234	GLU	OE1-CD-OE2	5.43	129.82	123.30
1	C	117	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	B	307	ASP	CB-CA-C	5.41	121.23	110.40
1	A	227	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	A	180	PHE	O-C-N	-5.40	114.06	122.70
1	B	32	GLY	CA-C-O	5.39	130.30	120.60
1	A	201	ARG	NH1-CZ-NH2	-5.38	113.48	119.40
1	C	95	GLU	CG-CD-OE2	5.37	129.03	118.30
1	A	227	ARG	NE-CZ-NH2	5.36	122.98	120.30
1	C	4	VAL	CA-C-N	-5.36	105.41	117.20
1	C	81	ILE	CA-C-O	-5.35	108.86	120.10
1	C	180	PHE	CB-CG-CD1	5.34	124.54	120.80
1	C	285	ARG	NH1-CZ-NH2	5.34	125.28	119.40
1	A	39	LEU	CB-CG-CD2	-5.32	101.95	111.00
1	A	4	VAL	N-CA-C	5.31	125.33	111.00
1	B	121	GLU	CG-CD-OE2	5.30	128.89	118.30
1	A	160	ASN	N-CA-CB	-5.29	101.08	110.60
1	A	164	ASP	CB-CA-C	5.29	120.98	110.40
1	A	194	PHE	CZ-CE2-CD2	-5.29	113.75	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	166	GLY	CA-C-N	-5.29	105.56	117.20
1	C	61	PHE	CA-C-N	5.29	126.77	116.20
1	A	84	LEU	CA-CB-CG	5.27	127.42	115.30
1	C	289	ARG	CA-CB-CG	5.26	124.97	113.40
1	C	3	GLN	O-C-N	5.25	131.10	122.70
1	B	237	LEU	CB-CA-C	5.24	120.16	110.20
1	A	291	ASN	CB-CA-C	5.24	120.89	110.40
1	C	227	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	A	4	VAL	CA-C-N	-5.22	105.71	117.20
1	A	251	LEU	CB-CA-C	5.22	120.11	110.20
1	C	311	ALA	CB-CA-C	5.21	117.92	110.10
1	C	292	PHE	CB-CG-CD1	-5.21	117.15	120.80
1	C	4	VAL	C-N-CA	5.21	134.72	121.70
1	C	95	GLU	CG-CD-OE1	-5.20	107.90	118.30
1	A	151[A]	ARG	NE-CZ-NH1	-5.19	117.70	120.30
1	A	151[B]	ARG	NE-CZ-NH1	-5.19	117.70	120.30
1	C	245	ARG	CG-CD-NE	5.18	122.68	111.80
1	B	203	VAL	CA-C-N	5.18	128.59	117.20
1	A	214	MET	CB-CG-SD	-5.17	96.88	112.40
1	A	286	LYS	CB-CG-CD	5.17	125.05	111.60
1	C	285	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	A	64	ASP	CB-CA-C	5.15	120.70	110.40
1	B	4	VAL	C-N-CA	5.14	134.55	121.70
1	C	201	ARG	NE-CZ-NH1	-5.14	117.73	120.30
1	A	280	ASP	OD1-CG-OD2	-5.13	113.55	123.30
1	B	119	PRO	O-C-N	5.13	130.90	122.70
1	A	3	GLN	CA-C-N	-5.12	105.92	117.20
1	B	50	ARG	NE-CZ-NH1	-5.12	117.74	120.30
1	B	223	GLU	CA-CB-CG	5.12	124.67	113.40
1	A	48	ALA	O-C-N	5.12	130.88	122.70
1	C	36	GLU	OE1-CD-OE2	5.09	129.41	123.30
1	C	185	LEU	CB-CA-C	5.09	119.86	110.20
1	C	291	ASN	N-CA-C	-5.05	97.38	111.00
1	A	130	GLU	CG-CD-OE1	-5.04	108.22	118.30
1	B	22	GLU	CG-CD-OE1	-5.02	108.27	118.30
1	A	17	GLU	CA-C-O	-5.02	109.57	120.10
1	B	278	GLU	CG-CD-OE1	-5.01	108.27	118.30
1	C	185	LEU	N-CA-CB	-5.01	100.37	110.40
1	C	227	ARG	CG-CD-NE	5.01	122.33	111.80
1	C	307	ASP	CB-CA-C	5.01	120.43	110.40
1	A	238	LEU	O-C-N	5.01	130.71	122.70
1	A	259	MET	C-N-CA	-5.00	109.19	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	300	ILE	O-C-N	5.00	130.71	122.70

There are no chirality outliers.

