



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:36 PM UTC

PDB ID : 3A6O / pdb_00003a6o
Title : Crystal structure of Thermoactinomyces vulgaris R-47 alpha-amylase 2/acarbose complex
Authors : Ohtaki, A.; Mizuno, M.; Tono-zuka, T.; Sakano, Y.; Kamitori, S.
Deposited on : 2009-09-07
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

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)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

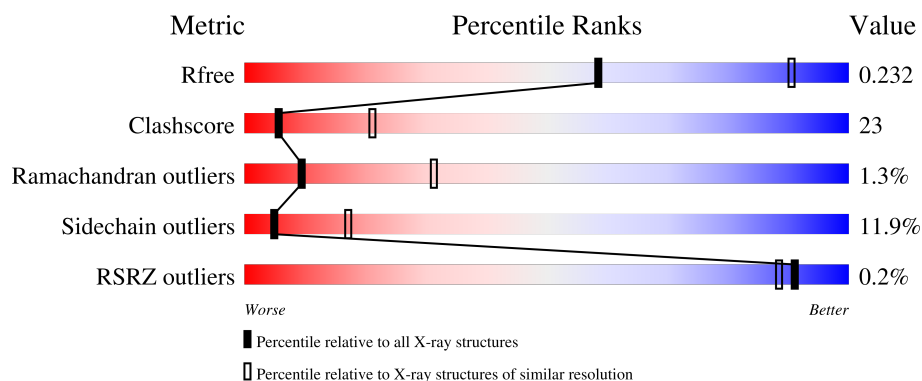
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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 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 $\leq 5\%$. 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	585	57% 31% 9% .
1	B	585	55% 34% 9% .

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 10068 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.

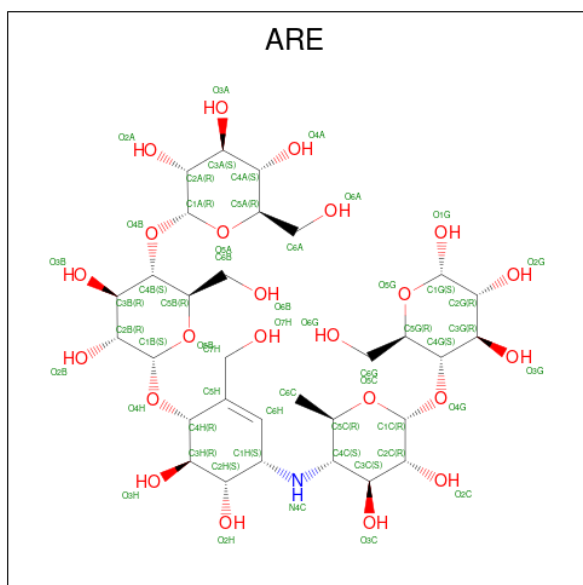
- Molecule 1 is a protein called Neopullulanase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	585	Total	C	N	O	S	0	0	0
			4775	3056	831	873	15			
1	B	585	Total	C	N	O	S	0	0	0
			4775	3056	831	873	15			

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		
2	B	1	Total	Ca	0	0
			1	1		

- Molecule 3 is ACARBOSE DERIVED PENTASACCHARIDE (CCD ID: ARE) (formula: C₃₁H₅₃NO₂₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			55	31	1	23		
3	B	1	Total	C	N	O	0	0
			55	31	1	23		

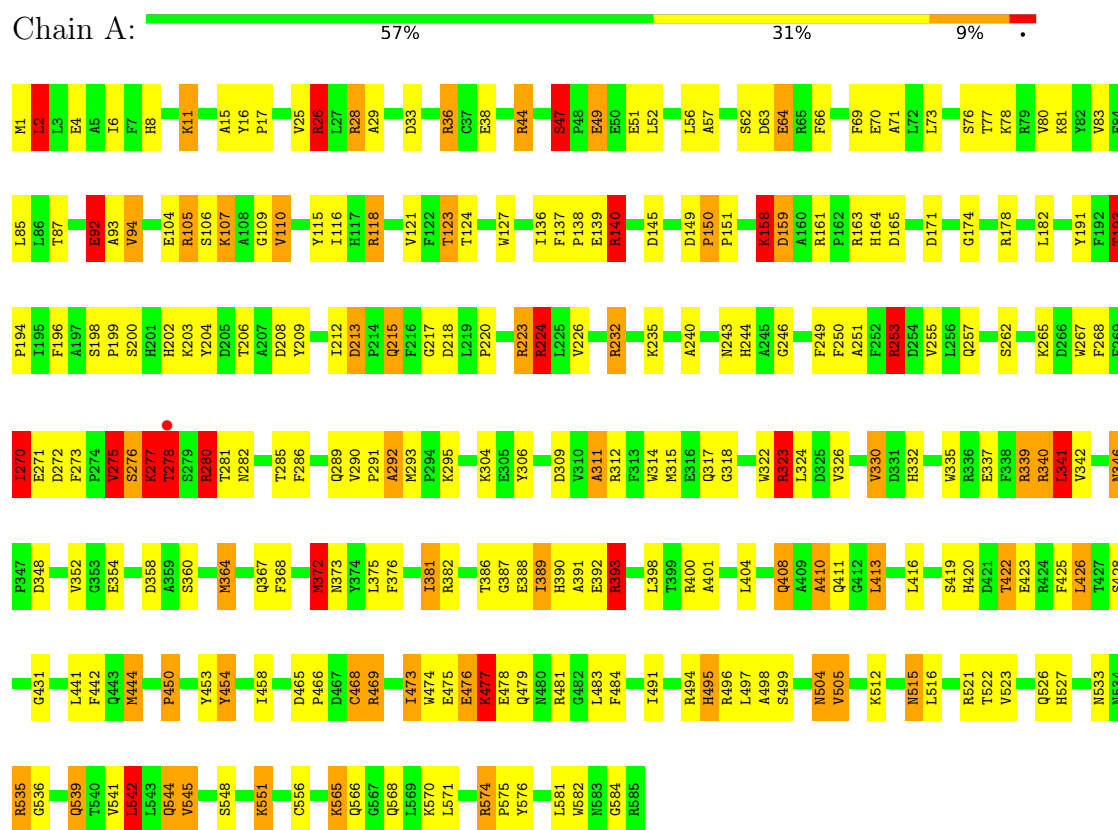
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	205	Total	O	0	0
			205	205		
4	B	201	Total	O	0	0
			201	201		

3 Residue-property plots

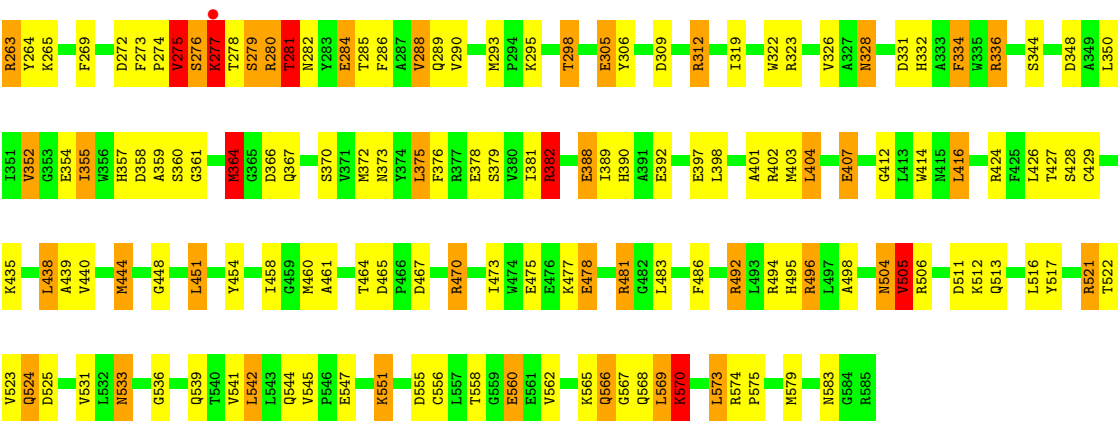
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Neopullulanase 2



• Molecule 1: Neopullulanase 2





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	114.60Å 119.26Å 113.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.81 – 2.80 38.81 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (38.81-2.80) 99.2 (38.81-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.19 (at 2.81Å)	Xtriage
Refinement program	CNS, REFMAC 5.2.0005	Depositor
R, R_{free}	0.157 , 0.231 0.163 , 0.232	Depositor DCC
R_{free} test set	3455 reflections (8.97%)	wwPDB-VP
Wilson B-factor (Å ²)	32.0	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 41.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.021 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10068	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.57% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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, ARE

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	1.67	46/4905 (0.9%)	1.58	65/6641 (1.0%)
1	B	1.65	36/4905 (0.7%)	1.51	38/6641 (0.6%)
All	All	1.66	82/9810 (0.8%)	1.55	103/13282 (0.8%)

