



# Full wwPDB X-ray Structure Validation Report ⓘ

May 27, 2020 – 10:48 pm BST

PDB ID : 3A6O  
Title : Crystal structure of Thermoactinomyces vulgaris R-47 alpha-amylase 2/acar-bose complex  
Authors : Ohtaki, A.; Mizuno, M.; Tonozuka, 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

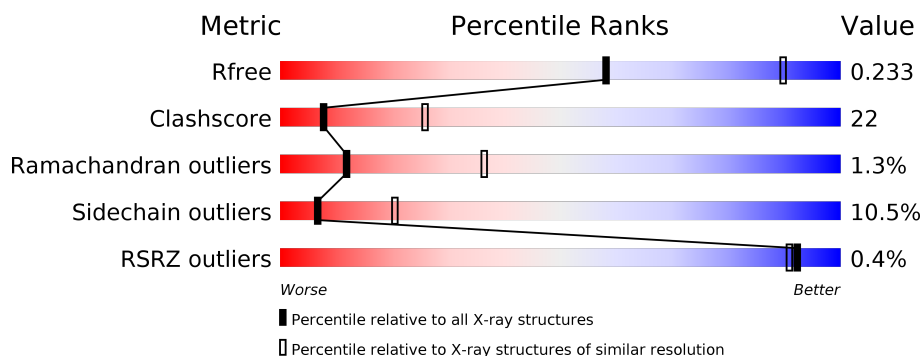
# 1 Overall quality at a glance

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))
$R_{free}$	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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	
1	B	585	

## 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.

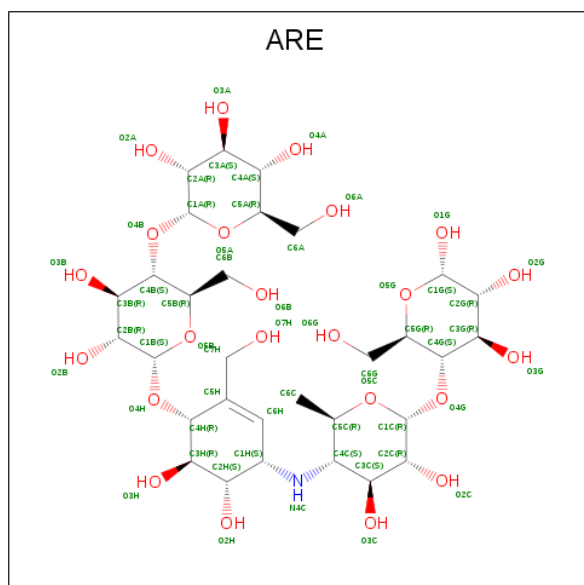
- Molecule 1 is a protein called Neopullulanase 2.

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 (three-letter code: CA) (formula: Ca).

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

- Molecule 3 is ACARBOSE DERIVED PENTASACCHARIDE (three-letter code: ARE) (formula:  $C_{31}H_{53}NO_{23}$ ).



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		

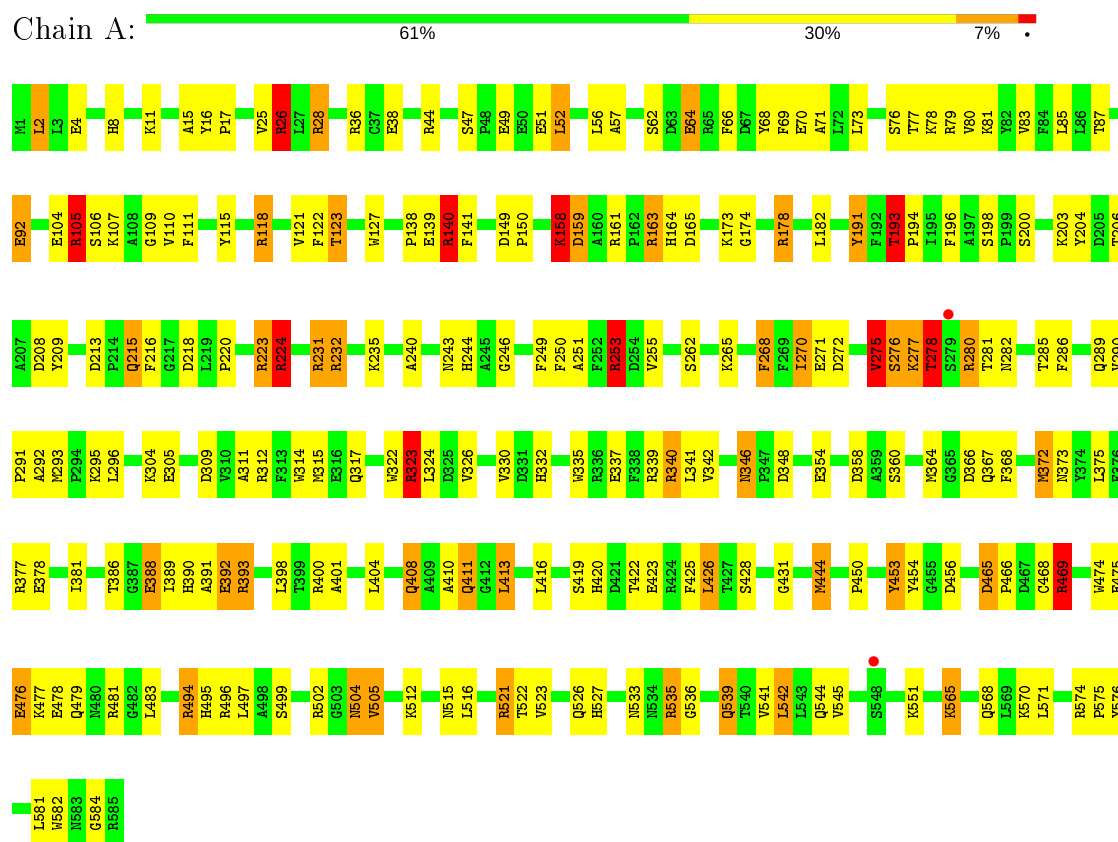
- Molecule 4 is water.