All (19) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	161	ARG	Sidechain
1	A	45	ARG	Sidechain
1	A	63	ARG	Sidechain
1	B	117	ARG	Sidechain
1	B	161	ARG	Sidechain
1	B	25	ARG	Sidechain
1	B	276	ARG	Sidechain
1	B	45	ARG	Sidechain
1	B	50	ARG	Sidechain
1	B	63	ARG	Sidechain
1	C	117	ARG	Sidechain
1	C	123	ARG	Sidechain
1	C	161	ARG	Sidechain
1	C	227	ARG	Sidechain
1	C	25	ARG	Sidechain
1	C	285	ARG	Sidechain
1	C	289	ARG	Sidechain
1	C	45	ARG	Sidechain
1	C	63	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	2519	0	2540	112	0
1	B	2513	0	2530	105	0
1	C	2513	0	2530	104	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
2	C	4	0	0	0	0
3	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	5	0	0	0	0
3	C	5	0	0	0	0
4	A	151	0	0	7	0
4	B	133	0	0	6	0
4	C	134	0	0	9	0
All	All	7990	0	7600	321	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 21.

All (321) 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:3:GLN:HG2	1:A:247:ILE:HD13	1.28	1.07
1:B:3:GLN:HG2	1:B:247:ILE:HD13	1.33	1.07
1:B:123:ARG:NH2	1:B:159:ALA:O	1.94	0.99
1:B:3:GLN:N	4:B:378:HOH:O	1.99	0.96
1:A:41:LEU:HD13	1:A:45:ARG:HH11	1.32	0.94
1:B:3:GLN:NE2	1:B:121:GLU:OE1	1.99	0.94
1:A:3:GLN:N	4:A:452:HOH:O	2.00	0.94
1:A:41:LEU:HD13	1:A:45:ARG:NH1	1.83	0.94
1:A:3:GLN:NE2	1:A:116:SER:O	2.02	0.91
1:B:261:GLY:O	1:B:262:ALA:C	2.12	0.87
1:C:3:GLN:NE2	1:C:121:GLU:OE1	2.09	0.85
1:A:3:GLN:HG3	1:A:118:THR:HG23	1.59	0.84
1:B:3:GLN:HG3	1:B:118:THR:HG23	1.61	0.82
1:A:286:LYS:HZ1	1:A:289:ARG:HH11	1.27	0.82
1:B:286:LYS:NZ	1:B:289:ARG:HE	1.76	0.82
1:C:3:GLN:OE1	1:C:247:ILE:HG21	1.79	0.81
1:B:6:ARG:H	1:B:283:ASN:HD21	1.25	0.81
1:C:6:ARG:H	1:C:283:ASN:HD21	1.23	0.81
1:B:273:MET:HE3	1:B:281:LEU:HD11	1.62	0.80
1:B:286:LYS:NZ	1:B:289:ARG:NE	2.29	0.80
1:B:41:LEU:HG	1:B:45:ARG:NH1	1.97	0.79
1:A:152:MET:HG2	1:A:236:LEU:HD13	1.65	0.79
1:B:100:LEU:HD11	1:B:110:LEU:HD11	1.64	0.78
1:B:6:ARG:HG3	1:B:6:ARG:HH11	1.45	0.78
1:B:286:LYS:HZ3	1:B:289:ARG:NE	1.81	0.77
1:B:286:LYS:HZ1	1:B:289:ARG:HE	1.30	0.77
1:B:289:ARG:HD3	4:B:381:HOH:O	1.83	0.77
1:B:261:GLY:O	1:B:263:GLY:N	2.18	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:LEU:HD13	1:A:110:LEU:HD11	1.68	0.75
1:A:96:LEU:HD13	1:A:113:ILE:HD12	1.66	0.75
1:A:265:ASP:O	1:A:269:LEU:HB2	1.85	0.75
1:A:297:TYR:CE1	1:A:313:LEU:HD13	2.21	0.75
1:B:102:GLY:O	1:B:103:ALA:CB	2.34	0.75
1:C:3:GLN:HG2	1:C:118:THR:HG23	1.68	0.74
1:A:285:ARG:HH11	1:A:289:ARG:HH22	1.33	0.74
1:C:293:ALA:O	1:C:294:THR:HB	1.88	0.73
1:A:305:SER:O	1:A:309:LYS:HB2	1.89	0.72
1:C:310:LYS:HE2	1:C:310:LYS:HA	1.70	0.72
1:B:3:GLN:OE1	1:B:247:ILE:HG21	1.89	0.72