All (82) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	193	THR	CA-C	9.85	1.65	1.52
1	A	340	ARG	CG-CD	8.57	1.78	1.52
1	A	11	LYS	N-CA	8.20	1.56	1.46
1	A	278	THR	N-CA	8.04	1.56	1.46
1	B	359	ALA	CA-CB	7.55	1.63	1.53
1	A	212	ILE	CA-CB	7.41	1.62	1.54
1	B	355	ILE	N-CA	7.38	1.55	1.46
1	A	277	LYS	CA-C	7.23	1.62	1.52
1	B	6	ILE	CA-CB	-7.05	1.45	1.54
1	A	92	GLU	N-CA	6.82	1.54	1.46
1	B	2	LEU	C-O	6.70	1.31	1.23
1	B	51	GLU	CA-C	6.64	1.61	1.52
1	B	570	LYS	N-CA	6.62	1.54	1.46
1	B	458	ILE	N-CA	6.62	1.52	1.46
1	B	249	PHE	CA-C	6.58	1.61	1.52
1	B	162	PRO	N-CA	6.56	1.55	1.47
1	A	280	ARG	CA-C	6.49	1.62	1.53
1	B	505	VAL	CA-CB	-6.45	1.46	1.54
1	B	348	ASP	N-CA	6.37	1.53	1.46
1	A	257	GLN	C-O	-6.34	1.17	1.24
1	B	334	PHE	C-O	6.32	1.31	1.24
1	A	36	ARG	C-O	6.20	1.31	1.23
1	B	193	THR	CA-C	6.11	1.60	1.52
1	A	477	LYS	C-O	-6.10	1.17	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	98	GLU	C-O	-6.08	1.16	1.24
1	B	198	SER	CA-C	6.08	1.58	1.52
1	A	381	ILE	C-O	6.06	1.30	1.24
1	A	28	ARG	C-O	6.05	1.31	1.23
1	B	273	PHE	CA-C	6.05	1.61	1.52
1	A	387	GLY	C-O	-6.01	1.15	1.23
1	A	4	GLU	CB-CG	-5.93	1.34	1.52
1	A	340	ARG	CD-NE	5.87	1.54	1.46
1	A	548	SER	CA-C	5.85	1.60	1.52
1	A	257	GLN	CA-C	-5.83	1.46	1.53
1	B	556	CYS	CA-C	-5.80	1.44	1.52
1	B	93	ALA	CA-C	5.72	1.59	1.52
1	A	372	MET	CA-C	-5.71	1.45	1.52
1	B	68	TYR	C-O	-5.69	1.17	1.24
1	B	35	VAL	C-O	-5.68	1.18	1.24
1	A	124	THR	CA-C	5.64	1.59	1.52
1	B	305	GLU	CG-CD	5.62	1.66	1.52
1	A	63	ASP	CA-C	-5.61	1.47	1.53
1	B	29	ALA	N-CA	5.61	1.53	1.45
1	A	270	ILE	N-CA	5.59	1.52	1.46
1	A	410	ALA	CA-C	5.59	1.60	1.52
1	B	381	ILE	CA-CB	5.52	1.60	1.54
1	A	116	ILE	C-O	-5.49	1.18	1.24
1	A	80	VAL	CA-C	5.49	1.59	1.52
1	A	275	VAL	CA-C	-5.48	1.46	1.53
1	B	275	VAL	CA-CB	-5.46	1.47	1.54
1	A	410	ALA	CA-CB	-5.44	1.44	1.53
1	A	542	LEU	N-CA	-5.39	1.40	1.46
1	A	171	ASP	C-O	5.38	1.30	1.23
1	A	318	GLY	C-O	-5.37	1.17	1.24
1	B	439	ALA	CA-C	5.36	1.59	1.52
1	A	47	SER	C-N	5.36	1.39	1.34
1	B	498	ALA	C-O	5.33	1.30	1.24
1	B	200	SER	CA-C	-5.31	1.46	1.53
1	B	496	ARG	N-CA	-5.29	1.39	1.46
1	B	207	ALA	CA-CB	-5.29	1.46	1.53
1	A	454	TYR	C-O	5.28	1.30	1.23
1	A	473	ILE	CA-CB	5.24	1.60	1.53
1	B	288	VAL	CA-CB	5.24	1.60	1.54
1	A	389	ILE	C-O	-5.22	1.18	1.24
1	A	26	ARG	C-O	5.17	1.30	1.23
1	B	169	GLY	C-N	5.16	1.38	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	64	GLU	N-CA	5.14	1.52	1.46
1	B	478	GLU	CA-C	5.13	1.59	1.52
1	B	521	ARG	C-O	-5.12	1.17	1.24
1	A	110	VAL	CA-CB	5.11	1.61	1.54
1	A	224	ARG	NE-CZ	5.11	1.38	1.33
1	B	306	TYR	N-CA	-5.10	1.40	1.46
1	A	566	GLN	CA-C	5.10	1.59	1.52
1	A	496	ARG	CA-C	5.09	1.59	1.52
1	A	393	ARG	C-O	5.08	1.30	1.24
1	A	208	ASP	CA-C	5.08	1.58	1.52
1	A	306	TYR	N-CA	-5.06	1.40	1.46
1	B	22	GLN	CA-C	-5.04	1.46	1.52
1	A	495	HIS	C-O	-5.02	1.18	1.24
1	B	364	MET	CA-C	5.02	1.59	1.52
1	A	450	PRO	CA-C	-5.02	1.46	1.52
1	A	340	ARG	CB-CG	5.01	1.67	1.52

All (103) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	340	ARG	N-CA-C	-11.69	98.56	111.07
1	A	496	ARG	N-CA-C	11.65	125.11	111.71
1	A	275	VAL	CB-CA-C	-10.22	100.19	111.23
1	B	193	THR	CA-C-N	-9.31	110.13	119.90
1	B	193	THR	C-N-CA	-9.31	110.13	119.90
1	A	224	ARG	N-CA-C	-9.03	101.52	111.36
1	B	202	HIS	N-CA-C	-8.39	103.17	113.41
1	B	505	VAL	CB-CA-C	-8.33	98.20	110.62
1	A	140	ARG	N-CA-C	8.22	123.47	111.87
1	B	18	ILE	N-CA-C	-8.19	104.50	113.43
1	A	145	ASP	CA-C-N	8.09	128.18	119.28
1	A	145	ASP	C-N-CA	8.09	128.18	119.28
1	A	364	MET	N-CA-C	-8.04	103.68	113.97
1	A	323	ARG	CG-CD-NE	7.80	129.15	112.00
1	A	140	ARG	NE-CZ-NH1	-7.67	113.83	121.50
1	A	232	ARG	NE-CZ-NH2	7.63	126.07	119.20
1	A	545	VAL	CB-CA-C	-7.34	104.10	111.08
1	B	352	VAL	CA-C-N	-7.27	115.31	122.36
1	B	352	VAL	C-N-CA	-7.27	115.31	122.36
1	B	173	LYS	N-CA-C	-7.25	103.41	111.82
1	B	381	ILE	N-CA-CB	7.25	118.52	110.62
1	B	350	LEU	N-CA-C	7.13	120.56	110.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	495	HIS	CA-C-N	-6.99	111.69	122.60
1	B	495	HIS	C-N-CA	-6.99	111.69	122.60
1	B	158	LYS	N-CA-C	6.96	118.87	111.28
1	A	150	PRO	CA-C-N	6.95	127.33	119.83
1	A	150	PRO	C-N-CA	6.95	127.33	119.83
1	A	311	ALA	N-CA-C	-6.90	103.81	111.82
1	A	123	THR	OG1-CB-CG2	-6.85	95.59	109.30
1	B	172	LEU	N-CA-C	6.85	118.75	111.28
1	B	492	ARG	N-CA-C	-6.82	103.92	111.36
1	A	340	ARG	N-CA-CB	6.79	119.86	110.01
1	B	276	SER	N-CA-C	6.75	119.24	107.49
1	A	232	ARG	NE-CZ-NH1	-6.73	114.77	121.50
1	A	323	ARG	N-CA-C	-6.72	97.94	108.90
1	B	382	ARG	NE-CZ-NH2	6.68	125.22	119.20
1	B	298	THR	N-CA-C	-6.62	105.06	113.01
1	A	323	ARG	NE-CZ-NH2	6.57	125.11	119.20
1	A	202	HIS	N-CA-C	-6.53	105.85	113.88
1	A	267	TRP	N-CA-C	-6.48	105.19	113.23
1	B	505	VAL	N-CA-C	6.47	117.81	108.48
1	A	473	ILE	CB-CA-C	-6.46	102.67	111.33
1	B	16	TYR	CA-C-N	6.41	126.92	119.99
1	B	16	TYR	C-N-CA	6.41	126.92	119.99
1	B	207	ALA	N-CA-C	-6.39	106.02	113.88
1	B	583	ASN	CA-C-N	-6.33	115.91	123.44
1	B	583	ASN	C-N-CA	-6.33	115.91	123.44
1	B	336	ARG	NE-CZ-NH1	-6.26	115.24	121.50
1	A	273	PHE	N-CA-C	6.20	118.45	110.39
1	A	63	ASP	CB-CA-C	-6.20	106.66	114.40
1	B	76	SER	CB-CA-C	-6.09	101.32	110.88
1	A	33	ASP	N-CA-C	6.01	117.83	111.28
1	B	232	ARG	N-CA-C	-5.99	106.22	112.93
1	A	468	CYS	N-CA-C	-5.94	105.99	113.18
1	A	505	VAL	CB-CA-C	-5.91	101.41	110.50
1	B	76	SER	N-CA-C	-5.88	104.78	111.07
1	A	341	LEU	CD1-CG-CD2	-5.86	97.91	110.80
1	A	224	ARG	NE-CZ-NH2	5.85	124.47	119.20
1	A	226	VAL	CA-C-N	-5.83	112.00	120.29
1	A	226	VAL	C-N-CA	-5.83	112.00	120.29
1	A	484	PHE	N-CA-C	-5.77	104.36	111.40
1	B	148	ASN	N-CA-C	-5.71	104.89	112.94
1	A	292	ALA	CA-C-N	-5.69	116.52	122.89
1	A	292	ALA	C-N-CA	-5.69	116.52	122.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	144	GLY	N-CA-C	-5.62	106.00	115.62
1	A	410	ALA	N-CA-C	5.62	118.17	111.71
1	A	352	VAL	CB-CA-C	-5.60	102.16	110.33
1	B	566	GLN	CB-CA-C	-5.58	103.49	112.09
1	A	93	ALA	CA-C-N	-5.49	114.46	122.58
1	A	93	ALA	C-N-CA	-5.49	114.46	122.58
1	A	217	GLY	N-CA-C	-5.46	103.31	110.29
1	A	473	ILE	N-CA-CB	5.42	116.83	110.82
1	A	29	ALA	CA-C-O	-5.39	114.80	121.06
1	B	35	VAL	N-CA-C	-5.36	107.15	113.42
1	A	382	ARG	CB-CA-C	5.32	120.22	110.11
1	A	339	ARG	CA-C-O	-5.31	114.89	120.63
1	A	2	LEU	N-CA-C	5.31	117.13	108.63
1	A	44	ARG	N-CA-C	5.31	117.06	111.28
1	B	312	ARG	N-CA-CB	5.30	118.51	110.14
1	A	137	PHE	N-CA-C	-5.28	98.15	109.81
1	A	213	ASP	CA-C-N	5.27	125.33	119.32
1	A	213	ASP	C-N-CA	5.27	125.33	119.32
1	B	388	GLU	CB-CA-C	-5.26	100.89	110.63
1	B	163	ARG	N-CA-C	-5.26	102.73	110.52
1	A	498	ALA	N-CA-C	-5.23	105.58	111.28
1	A	442	PHE	N-CA-C	-5.22	105.48	111.07
1	A	556	CYS	N-CA-C	5.18	117.83	111.82
1	A	199	PRO	CB-CA-C	-5.17	105.25	112.64
1	A	340	ARG	NE-CZ-NH2	5.17	123.85	119.20
1	A	491	ILE	N-CA-C	5.14	115.86	110.62
1	B	379	SER	N-CA-C	-5.14	105.86	111.82
1	A	551	LYS	N-CA-C	-5.14	106.83	114.64
1	A	253	ARG	N-CA-C	-5.08	105.82	111.36
1	A	574	ARG	CA-C-N	-5.08	114.49	119.93
1	A	574	ARG	C-N-CA	-5.08	114.49	119.93
1	A	199	PRO	CA-C-O	-5.06	116.00	121.77
1	A	535	ARG	NE-CZ-NH2	5.06	123.75	119.20
1	A	548	SER	N-CA-C	5.05	117.17	111.11
1	B	138	PRO	N-CA-C	5.04	120.15	113.40
1	A	140	ARG	NH1-CZ-NH2	5.03	125.84	119.30
1	B	127	TRP	N-CA-C	-5.03	105.99	111.82
1	A	441	LEU	N-CA-C	-5.03	105.88	111.36
1	A	270	ILE	CG1-CB-CG2	-5.02	95.65	110.70

There are no chirality outliers.