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

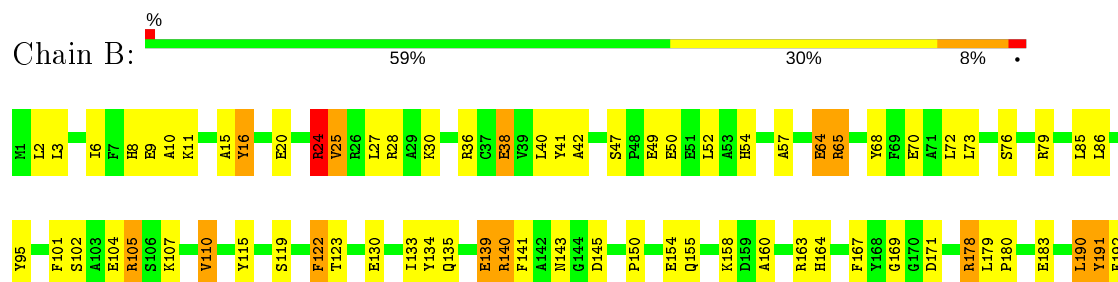
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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, $\alpha$ , $\beta$ , $\gamma$	114.60Å 119.26Å 113.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.81 – 2.80 38.80 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (38.81-2.80) 99.3 (38.80-2.80)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.19 (at 2.81Å)	Xtriage
Refinement program	CNS, REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.157 , 0.231 0.157 , 0.233	Depositor DCC
$R_{free}$ test set	3455 reflections (8.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.0	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 41.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.021 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10068	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	1.42	19/4905 (0.4%)	1.31	41/6641 (0.6%)
1	B	1.43	23/4905 (0.5%)	1.26	35/6641 (0.5%)
All	All	1.43	42/9810 (0.4%)	1.29	76/13282 (0.6%)