1:A:286:LYS:HZ1	1:A:289:ARG:NH1	1.87	0.71
1:C:259:MET:HG2	1:C:264:THR:HG23	1.71	0.71
1:A:291:ASN:O	1:A:293:ALA:N	2.20	0.71
1:C:22:GLU:O	1:C:26:LYS:HG2	1.90	0.71
1:C:3:GLN:O	1:C:280:ASP:OD2	2.08	0.71
1:B:39:LEU:O	1:B:43:THR:HB	1.91	0.70
1:A:310:LYS:O	1:A:314:LEU:HB2	1.92	0.70
1:A:285:ARG:HD2	1:A:289:ARG:NH2	2.07	0.69
1:B:102:GLY:O	1:B:103:ALA:HB3	1.92	0.69
1:A:304:THR:OG1	1:A:309:LYS:HG2	1.92	0.69
1:A:233:LEU:HG	1:A:237:LEU:HD22	1.73	0.69
1:C:297:TYR:CD2	1:C:318:GLU:HB2	2.28	0.69
1:A:259:MET:HG2	1:A:264:THR:HG23	1.73	0.69
1:C:108:LYS:HG3	4:C:380:HOH:O	1.91	0.68
1:B:310:LYS:O	1:B:314:LEU:HD22	1.93	0.68
1:B:273:MET:CE	1:B:281:LEU:HD11	2.21	0.68
1:A:97:LYS:HD3	1:A:133:TYR:CG	2.29	0.68
1:C:39:LEU:O	1:C:43:THR:HB	1.94	0.67
1:B:6:ARG:H	1:B:283:ASN:ND2	1.93	0.67
1:A:41:LEU:HD12	1:A:41:LEU:C	2.15	0.67
1:C:297:TYR:HD2	1:C:318:GLU:HB2	1.60	0.66
1:B:66:LEU:HD11	1:B:82:VAL:HG12	1.77	0.66
1:C:22:GLU:HB3	1:C:26:LYS:HE2	1.77	0.66
1:C:211:ASP:O	1:C:215:THR:HG23	1.94	0.66
1:A:43:THR:HG21	1:A:314:LEU:HG	1.78	0.66
1:A:293:ALA:O	1:A:294:THR:HB	1.95	0.65
1:A:261:GLY:O	1:A:263:GLY:N	2.30	0.65
1:B:297:TYR:CE1	1:B:313:LEU:HD13	2.32	0.65
1:A:286:LYS:HA	1:A:286:LYS:HZ2	1.62	0.65
1:B:220:GLN:NE2	4:B:396:HOH:O	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:GLU:O	1:B:26:LYS:HG2	1.97	0.65
1:A:39:LEU:O	1:A:43:THR:HB	1.97	0.64
1:C:286:LYS:HZ3	1:C:289:ARG:HD3	1.62	0.63
1:A:240:VAL:O	1:A:244:ILE:HG12	1.98	0.63
1:C:246:SER:HB3	1:C:249:ALA:HB3	1.80	0.63
1:C:259:MET:HE3	1:C:299:MET:HG2	1.80	0.63
1:B:291:ASN:O	1:B:293:ALA:N	2.26	0.63
1:B:147:GLY:O	1:B:151[A]:ARG:HD3	1.99	0.63
1:A:220:GLN:NE2	4:A:411:HOH:O	2.31	0.62
1:C:233:LEU:HG	1:C:237:LEU:HD22	1.81	0.62
1:A:297:TYR:CD1	1:A:313:LEU:HD22	2.34	0.62
1:C:12:PHE:HB2	1:C:44:SER:O	2.00	0.62
1:A:286:LYS:NZ	1:A:289:ARG:NH1	2.47	0.62
1:C:3:GLN:CG	1:C:118:THR:HG23	2.30	0.62
1:A:102:GLY:O	1:A:103:ALA:CB	2.47	0.62
1:B:214:MET:CE	1:B:219:PHE:C	2.68	0.62
1:B:3:GLN:O	1:B:280:ASP:OD2	2.17	0.62
1:B:246:SER:HB3	1:B:249:ALA:HB3	1.82	0.61
1:C:4:VAL:HA	1:C:280:ASP:HB3	1.82	0.61
1:B:3:GLN:HG2	1:B:247:ILE:CD1	2.22	0.61
1:C:291:ASN:O	1:C:293:ALA:N	2.29	0.61
1:A:294:THR:HG21	1:A:299:MET:CE	2.31	0.61
1:B:22:GLU:HB3	1:B:26:LYS:HE3	1.83	0.61
1:C:285:ARG:HH12	1:C:289:ARG:HH12	1.49	0.60
1:B:233:LEU:HG	1:B:237:LEU:HD22	1.83	0.60
1:A:299:MET:O	1:A:303:ASP:HB2	2.02	0.60
1:C:281:LEU:O	1:C:285:ARG:HG3	2.01	0.60
1:B:258:ALA:HB1	1:B:265:ASP:HB3	1.84	0.59
1:A:41:LEU:C	1:A:41:LEU:CD1	2.71	0.59
1:C:273:MET:HE3	1:C:281:LEU:HD21	1.84	0.59
1:B:172:VAL:HG12	1:B:212:LYS:HD2	1.84	0.59
1:B:6:ARG:N	1:B:283:ASN:HD21	1.98	0.59