There are no planarity outliers.

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	4775	0	4607	226	1
1	B	4775	0	4607	223	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	55	0	53	6	0
3	B	55	0	53	2	0
4	A	205	0	0	24	0
4	B	201	0	0	20	1
All	All	10068	0	9320	444	1

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 23.

All (444) 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:340:ARG:CD	1:A:340:ARG:CG	1.78	1.57
1:B:64:GLU:HB2	4:B:714:HOH:O	1.32	1.26
1:A:495:HIS:HB3	4:A:730:HOH:O	1.46	1.14
1:A:422:THR:HG22	1:A:423:GLU:O	1.48	1.14
1:A:277:LYS:HB3	1:A:280:ARG:O	1.49	1.12
1:A:158:LYS:HG3	1:A:478:GLU:HG3	1.35	1.08
1:A:158:LYS:O	1:A:158:LYS:HD3	1.56	1.05
1:B:256:LEU:HA	1:B:275:VAL:HG21	1.41	1.02
1:A:140:ARG:HD2	1:A:469:ARG:O	1.56	1.02
1:B:323:ARG:HH11	1:B:372:MET:HE1	1.20	1.01
1:A:545:VAL:O	1:A:545:VAL:HG23	1.61	1.00
1:B:328:ASN:H	1:B:328:ASN:HD22	1.02	0.99
1:B:105:ARG:HH11	1:B:105:ARG:HG2	1.28	0.99
1:A:340:ARG:HD3	4:A:783:HOH:O	1.69	0.93
1:A:323:ARG:HH21	1:A:372:MET:HE2	1.33	0.93
1:B:276:SER:HB2	1:B:282:ASN:OD1	1.70	0.92
1:A:200:SER:O	1:A:203:LYS:HD3	1.70	0.91
1:B:263:ARG:HH21	1:B:263:ARG:HG3	1.32	0.91
1:B:354:GLU:HG3	1:B:372:MET:HE3	1.55	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:544:GLN:HA	1:A:544:GLN:NE2	1.87	0.88
1:A:290:VAL:HG11	1:A:293:MET:HE2	1.56	0.87
1:A:309:ASP:OD2	1:A:312:ARG:NH1	2.08	0.87
1:A:393:ARG:HH21	1:A:393:ARG:HG3	1.40	0.86
1:A:83:VAL:HG11	4:A:634:HOH:O	1.74	0.86
1:A:275:VAL:O	1:A:276:SER:HB2	1.76	0.86
1:A:203:LYS:HE2	1:A:213:ASP:OD2	1.77	0.85
1:A:574:ARG:HG2	1:A:575:PRO:HD2	1.56	0.85
1:A:223:ARG:HD2	1:A:317:GLN:HE21	1.40	0.85
1:A:542:LEU:HD22	1:A:568:GLN:OE1	1.75	0.85
1:A:243:ASN:HD22	1:A:244:HIS:HD2	1.26	0.83
1:B:272:ASP:HB2	4:B:602:HOH:O	1.78	0.83
1:A:158:LYS:CG	1:A:478:GLU:HG3	2.09	0.82
1:A:499:SER:HB3	1:A:526:GLN:OE1	1.77	0.82
1:B:2:LEU:HD22	1:B:30:LYS:HE2	1.62	0.81
1:B:180:PRO:HG3	1:B:232:ARG:NH2	1.94	0.81
1:B:256:LEU:HD22	1:B:275:VAL:HG11	1.61	0.81
1:A:476:GLU:HG3	4:A:640:HOH:O	1.81	0.80
1:A:223:ARG:HD2	1:A:317:GLN:NE2	1.97	0.80
1:B:232:ARG:HH11	1:B:232:ARG:CG	1.97	0.78
1:A:545:VAL:O	1:A:545:VAL:CG2	2.33	0.77
1:B:332:HIS:HD2	1:B:367:GLN:OE1	1.65	0.77
1:A:140:ARG:CD	1:A:469:ARG:O	2.32	0.77
1:B:244:HIS:CD2	1:B:286:PHE:HB2	2.19	0.76
1:A:332:HIS:HE1	4:A:635:HOH:O	1.69	0.76
1:B:481:ARG:HG3	1:B:481:ARG:HH11	1.50	0.76
1:B:223:ARG:HB3	1:B:223:ARG:NH2	1.99	0.76
1:A:426:LEU:HD22	1:A:431:GLY:HA2	1.67	0.76
1:B:328:ASN:HD22	1:B:328:ASN:N	1.76	0.76
1:B:382:ARG:HH11	1:B:397:GLU:CD	1.93	0.76
1:A:105:ARG:HG2	1:A:105:ARG:HH21	1.49	0.76
1:B:232:ARG:HH11	1:B:232:ARG:HG2	1.49	0.75
1:B:551:LYS:NZ	1:B:566:GLN:H	1.85	0.74
1:A:341:LEU:HD23	1:A:342:VAL:N	2.02	0.74
1:B:243:ASN:HD21	1:B:295:LYS:NZ	1.85	0.74
1:B:263:ARG:HG3	1:B:263:ARG:NH2	1.99	0.74
1:A:386:THR:OG1	1:A:388:GLU:HG3	1.87	0.74
1:A:92:GLU:OE2	1:A:92:GLU:N	2.20	0.73
1:A:105:ARG:HG2	1:A:105:ARG:NH2	2.03	0.73
1:B:272:ASP:CB	4:B:602:HOH:O	2.33	0.73
1:B:133:ILE:HB	1:B:451:LEU:HD23	1.70	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280:ARG:HE	1:B:280:ARG:HA	1.53	0.72
1:A:178:ARG:CZ	4:A:702:HOH:O	2.35	0.72
1:B:10:ALA:O	1:B:11:LYS:HB3	1.90	0.72
1:A:323:ARG:NH2	1:A:372:MET:HE2	2.06	0.71
1:B:256:LEU:CA	1:B:275:VAL:HG21	2.19	0.70
1:A:83:VAL:HG12	1:A:109:GLY:O	1.92	0.70
1:B:257:GLN:HB3	4:B:629:HOH:O	1.92	0.69
1:B:256:LEU:CD2	1:B:275:VAL:HG11	2.23	0.69
1:A:293:MET:HE1	3:A:701:ARE:H6B1	1.75	0.69
1:A:51:GLU:OE2	1:A:51:GLU:HA	1.91	0.68
1:A:408:GLN:H	1:A:408:GLN:HE21	1.39	0.68
1:B:323:ARG:HE	1:B:372:MET:HE2	1.58	0.68
1:B:523:VAL:O	1:B:524:GLN:HB2	1.94	0.68
1:B:155:GLN:HA	1:B:155:GLN:NE2	2.09	0.67
1:B:243:ASN:HD21	1:B:295:LYS:HZ2	1.40	0.67
1:B:478:GLU:HA	1:B:478:GLU:OE2	1.94	0.67
1:A:416:LEU:H	1:A:416:LEU:HD23	1.58	0.67
1:A:223:ARG:CZ	1:A:223:ARG:HB3	2.24	0.67
1:A:272:ASP:O	1:A:282:ASN:ND2	2.28	0.67
1:B:478:GLU:HG3	4:B:766:HOH:O	1.95	0.67
1:A:255:VAL:HG12	1:A:275:VAL:HG21	1.74	0.67
1:A:477:LYS:H	1:A:477:LYS:HD2	1.59	0.67
1:A:422:THR:CG2	1:A:423:GLU:O	2.36	0.66
1:B:323:ARG:HH11	1:B:372:MET:CE	2.04	0.66
1:B:354:GLU:HG3	1:B:372:MET:CE	2.24	0.66
1:A:574:ARG:HG2	1:A:575:PRO:CD	2.26	0.65
1:B:551:LYS:HZ1	1:B:566:GLN:H	1.44	0.65
1:B:276:SER:CB	1:B:282:ASN:OD1	2.45	0.64
1:B:354:GLU:OE1	3:B:702:ARE:H1H	1.96	0.64
1:A:516:LEU:HD13	1:A:541:VAL:HG11	1.78	0.64
1:B:504:ASN:HD21	1:B:522:THR:HB	1.60	0.64
1:B:139:GLU:OE2	1:B:140:ARG:NH1	2.31	0.64
1:B:280:ARG:O	1:B:281:THR:HB	1.96	0.64
1:A:390:HIS:CD2	1:A:393:ARG:H	2.16	0.64
1:B:328:ASN:H	1:B:328:ASN:ND2	1.83	0.64
1:A:304:LYS:HE3	1:A:337:GLU:OE1	1.98	0.63
1:B:274:PRO:O	1:B:275:VAL:C	2.41	0.63
1:B:511:ASP:C	1:B:511:ASP:OD2	2.39	0.63
1:A:277:LYS:HZ2	1:A:278:THR:N	1.97	0.63
1:B:27:LEU:HD23	1:B:27:LEU:C	2.24	0.62
1:A:323:ARG:NH2	1:A:354:GLU:HG3	2.13	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:328:ASN:HB3	1:B:355:ILE:HG12	1.82	0.62
1:A:26:ARG:HA	1:A:69:PHE:O	1.99	0.62
1:B:323:ARG:NH1	1:B:372:MET:HE1	2.03	0.62
1:A:64:GLU:HB2	4:A:709:HOH:O	1.99	0.62
1:A:193:THR:CG2	4:A:605:HOH:O	2.47	0.61
1:B:47:SER:HB3	1:B:50:GLU:HG3	1.81	0.61
1:A:419:SER:H	1:A:422:THR:HB	1.66	0.61
1:A:339:ARG:HD2	1:A:367:GLN:O	1.99	0.61
1:A:499:SER:CB	1:A:526:GLN:OE1	2.47	0.61
1:A:544:GLN:HA	1:A:544:GLN:HE21	1.64	0.61
1:B:65:ARG:HH11	1:B:65:ARG:CG	2.13	0.61
1:B:202:HIS:CD2	1:B:204:TYR:H	2.19	0.61
1:A:544:GLN:HE22	1:A:568:GLN:HG2	1.64	0.60
1:A:178:ARG:HE	1:A:178:ARG:HA	1.65	0.60
1:A:243:ASN:HD22	1:A:244:HIS:CD2	2.15	0.60
1:A:341:LEU:HD23	1:A:341:LEU:C	2.26	0.60
1:B:358:ASP:OD1	1:B:358:ASP:C	2.44	0.60
1:A:36:ARG:NH1	1:A:38:GLU:OE2	2.29	0.60
1:A:138:PRO:HD2	1:A:193:THR:HG22	1.83	0.60
1:B:280:ARG:HA	1:B:280:ARG:NE	2.16	0.60
1:B:290:VAL:HG12	1:B:293:MET:HB2	1.82	0.60
1:A:178:ARG:NH1	4:A:702:HOH:O	2.33	0.60
1:A:393:ARG:HH21	1:A:393:ARG:CG	2.13	0.60
1:B:202:HIS:HD2	1:B:204:TYR:H	1.49	0.60
1:A:416:LEU:H	1:A:416:LEU:CD2	2.15	0.60
1:B:54:HIS:HB3	4:B:594:HOH:O	2.00	0.60
1:B:332:HIS:CD2	1:B:367:GLN:OE1	2.53	0.59
1:A:240:ALA:HB2	1:A:322:TRP:CE3	2.37	0.59
1:B:2:LEU:HD22	1:B:30:LYS:CE	2.32	0.59
1:B:68:TYR:CE2	1:B:403:MET:HG3	2.38	0.59
1:A:255:VAL:HA	1:A:262:SER:OG	2.02	0.59
1:A:290:VAL:HG11	1:A:293:MET:CE	2.31	0.59
1:A:83:VAL:HG13	1:A:110:VAL:HG12	1.85	0.59
1:A:277:LYS:O	1:A:281:THR:HA	2.03	0.59
1:A:8:HIS:HD2	1:A:26:ARG:O	1.86	0.58
1:B:155:GLN:HA	1:B:155:GLN:HE21	1.65	0.58
1:B:424:ARG:HB3	4:B:638:HOH:O	2.02	0.58
1:B:240:ALA:HB2	1:B:322:TRP:CE3	2.38	0.58
1:A:223:ARG:CD	1:A:317:GLN:NE2	2.66	0.58
1:A:200:SER:O	1:A:203:LYS:CD	2.49	0.58