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	340	ARG	CG-CD	10.49	1.78	1.51
1	B	305	GLU	CG-CD	9.43	1.66	1.51
1	A	4	GLU	CB-CG	-9.21	1.34	1.52
1	B	38	GLU	CD-OE2	7.75	1.34	1.25
1	A	305	GLU	CD-OE1	7.75	1.34	1.25
1	A	305	GLU	CG-CD	7.71	1.63	1.51
1	B	64	GLU	CG-CD	7.32	1.62	1.51
1	B	335	TRP	CZ3-CH2	6.88	1.51	1.40
1	B	388	GLU	CD-OE2	6.77	1.33	1.25
1	B	407	GLU	CB-CG	-6.54	1.39	1.52
1	A	388	GLU	CD-OE1	6.52	1.32	1.25
1	A	392	GLU	CD-OE1	6.36	1.32	1.25
1	B	38	GLU	CG-CD	6.28	1.61	1.51
1	A	141	PHE	CE2-CZ	6.28	1.49	1.37
1	A	68	TYR	CD1-CE1	-6.17	1.30	1.39
1	B	368	PHE	CE2-CZ	6.11	1.49	1.37
1	B	313	PHE	CE2-CZ	5.92	1.48	1.37
1	B	376	PHE	CE1-CZ	5.80	1.48	1.37
1	A	80	VAL	CB-CG1	-5.78	1.40	1.52
1	A	378	GLU	CD-OE1	5.74	1.31	1.25
1	B	119	SER	CB-OG	5.70	1.49	1.42
1	B	130	GLU	CB-CG	-5.67	1.41	1.52
1	B	340	ARG	CG-CD	5.63	1.66	1.51
1	A	411	GLN	CG-CD	5.62	1.64	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	484	PHE	CE2-CZ	5.62	1.48	1.37
1	A	340	ARG	CB-CG	5.54	1.67	1.52
1	B	16	TYR	CG-CD2	5.48	1.46	1.39
1	A	505	VAL	CB-CG2	-5.37	1.41	1.52
1	B	305	GLU	CB-CG	5.36	1.62	1.52
1	A	111	PHE	CE1-CZ	5.31	1.47	1.37
1	B	25	VAL	CB-CG1	-5.26	1.41	1.52
1	B	38	GLU	CD-OE1	5.23	1.31	1.25
1	B	359	ALA	CA-CB	5.21	1.63	1.52
1	B	486	PHE	CE2-CZ	5.19	1.47	1.37
1	B	531	VAL	CB-CG2	-5.19	1.42	1.52
1	A	392	GLU	CG-CD	5.18	1.59	1.51
1	A	268	PHE	CD1-CE1	5.17	1.49	1.39
1	A	216	PHE	CD1-CE1	5.16	1.49	1.39
1	A	278	THR	N-CA	5.10	1.56	1.46
1	B	453	TYR	CG-CD2	5.10	1.45	1.39
1	B	141	PHE	CE1-CZ	5.03	1.47	1.37
1	A	68	TYR	CG-CD2	5.02	1.45	1.39

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	140	ARG	NE-CZ-NH1	-12.93	113.83	120.30
1	A	232	ARG	NE-CZ-NH2	11.54	126.07	120.30
1	A	232	ARG	NE-CZ-NH1	-11.05	114.77	120.30
1	B	336	ARG	NE-CZ-NH1	-10.11	115.24	120.30
1	B	24	ARG	NE-CZ-NH1	9.94	125.27	120.30
1	B	382	ARG	NE-CZ-NH2	9.83	125.22	120.30
1	A	323	ARG	NE-CZ-NH2	9.62	125.11	120.30
1	A	469	ARG	NE-CZ-NH1	9.31	124.95	120.30
1	A	208	ASP	CB-CG-OD1	9.30	126.67	118.30
1	A	26	ARG	NE-CZ-NH2	-9.12	115.74	120.30
1	A	79	ARG	NE-CZ-NH1	8.35	124.47	120.30
1	A	224	ARG	NE-CZ-NH2	8.33	124.47	120.30
1	A	323	ARG	CG-CD-NE	8.26	129.15	111.80
1	B	481	ARG	NE-CZ-NH2	-8.19	116.20	120.30
1	B	535	ARG	NE-CZ-NH2	-8.01	116.30	120.30
1	A	465	ASP	CB-CG-OD1	-7.98	111.12	118.30
1	A	253	ARG	NE-CZ-NH2	-7.74	116.43	120.30
1	A	253	ARG	NE-CZ-NH1	7.44	124.02	120.30
1	B	239	ASP	CB-CG-OD1	7.38	124.94	118.30
1	B	79	ARG	NE-CZ-NH2	-7.29	116.65	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	364	MET	CG-SD-CE	7.26	111.81	100.20