1:A:318:GLU:O	1:A:318:GLU:OE1	2.21	0.59
1:B:280:ASP:O	1:B:284:ILE:HG13	2.04	0.58
1:C:5:LEU:HB3	1:C:283:ASN:OD1	2.03	0.58
1:A:3:GLN:CD	1:A:276:ARG:HH22	2.07	0.57
1:B:240:VAL:O	1:B:244:ILE:HG12	2.05	0.57
1:C:293:ALA:O	1:C:294:THR:CB	2.53	0.57
1:B:6:ARG:O	1:B:282:PHE:HB3	2.04	0.56
1:C:285:ARG:HH11	1:C:289:ARG:HH22	1.52	0.56
1:B:4:VAL:HA	1:B:280:ASP:HB3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:THR:HG21	1:A:299:MET:HE3	1.87	0.56
1:A:246:SER:HB3	1:A:249:ALA:HB3	1.87	0.56
1:C:22:GLU:HB3	1:C:26:LYS:CE	2.36	0.56
1:C:256:TYR:HD2	1:C:257:TYR:CE1	2.24	0.55
1:A:318:GLU:CD	1:A:318:GLU:O	2.46	0.54
1:A:5:LEU:HB3	1:A:283:ASN:OD1	2.08	0.54
1:B:41:LEU:O	1:B:45:ARG:HG2	2.07	0.54
1:C:263:GLY:O	4:C:413:HOH:O	2.19	0.54
1:C:308:TYR:CE1	1:C:312:LEU:HD11	2.43	0.54
1:B:100:LEU:HD11	1:B:110:LEU:CD1	2.36	0.54
1:C:105:THR:OG1	1:C:144:ASP:HB3	2.06	0.54
1:C:214:MET:HE1	1:C:219:PHE:C	2.27	0.53
1:B:47:ASN:O	1:B:51:GLN:HG2	2.07	0.53
1:A:11:ASP:OD1	1:A:46:SER:OG	2.15	0.53
1:C:6:ARG:N	1:C:283:ASN:HD21	2.01	0.53
1:B:96:LEU:O	1:B:100:LEU:HD13	2.09	0.53
1:C:285:ARG:HH11	1:C:289:ARG:NH2	2.07	0.53
1:B:151[B]:ARG:NH2	4:B:426:HOH:O	2.40	0.53
1:C:8:THR:HG23	1:C:281:LEU:HB3	1.91	0.53
1:C:285:ARG:NH1	1:C:289:ARG:HH12	2.07	0.53
1:B:286:LYS:N	1:B:286:LYS:HD2	2.24	0.52
1:B:3:GLN:OE1	1:B:276:ARG:NH2	2.42	0.52
1:B:15:PHE:CE2	1:B:52:GLU:HG3	2.44	0.52
1:C:18:ARG:NH2	4:C:326:HOH:O	2.43	0.52
1:A:282:PHE:O	1:A:285:ARG:HB2	2.09	0.52
1:A:28:MET:SD	1:A:72:GLU:HG3	2.49	0.52
1:B:66:LEU:CD1	1:B:82:VAL:HG12	2.40	0.52
1:C:253:GLU:HG3	1:C:257:TYR:HE1	1.74	0.52
1:A:152:MET:CG	1:A:236:LEU:HD13	2.38	0.52
1:B:3:GLN:NE2	1:B:117:ARG:HA	2.25	0.51
1:A:259:MET:HE3	1:A:299:MET:HG2	1.93	0.51
1:B:259:MET:HG2	1:B:264:THR:HG23	1.92	0.51
1:C:253:GLU:HG3	1:C:257:TYR:CE1	2.45	0.51
1:C:273:MET:HE3	1:C:281:LEU:HD11	1.92	0.51
1:A:3:GLN:HB2	4:A:415:HOH:O	2.10	0.51
1:C:292:PHE:O	1:C:293:ALA:O	2.29	0.51
1:A:214:MET:HA	1:A:219:PHE:O	2.10	0.51
1:B:15:PHE:HE2	1:B:52:GLU:HG3	1.74	0.51
1:B:211:ASP:O	1:B:215:THR:HG23	2.11	0.51
1:A:149:TYR:CD1	1:A:232:ASN:HB3	2.45	0.51
1:A:256:TYR:HD2	1:A:257:TYR:CD1	2.27	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:ASP:N	4:A:421:HOH:O	2.44	0.51
1:C:6:ARG:H	1:C:283:ASN:ND2	1.99	0.50
1:A:12:PHE:HB2	1:A:44:SER:O	2.12	0.50
1:A:118:THR:HB	1:A:119:PRO:CD	2.41	0.50
1:B:309:LYS:NZ	1:B:310:LYS:HZ2	2.09	0.50
1:A:97:LYS:HD3	1:A:133:TYR:CD1	2.46	0.49
1:A:147:GLY:O	1:A:151[B]:ARG:HG3	2.12	0.49
1:B:310:LYS:HE3	1:B:313:LEU:HD12	1.94	0.49
1:B:11:ASP:OD1	1:B:46:SER:OG	2.15	0.49
1:C:285:ARG:NH1	1:C:289:ARG:HH22	2.10	0.49