1:A:276:SER:O	1:A:277:LYS:C	2.46	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:THR:HB	1:B:194:PRO:CD	2.33	0.57
1:B:135:GLN:O	1:B:454:TYR:HB3	2.05	0.57
1:B:180:PRO:HG3	1:B:232:ARG:HH22	1.65	0.57
1:B:269:PHE:HB2	1:B:284:GLU:HB2	1.86	0.57
1:A:77:THR:O	1:A:78:LYS:HB2	2.05	0.57
1:A:293:MET:HE1	3:A:701:ARE:C6B	2.35	0.57
1:B:505:VAL:O	1:B:506:ARG:HD3	2.05	0.57
1:B:536:GLY:HA2	1:B:575:PRO:HB3	1.87	0.57
1:B:373:ASN:ND2	1:B:376:PHE:H	2.03	0.56
1:A:36:ARG:HB3	1:A:87:THR:HB	1.87	0.56
1:B:223:ARG:HB3	1:B:223:ARG:CZ	2.35	0.56
1:A:277:LYS:O	1:A:280:ARG:C	2.49	0.56
1:B:382:ARG:HG2	1:B:388:GLU:CD	2.30	0.56
1:A:295:LYS:HE2	1:B:115:TYR:CZ	2.39	0.56
1:A:330:VAL:HG22	1:A:335:TRP:NE1	2.21	0.56
1:B:200:SER:OG	1:B:205:ASP:OD1	2.23	0.56
1:B:232:ARG:HG2	1:B:232:ARG:NH1	2.20	0.56
1:B:277:LYS:O	1:B:279:SER:HB2	2.05	0.56
1:B:573:LEU:CD1	1:B:579:MET:HG3	2.36	0.56
1:B:460:MET:HG2	1:B:473:ILE:HD12	1.87	0.56
1:B:6:ILE:HD13	1:B:86:LEU:HD13	1.88	0.56
1:B:24:ARG:NH1	1:B:407:GLU:OE1	2.36	0.56
4:A:757:HOH:O	1:B:101:PHE:HD1	1.88	0.56
1:A:516:LEU:HD13	1:A:541:VAL:CG1	2.36	0.55
1:A:400:ARG:HG3	4:A:644:HOH:O	2.05	0.55
1:A:28:ARG:HD2	1:A:66:PHE:CG	2.41	0.55
1:B:65:ARG:HH11	1:B:65:ARG:HG2	1.71	0.55
1:A:250:PHE:HA	1:A:253:ARG:HH11	1.70	0.55
1:B:68:TYR:CD2	1:B:403:MET:HG3	2.40	0.55
1:A:411:GLN:HB3	4:A:641:HOH:O	2.07	0.55
1:A:15:ALA:O	4:A:656:HOH:O	2.17	0.55
1:A:104:GLU:OE1	1:A:107:LYS:HD3	2.07	0.55
1:A:277:LYS:NZ	1:A:278:THR:N	2.56	0.54
1:B:569:LEU:HD23	1:B:570:LYS:N	2.21	0.54
1:A:246:GLY:HA2	1:A:292:ALA:O	2.08	0.54
1:A:475:GLU:O	1:A:476:GLU:C	2.50	0.54
1:B:352:VAL:HG22	1:B:370:SER:HB3	1.90	0.54
1:B:533:ASN:ND2	1:B:539:GLN:HE21	2.06	0.54
1:B:12:GLY:C	1:B:364:MET:HE2	2.33	0.54
1:A:277:LYS:NZ	1:A:278:THR:H	2.06	0.54
1:B:382:ARG:NH1	1:B:397:GLU:OE2	2.40	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:309:ASP:OD2	1:B:312:ARG:NH2	2.42	0.53
1:A:158:LYS:O	1:A:158:LYS:CD	2.45	0.53
1:A:428:SER:HA	4:A:699:HOH:O	2.08	0.53
1:B:448:GLY:O	1:B:494:ARG:NH2	2.41	0.53
1:B:504:ASN:HD22	1:B:522:THR:H	1.53	0.53
1:A:293:MET:CE	3:A:701:ARE:H6B1	2.39	0.53
1:A:324:LEU:HD13	1:A:335:TRP:CZ3	2.44	0.53
1:B:16:TYR:OH	1:B:407:GLU:CG	2.55	0.53
1:B:219:LEU:HB3	1:B:220:PRO:HD3	1.89	0.53
1:A:159:ASP:HA	1:A:161:ARG:HH22	1.73	0.53
1:A:178:ARG:HD3	1:A:474:TRP:CH2	2.44	0.53
1:A:381:ILE:HD13	1:A:425:PHE:CE1	2.43	0.53
1:A:2:LEU:HD21	1:B:2:LEU:HD23	1.91	0.53
1:A:159:ASP:CA	1:A:161:ARG:HH22	2.22	0.53
1:A:178:ARG:HE	1:A:178:ARG:CA	2.22	0.53
1:B:427:THR:O	1:B:428:SER:C	2.48	0.52
1:A:1:MET:HE2	1:A:94:VAL:HG11	1.90	0.52
1:A:281:THR:H	1:A:289:GLN:HE22	1.55	0.52
1:A:420:HIS:O	1:A:469:ARG:NH1	2.43	0.52
1:A:115:TYR:CZ	1:B:295:LYS:HE2	2.44	0.52
1:A:150:PRO:HG3	1:A:215:GLN:NE2	2.24	0.52
1:B:243:ASN:ND2	1:B:295:LYS:NZ	2.56	0.52
1:A:104:GLU:O	1:A:105:ARG:C	2.52	0.52
1:A:251:ALA:O	1:A:255:VAL:HG23	2.10	0.52
1:B:223:ARG:HB3	1:B:223:ARG:HH21	1.71	0.52
1:A:332:HIS:HD2	1:A:367:GLN:OE1	1.93	0.52
1:A:191:TYR:CE1	1:A:323:ARG:HG3	2.45	0.51
1:A:232:ARG:NH1	4:A:746:HOH:O	2.25	0.51
1:B:323:ARG:HE	1:B:372:MET:CE	2.20	0.51
1:A:410:ALA:HA	1:A:413:LEU:HD22	1.92	0.51
1:B:155:GLN:HE21	1:B:155:GLN:CA	2.22	0.51
1:A:218:ASP:OD1	1:A:220:PRO:HD2	2.10	0.51
1:A:326:VAL:CG2	3:A:701:ARE:H6H	2.40	0.51
1:B:328:ASN:OD1	1:B:357:HIS:HE1	1.94	0.51
1:B:12:GLY:O	1:B:364:MET:HE2	2.11	0.51
1:B:122:PHE:HD1	1:B:123:THR:N	2.08	0.51
1:A:330:VAL:HG22	1:A:335:TRP:CE2	2.46	0.51
1:B:357:HIS:HD2	4:B:692:HOH:O	1.93	0.51
1:A:25:VAL:C	1:A:26:ARG:HG2	2.36	0.51
1:B:16:TYR:OH	1:B:407:GLU:HG3	2.11	0.51
1:B:183:GLU:OE2	1:B:232:ARG:NH1	2.44	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:238:LEU:HG	1:B:319:ILE:HG21	1.93	0.51
1:B:336:ARG:NH1	4:B:715:HOH:O	2.43	0.51
1:B:533:ASN:HD21	1:B:539:GLN:HE21	1.59	0.51
1:B:573:LEU:HD13	1:B:579:MET:HG3	1.92	0.51
1:B:191:TYR:CD1	1:B:191:TYR:C	2.88	0.50
1:B:154:GLU:OE1	1:B:163:ARG:NH2	2.45	0.50
1:A:11:LYS:HE3	1:B:360:SER:HB2	1.92	0.50
1:A:277:LYS:O	1:A:280:ARG:O	2.30	0.50
1:A:408:GLN:H	1:A:408:GLN:NE2	2.08	0.50
1:A:497:LEU:HA	4:A:703:HOH:O	2.12	0.50
1:A:193:THR:HG23	4:A:605:HOH:O	2.09	0.50
1:A:223:ARG:CD	1:A:317:GLN:HE21	2.17	0.50
1:A:390:HIS:HD2	1:A:393:ARG:H	1.59	0.50
1:A:392:GLU:OE1	1:A:512:LYS:HG2	2.11	0.50
1:A:346:ASN:ND2	1:A:348:ASP:H	2.09	0.50
1:B:516:LEU:HD23	1:B:517:TYR:N	2.26	0.50
1:A:390:HIS:HA	1:A:515:ASN:HD21	1.77	0.50
1:A:453:TYR:O	1:A:454:TYR:C	2.55	0.50
1:B:401:ALA:HA	1:B:404:LEU:HD22	1.93	0.50
1:A:368:PHE:N	1:A:368:PHE:CD2	2.77	0.49
1:B:197:ALA:HA	1:B:213:ASP:HA	1.92	0.49
1:B:105:ARG:HG2	1:B:105:ARG:NH1	2.07	0.49
1:B:542:LEU:HD11	1:B:568:GLN:HB3	1.95	0.49
1:A:390:HIS:CD2	1:A:392:GLU:H	2.30	0.49
1:B:478:GLU:OE2	1:B:478:GLU:CA	2.59	0.49
1:A:465:ASP:OD1	1:A:466:PRO:HA	2.13	0.49
1:B:483:LEU:O	1:B:486:PHE:HB3	2.12	0.49
1:A:83:VAL:CG1	1:A:109:GLY:O	2.58	0.49
1:A:544:GLN:HE22	1:A:568:GLN:CG	2.25	0.48
1:A:444:MET:HE3	1:A:450:PRO:HG3	1.96	0.48
1:A:275:VAL:HG23	4:A:784:HOH:O	2.12	0.48
1:A:275:VAL:HA	1:A:282:ASN:HD21	1.78	0.48
1:A:422:THR:CG2	1:A:423:GLU:N	2.74	0.48
1:B:143:ASN:CG	1:B:169:GLY:O	2.56	0.48
1:B:435:LYS:HD3	4:B:652:HOH:O	2.12	0.48
1:B:255:VAL:O	1:B:275:VAL:CG2	2.61	0.48
1:A:346:ASN:HD22	1:A:346:ASN:C	2.21	0.48
1:A:444:MET:O	1:A:494:ARG:NH1	2.46	0.48
1:B:193:THR:HB	1:B:194:PRO:HD3	1.95	0.48
1:A:311:ALA:O	1:A:315:MET:HG3	2.14	0.48
1:A:504:ASN:C	1:A:504:ASN:HD22	2.22	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:523:VAL:O	1:B:524:GLN:CB	2.60	0.48
1:B:15:ALA:HA	1:B:24:ARG:O	2.13	0.47
1:B:206:THR:HG21	1:B:209:TYR:CD2	2.49	0.47
1:B:354:GLU:CG	1:B:372:MET:HE3	2.35	0.47
1:B:416:LEU:HD23	1:B:416:LEU:H	1.79	0.47
1:A:127:TRP:CG	1:A:235:LYS:HE3	2.49	0.47
1:B:336:ARG:HD3	1:B:366:ASP:OD2	2.15	0.47
1:B:504:ASN:ND2	1:B:522:THR:H	2.11	0.47
1:B:551:LYS:NZ	1:B:566:GLN:N	2.60	0.47
1:A:504:ASN:HD21	1:A:522:THR:HB	1.78	0.47
1:B:269:PHE:CB	1:B:284:GLU:HB2	2.44	0.47
1:B:440:VAL:O	1:B:444:MET:HB2	2.14	0.47
1:B:511:ASP:OD2	1:B:513:GLN:N	2.44	0.47
1:B:352:VAL:HG21	1:B:414:TRP:CE2	2.49	0.47
1:A:354:GLU:HG3	1:A:372:MET:HE2	1.96	0.47
1:B:27:LEU:HD23	1:B:28:ARG:N	2.30	0.47
1:B:256:LEU:HA	1:B:275:VAL:CG2	2.29	0.47
1:B:416:LEU:H	1:B:416:LEU:CD2	2.27	0.47
1:A:286:PHE:CD1	1:A:293:MET:HE3	2.50	0.47
1:A:522:THR:HA	1:A:526:GLN:O	2.15	0.47
1:A:249:PHE:O	1:A:250:PHE:C	2.57	0.47
1:A:268:PHE:HB2	1:A:270:ILE:HD12	1.97	0.47
1:A:389:ILE:CG2	1:A:393:ARG:HD3	2.45	0.47
1:B:41:TYR:OH	4:B:782:HOH:O	2.15	0.47
1:B:255:VAL:O	1:B:275:VAL:HG21	2.15	0.47
1:B:298:THR:HB	1:B:334:PHE:CD2	2.50	0.47
1:B:562:VAL:HG11	1:B:569:LEU:HD21	1.97	0.47
1:B:533:ASN:ND2	1:B:533:ASN:C	2.72	0.46