1	A	270	ILE	CG1-CB-CG2	-7.16	95.65	111.40
1	A	340	ARG	NE-CZ-NH2	7.10	123.85	120.30
1	B	323	ARG	NE-CZ-NH1	-7.06	116.77	120.30
1	B	505	VAL	CB-CA-C	-6.95	98.20	111.40
1	B	437	ARG	NE-CZ-NH1	-6.94	116.83	120.30
1	A	535	ARG	NE-CZ-NH2	6.91	123.75	120.30
1	B	400	ARG	NE-CZ-NH1	-6.86	116.87	120.30
1	B	140	ARG	NE-CZ-NH1	-6.70	116.95	120.30
1	A	52	LEU	CA-CB-CG	-6.66	99.98	115.30
1	A	465	ASP	CB-CG-OD2	6.61	124.25	118.30
1	B	506	ARG	NE-CZ-NH1	-6.56	117.02	120.30
1	A	28	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	A	79	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	B	208	ASP	CB-CG-OD2	6.41	124.06	118.30
1	B	573	LEU	CA-CB-CG	6.39	129.99	115.30
1	A	105	ARG	NE-CZ-NH1	-6.33	117.13	120.30
1	B	232	ARG	NE-CZ-NH1	6.27	123.44	120.30
1	A	123	THR	OG1-CB-CG2	-6.26	95.59	110.00
1	A	231	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	B	145	ASP	CB-CG-OD1	6.01	123.71	118.30
1	B	331	ASP	CB-CG-OD2	5.99	123.69	118.30
1	B	72	LEU	CB-CG-CD1	-5.96	100.86	111.00
1	A	275	VAL	CB-CA-C	-5.90	100.19	111.40
1	B	178	ARG	NE-CZ-NH1	-5.87	117.36	120.30
1	A	140	ARG	NH1-CZ-NH2	5.85	125.84	119.40
1	A	494	ARG	NE-CZ-NH1	-5.83	117.38	120.30
1	B	263	ARG	NE-CZ-NH2	5.81	123.20	120.30
1	A	26	ARG	NE-CZ-NH1	5.77	123.19	120.30
1	B	339	ARG	NE-CZ-NH2	5.75	123.18	120.30
1	B	506	ARG	NE-CZ-NH2	5.75	123.18	120.30
1	B	79	ARG	NE-CZ-NH1	5.65	123.12	120.30
1	A	163	ARG	NE-CZ-NH1	5.57	123.09	120.30
1	A	366	ASP	CB-CG-OD2	-5.57	113.28	118.30
1	A	173	LYS	CD-CE-NZ	-5.53	98.97	111.70
1	A	296	LEU	CB-CG-CD2	-5.43	101.76	111.00
1	B	36	ARG	NE-CZ-NH1	-5.42	117.59	120.30
1	B	223	ARG	NE-CZ-NH2	5.42	123.01	120.30
1	A	521	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	B	470	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	B	521	ARG	NE-CZ-NH2	5.37	122.98	120.30
1	B	481	ARG	NE-CZ-NH1	5.35	122.97	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	521	ARG	NE-CZ-NH1	-5.35	117.62	120.30
1	B	395	ASP	CB-CG-OD1	5.35	123.11	118.30
1	A	456	ASP	CB-CG-OD2	5.35	123.11	118.30
1	A	453	TYR	CD1-CE1-CZ	-5.30	115.03	119.80
1	B	145	ASP	CB-CG-OD2	-5.30	113.53	118.30
1	A	505	VAL	CB-CA-C	-5.26	101.41	111.40
1	A	496	ARG	N-CA-C	5.23	125.11	111.00
1	B	190	LEU	CA-CB-CG	5.16	127.17	115.30
1	A	340	ARG	N-CA-CB	5.14	119.86	110.60
1	A	502	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	A	377	ARG	NE-CZ-NH2	5.05	122.82	120.30
1	B	219	LEU	CB-CG-CD2	5.04	119.57	111.00
1	A	469	ARG	NE-CZ-NH2	-5.03	117.78	120.30
1	B	511	ASP	CB-CG-OD2	-5.00	113.80	118.30