1:A:208:LYS:NZ	4:A:442:HOH:O	2.46	0.49
1:A:301:LYS:HA	1:A:309:LYS:HD3	1.95	0.49
1:B:18:ARG:O	1:B:22:GLU:HG3	2.12	0.49
1:A:3:GLN:O	1:A:280:ASP:OD2	2.31	0.49
1:C:294:THR:HG21	1:C:299:MET:CE	2.43	0.49
1:C:100:LEU:HD13	1:C:110:LEU:HD11	1.94	0.49
1:A:3:GLN:OE1	1:A:276:ARG:NH1	2.41	0.49
1:B:297:TYR:CD1	1:B:313:LEU:HD22	2.48	0.49
1:C:309:LYS:O	1:C:313:LEU:HD22	2.13	0.49
1:B:214:MET:HE2	1:B:219:PHE:C	2.32	0.48
1:B:263:GLY:O	4:B:452:HOH:O	2.20	0.48
1:A:102:GLY:O	1:A:103:ALA:HB3	2.13	0.48
1:C:282:PHE:O	1:C:285:ARG:HB2	2.13	0.48
1:B:82:VAL:O	1:B:86[A]:LYS:HG2	2.13	0.48
1:C:260:LYS:O	1:C:260:LYS:HE2	2.13	0.48
1:C:307:ASP:N	4:C:444:HOH:O	2.36	0.48
1:A:285:ARG:HH11	1:A:289:ARG:NH2	2.06	0.48
1:B:253:GLU:HA	1:B:292:PHE:CE2	2.48	0.48
1:B:259:MET:CE	1:B:299:MET:HG2	2.43	0.48
1:A:25:ARG:NH1	4:A:378:HOH:O	2.46	0.48
1:C:4:VAL:HG23	1:C:5:LEU:N	2.28	0.48
1:C:3:GLN:NE2	1:C:117:ARG:HA	2.28	0.48
1:A:297:TYR:HE1	1:A:313:LEU:HD13	1.74	0.48
1:B:161:ARG:HG3	1:B:201:ARG:O	2.14	0.48
1:A:43:THR:HG21	1:A:314:LEU:CG	2.42	0.48
1:C:108:LYS:HE3	4:C:380:HOH:O	2.13	0.48
1:B:309:LYS:HZ1	1:B:310:LYS:NZ	2.12	0.48
1:C:273:MET:CE	1:C:281:LEU:HD11	2.44	0.48
1:C:106:ASN:ND2	1:C:109:VAL:HG12	2.29	0.48
1:B:214:MET:HE3	1:B:220:GLN:N	2.29	0.47
1:B:292:PHE:O	1:B:293:ALA:O	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:MET:HE2	1:A:281:LEU:HD11	1.96	0.47
1:C:3:GLN:OE1	1:C:276:ARG:NH2	2.48	0.47
1:A:105:THR:OG1	1:A:144:ASP:HB3	2.15	0.47
1:B:309:LYS:NZ	1:B:310:LYS:NZ	2.62	0.47
1:B:6:ARG:HG3	1:B:6:ARG:NH1	2.20	0.47
1:B:101:LYS:HB3	1:B:102:GLY:H	1.40	0.47
1:A:305:SER:C	1:A:309:LYS:HB2	2.35	0.47
1:C:43:THR:HG21	1:C:314:LEU:HB3	1.96	0.47
1:A:161:ARG:HG3	1:A:161:ARG:HH11	1.80	0.47
1:C:167:ILE:HG22	1:C:169[B]:GLU:OE1	2.14	0.47
1:B:96:LEU:HD13	1:B:113:ILE:HD12	1.97	0.47
1:C:214:MET:CE	1:C:219:PHE:C	2.84	0.47
1:A:106:ASN:ND2	1:A:109:VAL:HG23	2.30	0.47
1:C:240:VAL:O	1:C:244:ILE:HG12	2.15	0.47
1:C:297:TYR:CE1	1:C:313:LEU:HG	2.49	0.46
1:B:264:THR:OG1	1:B:303:ASP:OD2	2.31	0.46
1:C:3:GLN:HA	1:C:247:ILE:HD13	1.98	0.46
1:A:286:LYS:CA	1:A:286:LYS:HZ2	2.28	0.46
1:A:118:THR:HB	1:A:119:PRO:HD2	1.97	0.46
1:C:108:LYS:HZ1	1:C:235:GLN:HB3	1.80	0.46
1:B:299:MET:O	1:B:303:ASP:HB2	2.15	0.46
1:C:256:TYR:CD2	1:C:292:PHE:CE1	3.04	0.46
1:B:39:LEU:HB3	1:B:77:PHE:CZ	2.51	0.46
1:B:149:TYR:CD1	1:B:232:ASN:HB3	2.50	0.46
1:B:273:MET:O	1:B:277:SER:HB3	2.16	0.46
1:A:285:ARG:NH1	1:A:318:GLU:HB3	2.31	0.45
1:B:297:TYR:HE1	1:B:313:LEU:HD13	1.79	0.45
1:B:18:ARG:NH2	4:B:371:HOH:O	2.12	0.45
1:B:260:LYS:HD2	1:B:260:LYS:HA	1.47	0.45
1:A:41:LEU:O	1:A:45:ARG:HG2	2.15	0.45