1:A:337:GLU:HA	1:A:340:ARG:HD2	1.98	0.46
1:B:150:PRO:HG3	1:B:167:PHE:CD2	2.50	0.46
1:A:198:SER:HB3	1:A:203:LYS:HB3	1.97	0.46
1:B:252:PHE:CE2	1:B:256:LEU:HD21	2.50	0.46
1:B:492:ARG:O	1:B:496:ARG:HG2	2.15	0.46
1:A:2:LEU:HD21	1:B:2:LEU:CD2	2.46	0.46
1:A:163:ARG:NH1	1:A:165:ASP:OD1	2.49	0.46
1:A:26:ARG:HD3	1:A:70:GLU:OE2	2.14	0.46
1:A:158:LYS:HG3	1:A:478:GLU:CG	2.25	0.46
1:A:393:ARG:NE	4:A:763:HOH:O	2.49	0.46
1:A:1:MET:HE3	1:A:6:ILE:HD11	1.97	0.46
1:A:28:ARG:NE	4:A:627:HOH:O	2.45	0.46
1:A:174:GLY:O	1:A:178:ARG:HG2	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:ARG:NE	4:A:746:HOH:O	2.23	0.46
1:A:391:ALA:H	1:A:515:ASN:HD22	1.62	0.46
1:A:533:ASN:O	1:A:576:TYR:HA	2.16	0.46
1:B:160:ALA:HB3	4:B:773:HOH:O	2.16	0.46
1:B:179:LEU:CD1	1:B:228:GLU:HB3	2.46	0.46
1:B:344:SER:HB3	4:B:597:HOH:O	2.15	0.46
1:B:378:GLU:HB3	1:B:382:ARG:NH2	2.31	0.46
1:B:558:THR:OG1	1:B:560:GLU:HB2	2.16	0.46
1:A:194:PRO:HD3	1:A:204:TYR:CZ	2.51	0.46
1:A:539:GLN:HB3	4:A:630:HOH:O	2.14	0.46
1:B:164:HIS:NE2	3:B:702:ARE:H2A	2.30	0.46
1:B:424:ARG:HG3	1:B:461:ALA:C	2.41	0.46
1:A:393:ARG:HG3	1:A:393:ARG:NH2	2.20	0.45
1:A:582:TRP:C	1:A:584:GLY:H	2.23	0.45
1:B:178:ARG:O	1:B:179:LEU:C	2.58	0.45
1:B:232:ARG:CG	1:B:232:ARG:NH1	2.65	0.45
1:A:293:MET:CE	3:A:701:ARE:C6B	2.94	0.45
1:A:565:LYS:HE3	1:A:565:LYS:HB3	1.50	0.45
1:A:401:ALA:O	1:A:404:LEU:HB2	2.15	0.45
1:A:522:THR:OG1	1:A:527:HIS:CD2	2.70	0.45
1:A:44:ARG:HA	1:A:81:LYS:HG2	1.97	0.45
1:A:140:ARG:NE	1:A:469:ARG:O	2.49	0.45
1:A:332:HIS:CE1	4:A:635:HOH:O	2.55	0.45
1:B:390:HIS:CE1	1:B:392:GLU:HB2	2.52	0.45
1:B:504:ASN:ND2	1:B:522:THR:HB	2.30	0.45
1:A:375:LEU:O	1:A:376:PHE:C	2.60	0.45
1:A:475:GLU:O	1:A:479:GLN:HG3	2.17	0.45
1:B:194:PRO:HD3	1:B:204:TYR:CZ	2.52	0.45
1:B:382:ARG:C	1:B:389:ILE:HG12	2.42	0.45
1:B:524:GLN:OE1	1:B:524:GLN:HA	2.16	0.45
1:A:121:VAL:O	1:A:123:THR:HG23	2.18	0.44
1:A:281:THR:CG2	1:A:291:PRO:HG3	2.47	0.44
1:B:427:THR:C	1:B:429:CYS:N	2.73	0.44
1:B:263:ARG:HG3	1:B:263:ARG:O	2.18	0.44
1:B:545:VAL:O	1:B:567:GLY:HA2	2.16	0.44
1:A:191:TYR:CD1	1:A:191:TYR:C	2.95	0.44
1:A:159:ASP:C	1:A:159:ASP:OD1	2.60	0.44
1:B:122:PHE:CD1	1:B:122:PHE:C	2.95	0.44
1:B:281:THR:O	1:B:281:THR:HG22	2.16	0.44
1:A:285:THR:HG21	1:A:290:VAL:H	1.83	0.44
1:B:464:THR:OG1	1:B:465:ASP:N	2.50	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:219:LEU:HB3	1:B:220:PRO:CD	2.48	0.44
1:B:352:VAL:HG21	1:B:414:TRP:CZ2	2.53	0.44
1:B:533:ASN:C	1:B:533:ASN:HD22	2.25	0.44
1:A:504:ASN:ND2	1:A:522:THR:HB	2.33	0.44
1:A:178:ARG:HD3	1:A:474:TRP:CZ2	2.53	0.44
1:B:524:GLN:HB3	1:B:525:ASP:H	1.42	0.44
1:A:253:ARG:HE	1:A:253:ARG:HB2	1.49	0.43
1:B:38:GLU:HB3	4:B:732:HOH:O	2.18	0.43
1:B:516:LEU:HD23	1:B:516:LEU:C	2.42	0.43
1:A:504:ASN:O	1:A:521:ARG:HA	2.18	0.43
1:B:133:ILE:HG22	1:B:134:TYR:N	2.32	0.43
1:B:219:LEU:O	1:B:220:PRO:C	2.59	0.43
1:B:412:GLY:HA3	4:B:700:HOH:O	2.17	0.43
1:B:438:LEU:HA	1:B:438:LEU:HD23	1.71	0.43
1:B:547:GLU:OE1	1:B:551:LYS:HD2	2.18	0.43
1:A:479:GLN:OE1	1:A:481:ARG:NH2	2.40	0.43
1:B:505:VAL:HG12	1:B:506:ARG:N	2.33	0.43
1:A:47:SER:C	1:A:49:GLU:H	2.26	0.43
1:A:422:THR:O	1:A:468:CYS:CB	2.66	0.43
1:B:288:VAL:HG12	1:B:289:GLN:HG2	2.01	0.43
1:B:481:ARG:HG3	1:B:481:ARG:NH1	2.26	0.43
1:A:360:SER:O	1:A:364:MET:HE2	2.19	0.43
1:A:512:LYS:HB2	1:A:512:LYS:HE2	1.25	0.43
1:A:286:PHE:HD1	1:A:293:MET:HE3	1.84	0.43
1:A:390:HIS:CD2	1:A:390:HIS:C	2.96	0.43
1:B:241:VAL:HG23	4:B:615:HOH:O	2.18	0.43
1:A:268:PHE:HB2	1:A:270:ILE:CD1	2.48	0.43
1:A:358:ASP:OD2	1:A:360:SER:HB3	2.19	0.43
1:A:389:ILE:HG21	1:A:393:ARG:HD3	1.99	0.43
1:A:389:ILE:HB	1:A:393:ARG:HB3	2.00	0.43
1:A:574:ARG:O	1:A:575:PRO:C	2.61	0.43
1:B:158:LYS:HB2	4:B:766:HOH:O	2.19	0.43
1:B:331:ASP:OD1	1:B:331:ASP:N	2.52	0.43
1:B:541:VAL:HG22	1:B:542:LEU:H	1.84	0.43
1:B:250:PHE:CG	1:B:251:ALA:N	2.87	0.43
1:B:57:ALA:HA	1:B:70:GLU:O	2.19	0.42
1:B:473:ILE:CG2	1:B:478:GLU:HB3	2.49	0.42
1:A:193:THR:HG23	1:A:194:PRO:HD2	2.01	0.42
1:B:223:ARG:CZ	1:B:223:ARG:CB	2.97	0.42
1:B:504:ASN:O	1:B:521:ARG:HA	2.19	0.42
1:A:391:ALA:N	1:A:515:ASN:ND2	2.67	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:ARG:HD2	4:B:693:HOH:O	2.19	0.42
1:A:277:LYS:O	1:A:281:THR:CA	2.68	0.42
1:A:499:SER:HA	1:A:523:VAL:HG12	2.00	0.42
1:B:551:LYS:HZ3	1:B:566:GLN:N	2.17	0.42
1:B:574:ARG:O	1:B:575:PRO:C	2.62	0.42
1:B:467:ASP:O	1:B:470:ARG:HG2	2.20	0.42
1:A:52:LEU:HD23	1:A:52:LEU:HA	1.71	0.42
1:A:92:GLU:H	1:A:92:GLU:CD	2.21	0.42
1:B:402:ARG:NH1	1:B:403:MET:HE1	2.35	0.42
1:A:346:ASN:ND2	1:A:346:ASN:C	2.78	0.42
1:B:290:VAL:CG1	1:B:293:MET:HB2	2.47	0.42
1:B:360:SER:O	1:B:361:GLY:C	2.62	0.42
1:B:551:LYS:HZ3	1:B:566:GLN:H	1.62	0.42
1:B:3:LEU:HD22	1:B:101:PHE:CD2	2.55	0.42
1:A:373:ASN:ND2	1:A:413:LEU:HD23	2.35	0.42
1:B:264:TYR:O	1:B:265:LYS:C	2.61	0.42
1:A:277:LYS:O	1:A:281:THR:N	2.53	0.41
1:B:376:PHE:CD1	1:B:376:PHE:C	2.98	0.41
1:B:544:GLN:HE22	1:B:568:GLN:HG2	1.84	0.41
1:B:6:ILE:HA	1:B:28:ARG:O	2.20	0.41
1:A:244:HIS:CD2	1:A:286:PHE:HB2	2.54	0.41
1:A:422:THR:O	1:A:468:CYS:HB3	2.19	0.41
1:A:138:PRO:CD	1:A:193:THR:HG22	2.51	0.41
1:A:196:PHE:CE2	1:A:314:TRP:CE2	3.08	0.41
1:A:375:LEU:HD23	4:A:663:HOH:O	2.20	0.41
1:B:234:ILE:HG22	1:B:235:LYS:N	2.34	0.41
1:B:426:LEU:HD23	1:B:461:ALA:HB2	2.01	0.41
1:A:139:GLU:OE2	1:A:140:ARG:NH1	2.48	0.41
1:B:16:TYR:C	1:B:23:LEU:HD12	2.46	0.41
1:B:75:CYS:O	1:B:76:SER:C	2.62	0.41
1:B:95:TYR:HB2	1:B:102:SER:O	2.21	0.41
1:A:118:ARG:H	1:A:118:ARG:HG3	1.34	0.41
1:A:536:GLY:O	1:A:575:PRO:HB3	2.20	0.41
1:B:285:THR:O	1:B:286:PHE:C	2.63	0.41
1:A:164:HIS:CE1	3:A:701:ARE:O2A	2.74	0.41
1:A:224:ARG:NH2	1:A:224:ARG:HA	2.36	0.41
1:B:104:GLU:OE1	1:B:107:LYS:HE2	2.20	0.41
1:B:541:VAL:HG22	1:B:542:LEU:N	2.36	0.41
1:A:391:ALA:H	1:A:515:ASN:ND2	2.19	0.41
1:B:542:LEU:HD11	1:B:568:GLN:CD	2.46	0.41
1:B:8:HIS:CG	1:B:9:GLU:N	2.89	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:192:PHE:O	1:B:239:ASP:HB2	2.21	0.40
1:A:16:TYR:HA	1:A:17:PRO:HD3	1.82	0.40
1:A:497:LEU:HA	1:A:497:LEU:HD23	1.87	0.40
1:B:328:ASN:N	1:B:328:ASN:ND2	2.51	0.40
1:A:57:ALA:HB2	1:A:71:ALA:HB2	2.03	0.40
1:A:206:THR:HG21	1:A:209:TYR:CD2	2.57	0.40
1:A:516:LEU:C	1:A:516:LEU:HD23	2.46	0.40
1:B:42:ALA:HB2	1:B:52:LEU:HD23	2.04	0.40
1:B:160:ALA:N	4:B:773:HOH:O	2.50	0.40
1:B:416:LEU:HD23	1:B:416:LEU:N	2.37	0.40
1:B:426:LEU:O	1:B:429:CYS:HB2	2.21	0.40
1:B:555:ASP:OD2	1:B:555:ASP:C	2.64	0.40
1:A:1:MET:HE2	1:A:94:VAL:CG1	2.51	0.40
1:A:163:ARG:NH1	1:A:163:ARG:HB2	2.37	0.40
1:B:375:LEU:HD12	4:B:604:HOH:O	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:ASP:OD1	4:B:765:HOH:O[2_565]	2.19	0.01