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	212	1
1	B	4775	0	4607	207	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	55	0	53	7	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	414	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 22.

All (414) 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:HD3	1:A:158:LYS:O	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: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	1.54	0.89
1:A:544:GLN:HA	1:A:544:GLN:NE2	1.87	0.88
1:A:309:ASP:OD2	1:A:312:ARG:NH1	2.08	0.87
1:A:393:ARG:HG3	1:A:393:ARG:HH21	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:CG	1:B:232:ARG:HH11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:481:ARG:HH11	1:B:481:ARG:HG3	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:N	1:B:328:ASN:HD22	1.76	0.76
1:A:105:ARG:HH21	1:A:105:ARG:HG2	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:NH2	1:A:105:ARG:HG2	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
1:B:280:ARG:HA	1:B:280:ARG:HE	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:B:382:ARG:HH11	1:B:397:GLU:CD	1.93	0.71
1:B:328:ASN:H	1:B:328:ASN:ND2	1.83	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:A:290:VAL:HG11	1:A:293:MET:HE2	1.74	0.69
1:B:256:LEU:CD2	1:B:275:VAL:HG11	2.23	0.69
1:A:51:GLU:OE2	1:A:51:GLU:HA	1.91	0.68
1:A:408:GLN:HE21	1:A:408:GLN:H	1.39	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:478:GLU:HA	1:B:478:GLU:OE2	1.94	0.67
1:A:416:LEU:HD23	1:A:416:LEU:H	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:323:ARG:HE	1:B:372:MET:HE2	1.60	0.66
1:B:243:ASN:HD21	1:B:295:LYS:HZ3	1.41	0.66
1:B:354:GLU:HG3	1:B:372:MET:CE	2.24	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:280:ARG:O	1:B:281:THR:HB	1.96	0.64
1:B:139:GLU:OE2	1:B:140:ARG:NH1	2.31	0.64
1:A:390:HIS:CD2	1:A:393:ARG:H	2.16	0.64
1:A:304:LYS:HE3	1:A:337:GLU:OE1	1.98	0.63
1:B:323:ARG:NH1	1:B:372:MET:HE1	2.03	0.62
1:A:323:ARG:NH2	1:A:354:GLU:HG3	2.13	0.62
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: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:354:GLU:HG3	1:A:372:MET:HE2	1.82	0.61
1:A:544:GLN:HE21	1:A:544:GLN:HA	1.64	0.61
1:B:202:HIS:CD2	1:B:204:TYR:H	2.19	0.61
1:B:65:ARG:CG	1:B:65:ARG:HH11	2.13	0.61
1:A:544:GLN:HE22	1:A:568:GLN:HG2	1.64	0.60
1:A:178:ARG:HA	1:A:178:ARG:HE	1.65	0.60
1:A:243:ASN:HD22	1:A:244:HIS:CD2	2.15	0.60
1:A:138:PRO:HD2	1:A:193:THR:HG22	1.83	0.60
1:A:36:ARG:NH1	1:A:38:GLU:OE2	2.29	0.60
1:B:280:ARG:NE	1:B:280:ARG:HA	2.16	0.60
1:A:277:LYS:HZ2	1:A:278:THR:N	2.00	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:A:290:VAL:HG11	1:A:293:MET:CE	2.31	0.59
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:274:PRO:O	1:B:275:VAL:C	2.41	0.58
1:B:424:ARG:HB3	4:B:638:HOH:O	2.02	0.58
1:B:511:ASP:C	1:B:511:ASP:OD2	2.39	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:B:27:LEU:HD23	1:B:27:LEU:C	2.24	0.58
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: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: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:A:341:LEU:HD23	1:A:341:LEU:C	2.26	0.56
1:B:232:ARG:NH1	1:B:232:ARG:HG2	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:358:ASP:C	1:B:358:ASP:OD1	2.44	0.56
1:B:24:ARG:NH1	1:B:407:GLU:OE1	2.36	0.56
1:B:6:ILE:HD13	1:B:86:LEU:HD13	1.88	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:HG2	1:B:65:ARG:HH11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:GLU:OE1	1:A:107:LYS:HD3	2.07	0.55
1:A:15:ALA:O	4:A:656:HOH:O	2.17	0.55
1:A:323:ARG:HH21	1:A:372:MET:CE	2.20	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: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: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
1:B:309:ASP:OD2	1:B:312:ARG:NH2	2.42	0.53
1:A:158:LYS:CD	1:A:158:LYS:O	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:276:SER:O	1:A:277:LYS:C	2.46	0.53
1:A:324:LEU:HD13	1:A:335:TRP:CZ3	2.44	0.53
1:A:293:MET:CE	3:A:701:ARE:H6B1	2.39	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:381:ILE:HD13	1:A:425:PHE:CE1	2.43	0.53
1:A:178:ARG:HD3	1:A:474:TRP:CH2	2.44	0.53
1:A:159:ASP:CA	1:A:161:ARG:HH22	2.22	0.53
1:A:178:ARG:CA	1:A:178:ARG:HE	2.22	0.53
1:A:2:LEU:HD21	1:B:2:LEU:HD23	1.91	0.53
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:251:ALA:O	1:A:255:VAL:HG23	2.10	0.52
1:A:444:MET:HE3	1:A:450:PRO:HG3	1.92	0.52
1:A:293:MET:HE1	3:A:701:ARE:H6B1	1.92	0.52
1:B:223:ARG:HH21	1:B:223:ARG:HB3	1.71	0.52
1:A:332:HIS:HD2	1:A:367:GLN:OE1	1.93	0.52
1:B:382:ARG:HG2	1:B:388:GLU:CD	2.30	0.52
1:A:277:LYS:O	1:A:280:ARG:C	2.49	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:ALA:HA	1:A:413:LEU:HD22	1.92	0.51
1:B:155:GLN:CA	1:B:155:GLN:HE21	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: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:B:183:GLU:OE2	1:B:232:ARG:NH1	2.44	0.51
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:16:TYR:OH	1:B:407:GLU:HG3	2.11	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: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:NE2	1:A:408:GLN:H	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:422:THR:CG2	1:A:423:GLU:N	2.74	0.50
1:A:390:HIS:HA	1:A:515:ASN:HD21	1.77	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:NH1	1:B:105:ARG:HG2	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:A:475:GLU:O	1:A:476:GLU:C	2.50	0.49
1:A:323:ARG:HH21	1:A:372:MET:HE1	1.78	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:275:VAL:HG23	4:A:784:HOH:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:VAL:HA	1:A:282:ASN:HD21	1.78	0.48
1:B:354:GLU:CG	1:B:372:MET:HE3	2.34	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:B:427:THR:O	1:B:428:SER:C	2.48	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: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:416:LEU:H	1:B:416:LEU:HD23	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:A:104:GLU:O	1:A:105:ARG:C	2.52	0.47
1:B:352:VAL:HG21	1:B:414:TRP:CE2	2.49	0.47
1:B:256:LEU:HA	1:B:275:VAL:CG2	2.29	0.47
1:B:27:LEU:HD23	1:B:28:ARG:N	2.30	0.47
1:B:416:LEU:CD2	1:B:416:LEU:H	2.27	0.47
1:A:522:THR:HA	1:A:526:GLN:O	2.15	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: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:41:TYR:OH	4:B:782:HOH:O	2.15	0.47
1:B:562:VAL:HG11	1:B:569:LEU:HD21	1.97	0.47
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:158:LYS:HG3	1:A:478:GLU:CG	2.25	0.46
1:A:26:ARG:HD3	1:A:70:GLU:OE2	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:VAL:C	1:A:26:ARG:HG2	2.36	0.46
1:A:393:ARG:NE	4:A:763:HOH:O	2.49	0.46
1:A:174:GLY:O	1:A:178:ARG:HG2	2.16	0.46
1:A:232:ARG:NE	4:A:746:HOH:O	2.23	0.46
1:A:28:ARG:NE	4:A:627:HOH:O	2.45	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:191:TYR:C	1:B:191:TYR:CD1	2.88	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:A:393:ARG:HG3	1:A:393:ARG:NH2	2.20	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: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:A:44:ARG:HA	1:A:81:LYS:HG2	1.97	0.45
1:A:453:TYR:O	1:A:454:TYR:C	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:293:MET:HE2	3:A:701:ARE:C6B	2.46	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:524:GLN:HA	1:B:524:GLN:OE1	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: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:B:281:THR:HG22	1:B:281:THR:O	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
1:B:133:ILE:HG22	1:B:134:TYR:N	2.32	0.44
1:B:155:GLN:CA	1:B:155:GLN:NE2	2.76	0.44