1:C:247:ILE:N	1:C:248:PRO:CD	2.80	0.45
1:B:84:LEU:HD13	1:B:274:VAL:HG22	1.97	0.45
1:B:4:VAL:HB	1:B:5:LEU:H	1.44	0.45
1:B:310:LYS:HD3	1:B:310:LYS:HA	1.63	0.45
1:A:4:VAL:HB	1:A:5:LEU:H	1.39	0.45
1:C:192:GLU:HG3	4:C:404:HOH:O	2.16	0.45
1:A:48:ALA:O	1:A:52:GLU:HG3	2.16	0.45
1:C:97:LYS:HD3	1:C:133:TYR:CG	2.51	0.45
1:C:15:PHE:CZ	1:C:17:GLU:HB3	2.52	0.44
1:C:24:LEU:HD12	1:C:53:ILE:HG21	1.99	0.44
1:A:174:GLN:HG3	4:A:439:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:161:ARG:HG3	1:C:201:ARG:O	2.16	0.44
1:B:247:ILE:N	1:B:248:PRO:CD	2.80	0.44
1:A:79:LYS:HD2	1:A:79:LYS:N	2.33	0.44
1:B:35:GLU:HA	1:B:38:ILE:HD12	2.00	0.44
1:A:247:ILE:N	1:A:248:PRO:CD	2.80	0.44
1:C:253:GLU:O	1:C:257:TYR:HD1	2.00	0.44
1:B:3:GLN:HB3	1:B:276:ARG:HH22	1.82	0.44
1:A:69:LEU:HG	1:A:81:ILE:HG21	2.00	0.44
1:B:39:LEU:HB3	1:B:77:PHE:HZ	1.82	0.44
1:C:285:ARG:HG2	1:C:296:LEU:HD23	1.98	0.44
1:C:280:ASP:HA	1:C:283:ASN:HD22	1.82	0.44
1:A:123:ARG:NH2	1:A:159:ALA:O	2.50	0.44
1:A:190:ASP:OD2	1:A:193[A]:LYS:HE2	2.17	0.44
1:C:280:ASP:O	1:C:284:ILE:HG13	2.18	0.44
1:C:43:THR:CG2	1:C:314:LEU:HB3	2.48	0.44
1:A:46:SER:O	1:A:50:ARG:HG3	2.18	0.44
1:C:5:LEU:HD22	1:C:5:LEU:HA	1.77	0.43
1:C:257:TYR:CD1	1:C:257:TYR:N	2.86	0.43
1:B:97:LYS:HD3	1:B:133:TYR:CD1	2.53	0.43
1:C:123:ARG:HD2	4:C:351:HOH:O	2.17	0.43
1:A:101:LYS:HG2	1:A:102:GLY:H	1.82	0.43
1:B:5:LEU:HB3	1:B:283:ASN:OD1	2.18	0.43
1:A:261:GLY:C	1:A:263:GLY:N	2.69	0.43
1:A:245:ARG:HG2	1:A:245:ARG:HH11	1.83	0.43
1:A:66:LEU:HA	1:A:66:LEU:HD12	1.79	0.43
1:C:147:GLY:O	1:C:151[A]:ARG:HD2	2.18	0.43
1:A:285:ARG:HH12	1:A:318:GLU:HB3	1.84	0.43
1:C:43:THR:HG21	1:C:314:LEU:HG	2.00	0.43
1:A:214:MET:CE	1:A:220:GLN:OE1	2.67	0.43
1:A:15:PHE:CZ	1:A:17:GLU:HB3	2.53	0.43
1:A:3:GLN:HB3	1:A:276:ARG:HH22	1.84	0.43
1:C:108:LYS:NZ	1:C:235:GLN:HB3	2.34	0.43
1:B:5:LEU:HD22	1:B:5:LEU:HA	1.91	0.43
1:B:208:LYS:NZ	1:B:208:LYS:HB3	2.34	0.43
1:C:94:TYR:O	1:C:98:HIS:HD2	2.02	0.43
1:C:4:VAL:CG2	1:C:5:LEU:N	2.78	0.42
1:C:3:GLN:CD	1:C:276:ARG:HH22	2.23	0.42
1:C:43:THR:HG21	1:C:314:LEU:CG	2.49	0.42
1:C:151[B]:ARG:NH2	4:C:425:HOH:O	2.49	0.42
1:A:41:LEU:HD22	1:A:45:ARG:HH12	1.85	0.42
1:B:15:PHE:HZ	1:B:53:ILE:HG13	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:TYR:CE1	1:B:151[B]:ARG:NH1	2.88	0.42
1:A:260:LYS:HA	1:A:260:LYS:HD2	1.57	0.42
1:C:267:HIS:HD2	1:C:267:HIS:O	2.03	0.42
1:B:106:ASN:OD1	1:B:108:LYS:HB3	2.19	0.42
1:C:96:LEU:HD12	1:C:110:LEU:HD12	2.02	0.42
1:B:100:LEU:HD23	1:B:140:ASP:HB3	2.02	0.42
1:A:114:ILE:HD12	1:A:153:LEU:HD22	2.01	0.42
1:A:145:THR:O	1:A:150:GLN:NE2	2.53	0.42
1:C:276:ARG:HH21	1:C:280:ASP:CG	2.23	0.42