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	583/585 (100%)	520 (89%)	56 (10%)	7 (1%)	10	34
1	B	583/585 (100%)	523 (90%)	52 (9%)	8 (1%)	9	30
All	All	1166/1170 (100%)	1043 (90%)	108 (9%)	15 (1%)	9	31

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	158	LYS
1	A	159	ASP
1	A	276	SER
1	A	278	THR
1	B	275	VAL
1	B	277	LYS
1	B	278	THR
1	B	279	SER
1	B	281	THR
1	A	105	ARG
1	B	139	GLU
1	A	106	SER
1	B	110	VAL
1	B	193	THR
1	A	193	THR

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	493/493 (100%)	433 (88%)	60 (12%)	5	16
1	B	493/493 (100%)	436 (88%)	57 (12%)	5	18
All	All	986/986 (100%)	869 (88%)	117 (12%)	5	17

All (117) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LEU
1	A	26	ARG
1	A	47	SER
1	A	49	GLU
1	A	56	LEU
1	A	62	SER
1	A	73	LEU
1	A	76	SER
1	A	85	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	92	GLU
1	A	94	VAL
1	A	107	LYS
1	A	118	ARG
1	A	136	ILE
1	A	140	ARG
1	A	151	PRO
1	A	158	LYS
1	A	182	LEU
1	A	193	THR
1	A	215	GLN
1	A	223	ARG
1	A	224	ARG
1	A	253	ARG
1	A	265	LYS
1	A	270	ILE
1	A	271	GLU
1	A	275	VAL
1	A	277	LYS
1	A	278	THR
1	A	280	ARG
1	A	323	ARG
1	A	330	VAL
1	A	341	LEU
1	A	346	ASN
1	A	372	MET
1	A	393	ARG
1	A	398	LEU
1	A	408	GLN
1	A	413	LEU
1	A	422	THR
1	A	426	LEU
1	A	444	MET
1	A	458	ILE
1	A	469	ARG
1	A	473	ILE
1	A	476	GLU
1	A	477	LYS
1	A	483	LEU
1	A	504	ASN
1	A	505	VAL
1	A	515	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	535	ARG
1	A	539	GLN
1	A	542	LEU
1	A	544	GLN
1	A	551	LYS
1	A	565	LYS
1	A	570	LYS
1	A	571	LEU
1	A	581	LEU
1	B	4	GLU
1	B	20	GLU
1	B	24	ARG
1	B	25	VAL
1	B	40	LEU
1	B	49	GLU
1	B	65	ARG
1	B	70	GLU
1	B	73	LEU
1	B	76	SER
1	B	85	LEU
1	B	94	VAL
1	B	105	ARG
1	B	110	VAL
1	B	139	GLU
1	B	187	VAL
1	B	190	LEU
1	B	220	PRO
1	B	223	ARG
1	B	232	ARG
1	B	248	GLN
1	B	256	LEU
1	B	263	ARG
1	B	277	LYS
1	B	280	ARG
1	B	281	THR
1	B	284	GLU
1	B	305	GLU
1	B	326	VAL
1	B	328	ASN
1	B	364	MET
1	B	375	LEU
1	B	382	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	398	LEU
1	B	404	LEU
1	B	407	GLU
1	B	416	LEU
1	B	438	LEU
1	B	444	MET
1	B	451	LEU
1	B	470	ARG
1	B	475	GLU
1	B	477	LYS
1	B	481	ARG
1	B	504	ASN
1	B	505	VAL
1	B	512	LYS
1	B	524	GLN
1	B	531	VAL
1	B	533	ASN
1	B	542	LEU
1	B	551	LYS
1	B	560	GLU
1	B	565	LYS
1	B	569	LEU
1	B	570	LYS
1	B	573	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	135	GLN
1	A	244	HIS
1	A	289	GLN
1	A	317	GLN
1	A	332	HIS
1	A	346	ASN
1	A	367	GLN
1	A	390	HIS
1	A	408	GLN
1	A	443	GLN
1	A	504	ASN
1	A	509	HIS
1	A	515	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	527	HIS
1	A	539	GLN
1	A	544	GLN
1	A	566	GLN
1	B	22	GLN
1	B	135	GLN
1	B	155	GLN
1	B	202	HIS
1	B	243	ASN
1	B	244	HIS
1	B	257	GLN
1	B	289	GLN
1	B	328	ASN
1	B	332	HIS
1	B	357	HIS
1	B	373	ASN
1	B	443	GLN
1	B	495	HIS
1	B	504	ASN
1	B	533	ASN
1	B	539	GLN
1	B	544	GLN
1	B	566	GLN