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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:A:504:ASN:ND2	1:A:522:THR:HB	2.33	0.44
1:A:346:ASN:HD22	1:A:346:ASN:C	2.21	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:HB2	1:A:253:ARG:HE	1.49	0.43
1:B:38:GLU:HB3	4:B:732:HOH:O	2.18	0.43
1:A:504:ASN:C	1:A:504:ASN:HD22	2.22	0.43
1:A:504:ASN:O	1:A:521:ARG:HA	2.18	0.43
1:B:143:ASN:CG	1:B:169:GLY:O	2.56	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: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:512:LYS:HB2	1:A:512:LYS:HE2	1.25	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:B:158:LYS:HB2	4:B:766:HOH:O	2.19	0.43
1:B:331:ASP:N	1:B:331:ASP:OD1	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:473:ILE:CG2	1:B:478:GLU:HB3	2.49	0.42
1:B:57:ALA:HA	1:B:70:GLU:O	2.19	0.42
1:A:249:PHE:O	1:A:250:PHE:C	2.57	0.42
1:A:193:THR:HG23	1:A:194:PRO:HD2	2.01	0.42
1:B:223:ARG:CB	1:B:223:ARG:CZ	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
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:467:ASP:O	1:B:470:ARG:HG2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:LEU:HD23	1:A:52:LEU:HA	1.71	0.42
1:B:290:VAL:CG1	1:B:293:MET:HB2	2.47	0.42
1:B:533:ASN:ND2	1:B:533:ASN:C	2.72	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:A:277:LYS:O	1:A:281:THR:N	2.53	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:95:TYR:HB2	1:B:102:SER:O	2.21	0.41
1:A:118:ARG:HG3	1:A:118:ARG:H	1.34	0.41
1:A:536:GLY:O	1:A:575:PRO:HB3	2.20	0.41
1:B:424:ARG:HG3	1:B:461:ALA:C	2.41	0.41
1:A:164:HIS:CE1	3:A:701:ARE:O2A	2.74	0.41
1:B:104:GLU:OE1	1:B:107:LYS:HE2	2.20	0.41
1:B:200:SER:OG	1:B:205:ASP:OD1	2.23	0.41
1:B:541:VAL:HG22	1:B:542:LEU:N	2.36	0.41
1:A:224:ARG:NH2	1:A:224:ARG:HA	2.36	0.41
1:A:582:TRP:C	1:A:584:GLY:H	2.23	0.41
1:B:178:ARG:O	1:B:179:LEU:C	2.58	0.41
1:B:234:ILE:CG2	1:B:235:LYS:N	2.84	0.41
1:A:391:ALA:H	1:A:515:ASN:ND2	2.19	0.41
1:A:293:MET:HE2	3:A:701:ARE:H6B2	2.02	0.40
1:B:192:PHE:O	1:B:239:ASP:HB2	2.21	0.40
1:B:8:HIS:CG	1:B:9:GLU:N	2.89	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:ND2	1:B:328:ASN:N	2.51	0.40
1:A:206:THR:HG21	1:A:209:TYR:CD2	2.57	0.40
1:A:57:ALA:HB2	1:A:71:ALA:HB2	2.03	0.40
1:B:160:ALA:N	4:B:773:HOH:O	2.50	0.40
1:B:416:LEU:N	1:B:416:LEU:HD23	2.37	0.40
1:B:426:LEU:O	1:B:429:CYS:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:ALA:HB2	1:B:52:LEU:HD23	2.04	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 ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	583/585 (100%)	520 (89%)	56 (10%)	7 (1%)	13	39
1	B	583/585 (100%)	523 (90%)	52 (9%)	8 (1%)	11	34
All	All	1166/1170 (100%)	1043 (90%)	108 (9%)	15 (1%)	12	36