1:A:101:LYS:C	1:A:103:ALA:H	2.21	0.42
1:A:152:MET:HE2	1:A:156:LEU:HD21	2.01	0.42
1:B:251:LEU:HB3	1:B:284:ILE:HD13	2.02	0.41
1:A:273:MET:CE	1:A:281:LEU:HD11	2.50	0.41
1:A:47:ASN:O	1:A:51:GLN:HG2	2.19	0.41
1:A:75:GLY:O	1:A:79:LYS:HD3	2.19	0.41
1:B:247:ILE:HB	1:B:248:PRO:HD3	2.01	0.41
1:A:151[B]:ARG:HD2	1:A:151[B]:ARG:HH11	1.58	0.41
1:A:221:ILE:HD12	1:A:221:ILE:HA	1.91	0.41
1:C:91:TYR:OH	4:C:361:HOH:O	2.15	0.41
1:C:299:MET:HB2	1:C:299:MET:HE3	1.92	0.41
1:C:82:VAL:O	1:C:86[B]:LYS:HG2	2.21	0.41
1:C:114:ILE:HD12	1:C:153:LEU:HD22	2.03	0.41
1:A:286:LYS:NZ	1:A:289:ARG:HD2	2.36	0.41
1:C:310:LYS:O	1:C:314:LEU:HD22	2.21	0.41
1:A:259:MET:CE	1:A:299:MET:HG2	2.50	0.41
1:B:214:MET:HE3	1:B:219:PHE:C	2.40	0.41
1:B:276:ARG:HH21	1:B:280:ASP:CG	2.23	0.41
1:A:294:THR:CG2	1:A:299:MET:HE3	2.49	0.41
1:C:285:ARG:HD2	1:C:285:ARG:HH11	1.64	0.41
1:A:161:ARG:HG3	1:A:201:ARG:O	2.20	0.41
1:B:60:LEU:HD12	1:B:60:LEU:HA	1.90	0.41
1:C:285:ARG:O	1:C:289:ARG:HD2	2.20	0.41
1:A:182:ALA:HB1	1:A:190:ASP:HB3	2.03	0.41
1:A:157:LEU:HA	1:A:157:LEU:HD23	1.92	0.41
1:B:76:LYS:HE2	1:B:266:ASP:OD2	2.21	0.40
1:C:3:GLN:NE2	1:C:276:ARG:HH12	2.20	0.40
1:C:299:MET:O	1:C:303:ASP:HB2	2.21	0.40
1:C:286:LYS:HA	1:C:289:ARG:HG2	2.03	0.40
1:C:4:VAL:HB	1:C:5:LEU:H	1.37	0.40
1:A:256:TYR:HB2	1:A:288:PHE:CE1	2.57	0.40
1:B:41:LEU:HG	1:B:45:ARG:HH12	1.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:285:ARG:HD3	1:B:316:CYS:SG	2.62	0.40
1:C:310:LYS:NZ	1:C:314:LEU:HD22	2.37	0.40
1:C:26:LYS:HD3	1:C:26:LYS:N	2.37	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	319/319 (100%)	293 (92%)	18 (6%)	8 (2%)	7	1
1	B	318/319 (100%)	296 (93%)	13 (4%)	9 (3%)	6	1
1	C	318/319 (100%)	294 (92%)	17 (5%)	7 (2%)	8	1
All	All	955/957 (100%)	883 (92%)	48 (5%)	24 (2%)	7	1

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	103	ALA
1	A	292	PHE
1	A	294	THR
1	B	5	LEU
1	B	292	PHE
1	B	293	ALA
1	B	294	THR
1	C	5	LEU
1	C	103	ALA
1	C	292	PHE
1	C	294	THR
1	A	291	ASN
1	A	293	ALA

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Mol	Chain	Res	Type
1	B	103	ALA
1	B	262	ALA
1	C	293	ALA
1	A	4	VAL
1	B	30	GLY
1	A	166	GLY
1	C	4	VAL
1	B	166	GLY
1	B	4	VAL
1	C	166	GLY

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	274/271 (101%)	233 (85%)	41 (15%)	3	1
1	B	273/271 (101%)	236 (86%)	37 (14%)	5	1
1	C	273/271 (101%)	226 (83%)	47 (17%)	2	0
All	All	820/813 (101%)	695 (85%)	125 (15%)	3	1

All (125) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	10	THR
1	A	26	LYS
1	A	31	LEU
1	A	33	THR
1	A	39	LEU
1	A	41	LEU
1	A	42	LEU
1	A	43	THR
1	A	59	THR
1	A	60	LEU
1	A	69	LEU