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 4 ligands modelled in this entry, 2 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	ARE	B	702	-	58,59,59	2.54	12 (20%)	76,88,88	2.25	24 (31%)
3	ARE	A	701	-	58,59,59	2.92	18 (31%)	76,88,88	1.74	16 (21%)

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	ARE	B	702	-	-	6/24/124/124	0/5/5/5
3	ARE	A	701	-	-	9/24/124/124	0/5/5/5

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	702	ARE	C6H-C5H	16.01	1.55	1.32
3	A	701	ARE	C6H-C5H	15.06	1.54	1.32
3	A	701	ARE	C4H-C5H	7.47	1.58	1.51
3	A	701	ARE	O5A-C5A	6.11	1.59	1.44
3	A	701	ARE	O4G-C1C	4.28	1.53	1.41
3	A	701	ARE	O4H-C1B	3.86	1.52	1.41
3	B	702	ARE	C1H-C6H	3.72	1.55	1.50
3	A	701	ARE	C1H-C6H	3.61	1.55	1.50
3	B	702	ARE	O5B-C5B	3.60	1.53	1.44
3	A	701	ARE	C4A-C5A	3.33	1.60	1.53
3	A	701	ARE	C3C-C4C	3.07	1.58	1.53
3	A	701	ARE	O5A-C1A	2.99	1.49	1.41
3	A	701	ARE	O5B-C1B	2.93	1.49	1.41
3	B	702	ARE	O5A-C5A	2.80	1.51	1.44
3	A	701	ARE	C3A-C2A	2.77	1.59	1.52
3	A	701	ARE	O3C-C3C	2.73	1.49	1.43
3	A	701	ARE	C6A-C5A	2.73	1.61	1.51
3	B	702	ARE	O2G-C2G	2.62	1.49	1.43
3	B	702	ARE	O1G-C1G	2.56	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	702	ARE	O3C-C3C	2.51	1.49	1.43
3	B	702	ARE	C3G-C2G	2.29	1.58	1.52
3	A	701	ARE	O4B-C1A	2.24	1.48	1.41
3	B	702	ARE	C3C-C4C	2.21	1.57	1.53
3	A	701	ARE	O4G-C4G	2.20	1.49	1.43
3	B	702	ARE	C3H-C4H	2.17	1.56	1.53
3	A	701	ARE	C3G-C4G	2.12	1.58	1.52
3	A	701	ARE	O1G-C1G	2.10	1.46	1.39
3	B	702	ARE	O5A-C1A	2.10	1.47	1.41
3	B	702	ARE	C6A-C5A	2.08	1.58	1.51
3	A	701	ARE	O2G-C2G	2.04	1.48	1.43

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	701	ARE	O4G-C1C-C2C	6.70	124.58	108.09
3	B	702	ARE	C1G-O5G-C5G	6.35	125.93	113.65
3	B	702	ARE	C2G-C3G-C4G	4.93	120.87	109.68
3	B	702	ARE	C6G-C5G-C4G	-4.90	99.60	113.38
3	B	702	ARE	C1C-O5C-C5C	4.60	121.48	113.63
3	B	702	ARE	C3G-C4G-C5G	-4.46	101.05	110.93
3	B	702	ARE	C1B-O5B-C5B	-4.19	105.54	113.72
3	B	702	ARE	O1G-C1G-O5G	-4.12	98.19	110.41
3	B	702	ARE	O1G-C1G-C2G	4.10	120.87	108.98
3	B	702	ARE	C1A-O4B-C4B	-3.98	108.54	117.98
3	B	702	ARE	O5B-C5B-C6B	3.90	116.11	106.44
3	A	701	ARE	O5C-C1C-C2C	-3.86	102.44	110.37
3	A	701	ARE	O5G-C1G-C2G	3.85	117.07	110.30
3	A	701	ARE	C2G-C3G-C4G	3.78	118.25	109.68
3	B	702	ARE	C6C-C5C-C4C	3.60	120.16	113.57
3	A	701	ARE	O5A-C5A-C6A	3.53	115.18	106.44
3	B	702	ARE	O5C-C1C-C2C	3.38	117.31	110.37
3	B	702	ARE	C6H-C1H-N4C	3.33	115.59	110.68
3	B	702	ARE	O5A-C5A-C4A	3.30	115.65	109.70
3	B	702	ARE	O4B-C1A-C2A	3.18	115.92	108.09
3	A	701	ARE	C6C-C5C-C4C	3.12	119.28	113.57
3	B	702	ARE	O5G-C5G-C4G	-3.09	103.34	109.72
3	B	702	ARE	O3C-C3C-C4C	3.07	115.70	109.58
3	A	701	ARE	C1G-O5G-C5G	2.93	119.33	113.65
3	A	701	ARE	O4H-C1B-O5B	2.79	118.02	110.69
3	B	702	ARE	O5G-C5G-C6G	2.69	113.10	106.44
3	A	701	ARE	O5C-C5C-C6C	2.67	112.67	106.74

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	701	ARE	O3C-C3C-C4C	2.66	114.87	109.58
3	B	702	ARE	C1B-C2B-C3B	2.66	115.60	110.01
3	B	702	ARE	O4H-C1B-C2B	2.58	114.44	108.09
3	A	701	ARE	C1A-O4B-C4B	2.51	123.93	117.98
3	B	702	ARE	C1A-O5A-C5A	2.43	118.47	113.72
3	A	701	ARE	O1G-C1G-O5G	-2.42	103.23	110.41
3	A	701	ARE	O3A-C3A-C2A	2.38	115.98	110.38
3	A	701	ARE	C2B-C3B-C4B	2.22	114.71	109.68
3	B	702	ARE	C2B-C3B-C4B	2.20	114.67	109.68
3	B	702	ARE	O2H-C2H-C1H	2.18	113.37	109.08
3	A	701	ARE	O2A-C2A-C1A	-2.16	104.93	110.08
3	B	702	ARE	O4A-C4A-C3A	-2.14	105.33	110.38
3	A	701	ARE	O2H-C2H-C1H	-2.12	104.91	109.08

There are no chirality outliers.

All (15) torsion outliers are listed below:

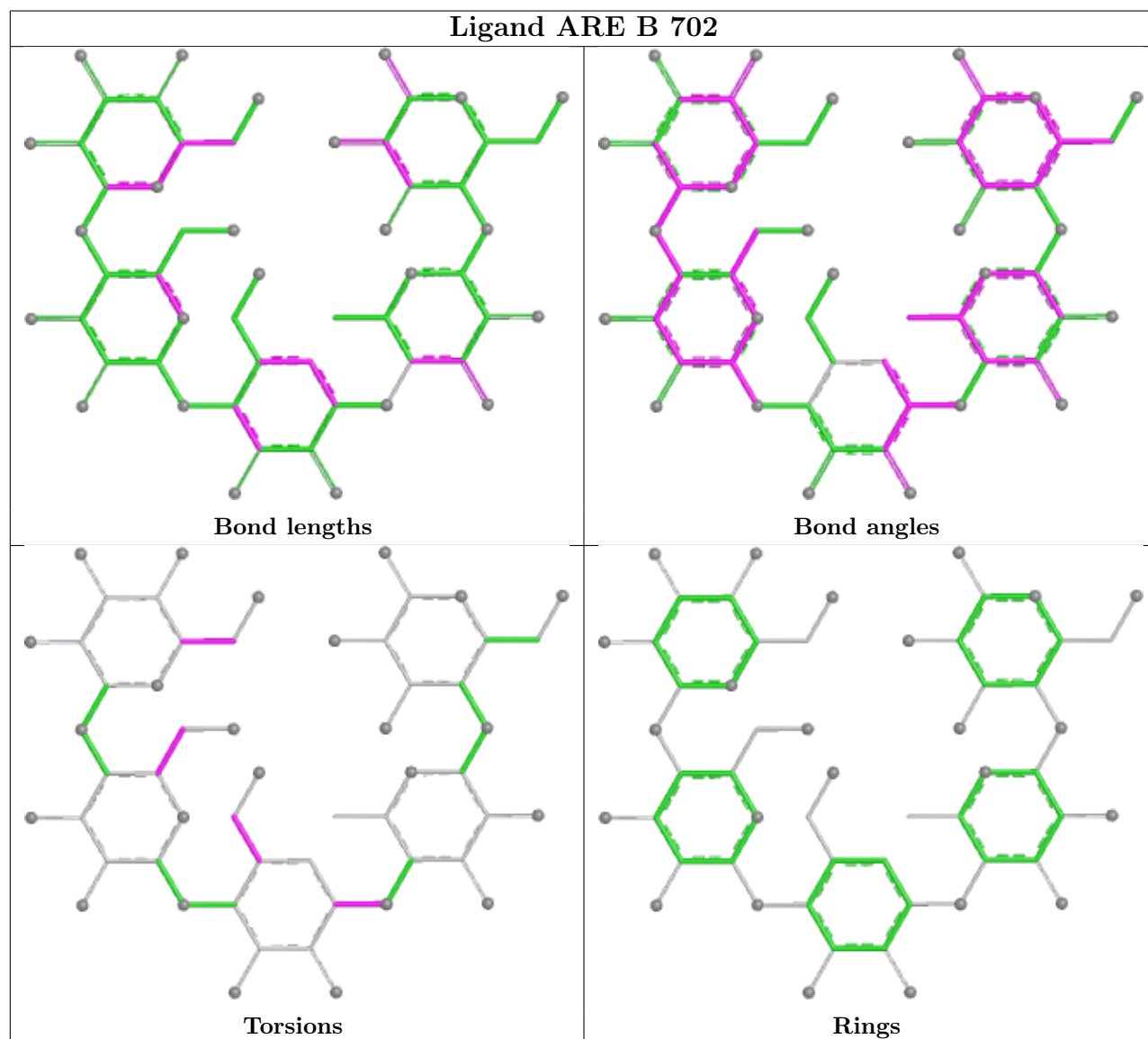
Mol	Chain	Res	Type	Atoms
3	A	701	ARE	C6H-C1H-N4C-C4C
3	A	701	ARE	C6H-C5H-C7H-O7H
3	B	702	ARE	C6H-C1H-N4C-C4C
3	B	702	ARE	C6H-C5H-C7H-O7H
3	A	701	ARE	C4A-C5A-C6A-O6A
3	A	701	ARE	O5B-C5B-C6B-O6B
3	A	701	ARE	O5G-C5G-C6G-O6G
3	A	701	ARE	O5A-C5A-C6A-O6A
3	A	701	ARE	C4G-C5G-C6G-O6G
3	B	702	ARE	O5A-C5A-C6A-O6A
3	A	701	ARE	C4B-C5B-C6B-O6B
3	B	702	ARE	O5B-C5B-C6B-O6B
3	B	702	ARE	C4B-C5B-C6B-O6B
3	B	702	ARE	C4A-C5A-C6A-O6A
3	A	701	ARE	C5H-C4H-O4H-C1B