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

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Mol	Chain	Res	Type
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%)	441 (90%)	52 (10%)	7	20
1	B	493/493 (100%)	441 (90%)	52 (10%)	7	20
All	All	986/986 (100%)	882 (90%)	104 (10%)	7	20

All (104) 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	64	GLU
1	A	73	LEU
1	A	76	SER
1	A	85	LEU
1	A	92	GLU
1	A	118	ARG
1	A	122	PHE
1	A	140	ARG
1	A	158	LYS
1	A	178	ARG
1	A	182	LEU
1	A	191	TYR

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Mol	Chain	Res	Type
1	A	193	THR
1	A	215	GLN
1	A	223	ARG
1	A	224	ARG
1	A	231	ARG
1	A	253	ARG
1	A	265	LYS
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	346	ASN
1	A	372	MET
1	A	393	ARG
1	A	398	LEU
1	A	408	GLN
1	A	413	LEU
1	A	426	LEU
1	A	444	MET
1	A	469	ARG
1	A	476	GLU
1	A	483	LEU
1	A	504	ASN
1	A	505	VAL
1	A	535	ARG
1	A	539	GLN
1	A	542	LEU
1	A	551	LYS
1	A	565	LYS
1	A	570	LYS
1	A	571	LEU
1	A	581	LEU
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	73	LEU
1	B	76	SER

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Mol	Chain	Res	Type
1	B	85	LEU
1	B	105	ARG
1	B	110	VAL
1	B	122	PHE
1	B	171	ASP
1	B	190	LEU
1	B	191	TYR
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	272	ASP
1	B	277	LYS
1	B	280	ARG
1	B	281	THR
1	B	284	GLU
1	B	305	GLU
1	B	320	ASP
1	B	323	ARG
1	B	328	ASN
1	B	364	MET
1	B	373	ASN
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	481	ARG
1	B	504	ASN
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

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Mol	Chain	Res	Type
1	B	569	LEU
1	B	573	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) 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	390	HIS
1	A	408	GLN
1	A	443	GLN
1	A	504	ASN
1	A	515	ASN
1	A	527	HIS
1	A	539	GLN
1	A	544	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	328	ASN
1	B	332	HIS
1	B	357	HIS
1	B	373	ASN
1	B	504	ASN
1	B	533	ASN
1	B	544	GLN
1	B	566	GLN

### 5.3.3 RNA ⓘ

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 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	2.56	12 (20%)	74,88,88	2.21	23 (31%)
3	ARE	A	701	-	58,59,59	2.93	18 (31%)	74,88,88	1.70	15 (20%)