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Mol	Chain	Res	Type
1	A	71	SER
1	A	78	GLU
1	A	79	LYS
1	A	84	LEU
1	A	89	ARG
1	A	96	LEU
1	A	100	LEU
1	A	108	LYS
1	A	110	LEU
1	A	128	VAL
1	A	136	SER
1	A	160	ASN
1	A	163	PRO
1	A	236	LEU
1	A	237	LEU
1	A	251	LEU
1	A	260	LYS
1	A	269	LEU
1	A	281	LEU
1	A	283	ASN
1	A	286	LYS
1	A	290	LYS
1	A	291	ASN
1	A	294	THR
1	A	297	TYR
1	A	298	SER
1	A	303	ASP
1	A	309	LYS
1	A	310	LYS
1	B	5	LEU
1	B	6	ARG
1	B	10	THR
1	B	33	THR
1	B	36	GLU
1	B	39	LEU
1	B	42	LEU
1	B	43	THR
1	B	52	GLU
1	B	59	THR
1	B	60	LEU
1	B	69	LEU
1	B	84	LEU

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Mol	Chain	Res	Type
1	B	90	LEU
1	B	96	LEU
1	B	97	LYS
1	B	123	ARG
1	B	151[A]	ARG
1	B	151[B]	ARG
1	B	164	ASP
1	B	169[A]	GLU
1	B	169[B]	GLU
1	B	212	LYS
1	B	214	MET
1	B	237	LEU
1	B	251	LEU
1	B	260	LYS
1	B	281	LEU
1	B	286	LYS
1	B	289	ARG
1	B	290	LYS
1	B	291	ASN
1	B	297	TYR
1	B	299	MET
1	B	303	ASP
1	B	310	LYS
1	B	314	LEU
1	C	5	LEU
1	C	22	GLU
1	C	25	ARG
1	C	33	THR
1	C	36	GLU
1	C	39	LEU
1	C	42	LEU
1	C	43	THR
1	C	45	ARG
1	C	59	THR
1	C	60	LEU
1	C	69	LEU
1	C	76	LYS
1	C	84	LEU
1	C	86[A]	LYS
1	C	86[B]	LYS
1	C	89	ARG
1	C	96	LEU

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Mol	Chain	Res	Type
1	C	97	LYS
1	C	100	LEU
1	C	108	LYS
1	C	109	VAL
1	C	110	LEU
1	C	123	ARG
1	C	127	GLN
1	C	136	SER
1	C	137	LEU
1	C	160	ASN
1	C	185	LEU
1	C	214	MET
1	C	227	ARG
1	C	237	LEU
1	C	251	LEU
1	C	260	LYS
1	C	269	LEU
1	C	273	MET
1	C	281	LEU
1	C	286	LYS
1	C	289	ARG
1	C	297	TYR
1	C	298	SER
1	C	299	MET
1	C	303	ASP
1	C	305	SER
1	C	310	LYS
1	C	313	LEU
1	C	314	LEU

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

Mol	Chain	Res	Type
1	A	127	GLN
1	A	177	GLN
1	A	181	GLN
1	A	283	ASN
1	B	98	HIS
1	B	150	GLN
1	B	220	GLN
1	B	283	ASN
1	C	98	HIS

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Mol	Chain	Res	Type
1	C	150	GLN
1	C	232	ASN
1	C	283	ASN
1	C	291	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 12 are monoatomic - leaving 3 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	SO4	A	322	2	4,4,4	2.66	2 (50%)	6,6,6	0.88	0
3	SO4	B	322	2	4,4,4	2.56	2 (50%)	6,6,6	0.39	0
3	SO4	C	322	2	4,4,4	2.83	2 (50%)	6,6,6	0.73	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	A	322	2	-	0/0/0/0	0/0/0/0
3	SO4	B	322	2	-	0/0/0/0	0/0/0/0
3	SO4	C	322	2	-	0/0/0/0	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	322	SO4	O4-S	3.21	1.58	1.47
3	A	322	SO4	O1-S	3.54	1.59	1.47
3	C	322	SO4	O4-S	3.77	1.60	1.47
3	B	322	SO4	O1-S	3.84	1.60	1.47
3	A	322	SO4	O4-S	3.85	1.61	1.47
3	C	322	SO4	O1-S	4.14	1.61	1.47

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.