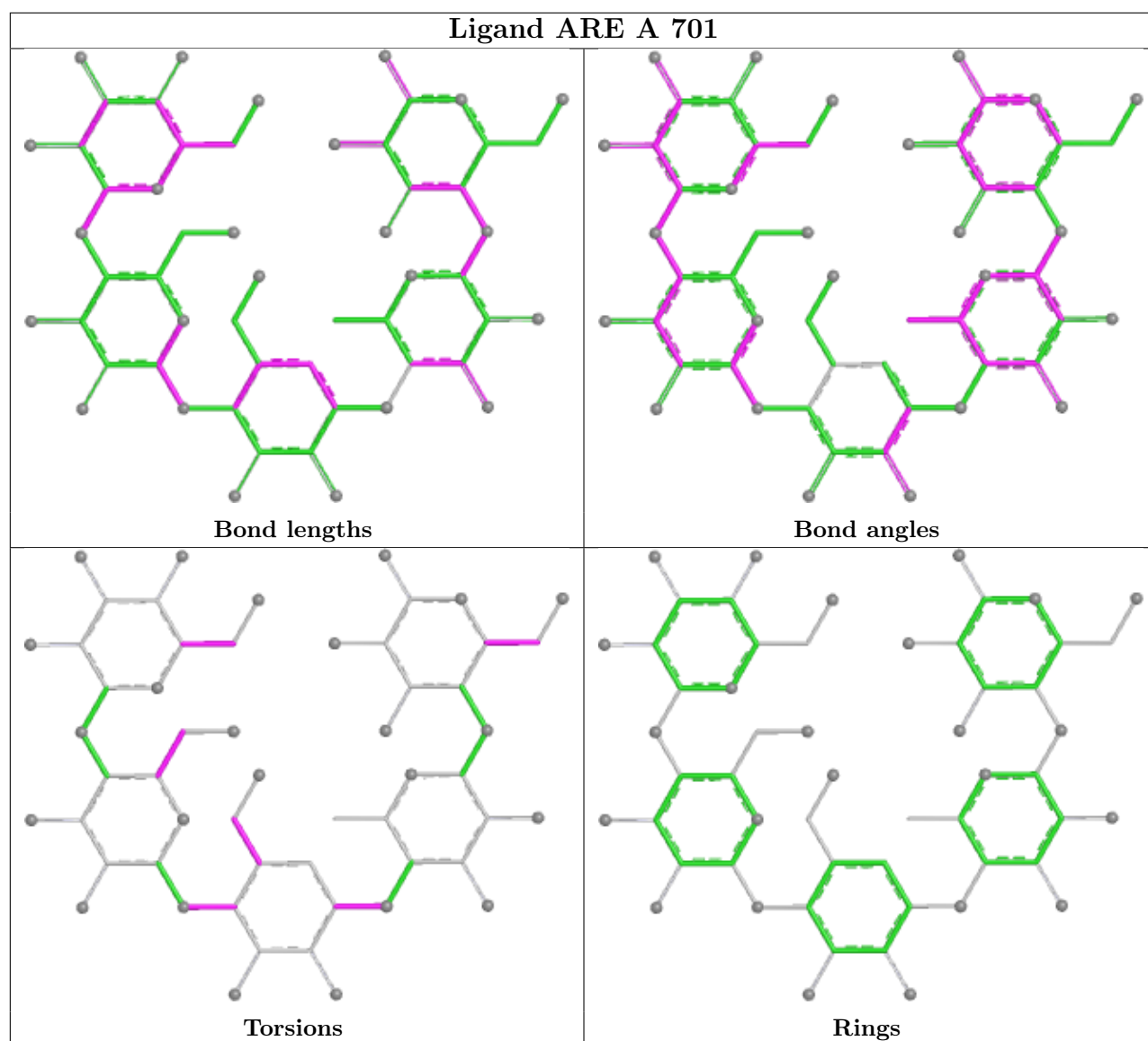
There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	702	ARE	2	0
3	A	701	ARE	6	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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, 95th 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 ²)	Q<0.9
1	A	585/585 (100%)	-0.85	1 (0%) 91 88	8, 23, 47, 77	0
1	B	585/585 (100%)	-0.84	1 (0%) 91 88	9, 23, 48, 90	0
All	All	1170/1170 (100%)	-0.85	2 (0%) 91 88	8, 23, 48, 90	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	278	THR	3.2
1	B	277	LYS	2.4

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 oligosaccharides 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. The B-factors column lists the minimum, median, 95th 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	B-factors(Å ²)	Q<0.9
3	ARE	A	701	55/55	0.95	0.09	17,35,76,78	0
3	ARE	B	702	55/55	0.95	0.07	24,38,67,71	0
2	CA	A	586	1/1	1.00	0.01	19,19,19,19	0

Continued on next page...

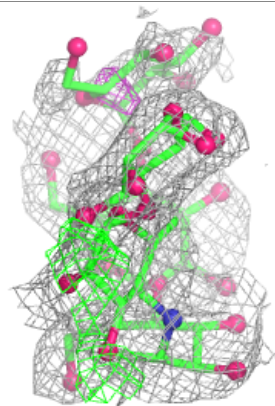
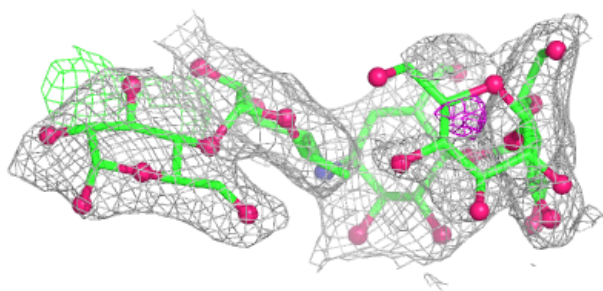
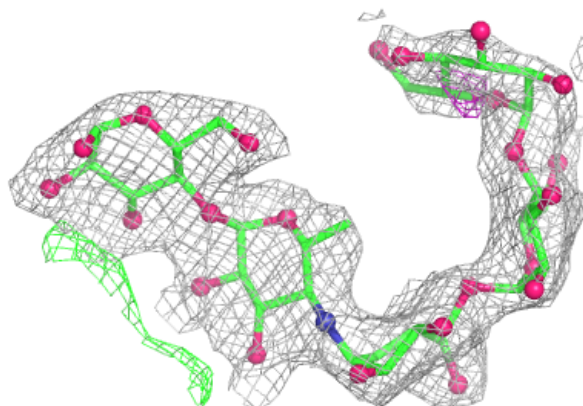
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CA	B	586	1/1	1.00	0.02	28,28,28,28	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

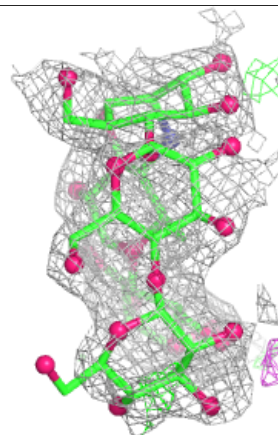
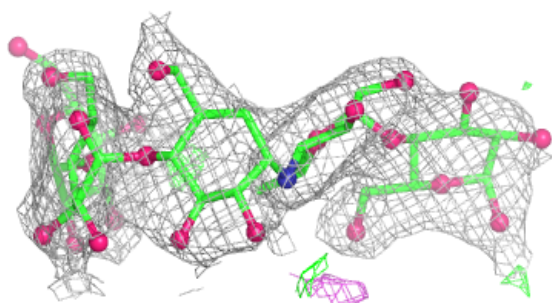
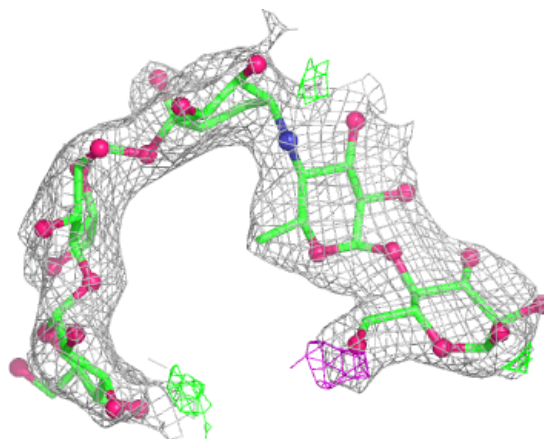
Electron density around ARE A 701:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ARE B 702:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.