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	-	-	8/24/124/124	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	16.15	1.55	1.32
3	A	701	ARE	C6H-C5H	15.20	1.54	1.32
3	A	701	ARE	C4H-C5H	7.05	1.58	1.51
3	A	701	ARE	O5A-C5A	6.16	1.59	1.44
3	A	701	ARE	O4G-C1C	4.29	1.53	1.41
3	A	701	ARE	O4H-C1B	3.87	1.52	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	702	ARE	C1H-C6H	3.71	1.55	1.50
3	B	702	ARE	O5B-C5B	3.64	1.53	1.44
3	A	701	ARE	C1H-C6H	3.60	1.55	1.50
3	A	701	ARE	C4A-C5A	3.36	1.60	1.53
3	A	701	ARE	O5A-C1A	3.01	1.49	1.41
3	A	701	ARE	C3C-C4C	2.96	1.58	1.53
3	A	701	ARE	O5B-C1B	2.96	1.49	1.41
3	A	701	ARE	O3C-C3C	2.87	1.49	1.43
3	B	702	ARE	O5A-C5A	2.84	1.51	1.44
3	A	701	ARE	C3A-C2A	2.82	1.59	1.52
3	B	702	ARE	O2G-C2G	2.74	1.49	1.43
3	A	701	ARE	C6A-C5A	2.72	1.61	1.51
3	B	702	ARE	O3C-C3C	2.63	1.49	1.43
3	B	702	ARE	O1G-C1G	2.52	1.47	1.39
3	B	702	ARE	C3G-C2G	2.34	1.58	1.52
3	A	701	ARE	O4B-C1A	2.25	1.48	1.41
3	A	701	ARE	O4G-C4G	2.15	1.49	1.43
3	A	701	ARE	O2G-C2G	2.13	1.48	1.43
3	A	701	ARE	C3G-C4G	2.13	1.58	1.52
3	B	702	ARE	C3C-C4C	2.13	1.57	1.53
3	B	702	ARE	C3H-C4H	2.13	1.56	1.53
3	B	702	ARE	O5A-C1A	2.12	1.47	1.41
3	B	702	ARE	C6A-C5A	2.07	1.58	1.51
3	A	701	ARE	O1G-C1G	2.06	1.46	1.39

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	702	ARE	C1G-O5G-C5G	6.50	125.93	113.66
3	A	701	ARE	O4G-C1C-C2C	6.36	124.58	108.10
3	B	702	ARE	C2G-C3G-C4G	4.90	120.87	109.68
3	B	702	ARE	C6G-C5G-C4G	-4.72	99.60	113.33
3	B	702	ARE	C1C-O5C-C5C	4.55	121.48	113.67
3	B	702	ARE	C3G-C4G-C5G	-4.31	101.05	110.93
3	B	702	ARE	O1G-C1G-C2G	4.20	120.87	109.03
3	B	702	ARE	C1B-O5B-C5B	-4.15	105.54	113.69
3	B	702	ARE	O1G-C1G-O5G	-4.06	98.19	110.38
3	B	702	ARE	O5B-C5B-C6B	3.89	116.11	106.44
3	B	702	ARE	C1A-O4B-C4B	-3.81	108.54	117.96
3	A	701	ARE	O5G-C1G-C2G	3.80	117.07	110.28
3	A	701	ARE	C2G-C3G-C4G	3.75	118.25	109.68
3	A	701	ARE	O5C-C1C-C2C	-3.73	102.44	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	701	ARE	O5A-C5A-C6A	3.52	115.18	106.44
3	B	702	ARE	O5C-C1C-C2C	3.29	117.31	110.35
3	B	702	ARE	O5A-C5A-C4A	3.28	115.65	109.69
3	B	702	ARE	C6H-C1H-N4C	3.27	115.59	110.68
3	B	702	ARE	O5G-C5G-C4G	-3.04	103.34	109.75
3	B	702	ARE	O4B-C1A-C2A	3.02	115.92	108.10
3	A	701	ARE	C1G-O5G-C5G	3.00	119.33	113.66
3	B	702	ARE	O3C-C3C-C4C	2.99	115.70	109.66
3	A	701	ARE	O5C-C5C-C6C	2.76	112.67	106.70
3	B	702	ARE	C1B-C2B-C3B	2.69	115.60	110.00
3	B	702	ARE	O5G-C5G-C6G	2.68	113.10	106.44
3	A	701	ARE	O4H-C1B-O5B	2.63	118.02	110.67
3	A	701	ARE	O3C-C3C-C4C	2.58	114.87	109.66
3	B	702	ARE	O4H-C1B-C2B	2.45	114.44	108.10
3	B	702	ARE	C1A-O5A-C5A	2.43	118.47	113.69
3	A	701	ARE	O3A-C3A-C2A	2.43	115.98	110.35
3	A	701	ARE	C1A-O4B-C4B	2.41	123.93	117.96
3	A	701	ARE	O1G-C1G-O5G	-2.38	103.23	110.38
3	A	701	ARE	C2B-C3B-C4B	2.20	114.71	109.68
3	B	702	ARE	C2B-C3B-C4B	2.18	114.67	109.68
3	B	702	ARE	O4A-C4A-C3A	-2.17	105.33	110.35
3	B	702	ARE	O2H-C2H-C1H	2.12	113.37	109.12
3	A	701	ARE	O2A-C2A-C1A	-2.11	104.93	110.05
3	A	701	ARE	O2H-C2H-C1H	-2.10	104.91	109.12

There are no chirality outliers.

All (14) torsion outliers are listed below:

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

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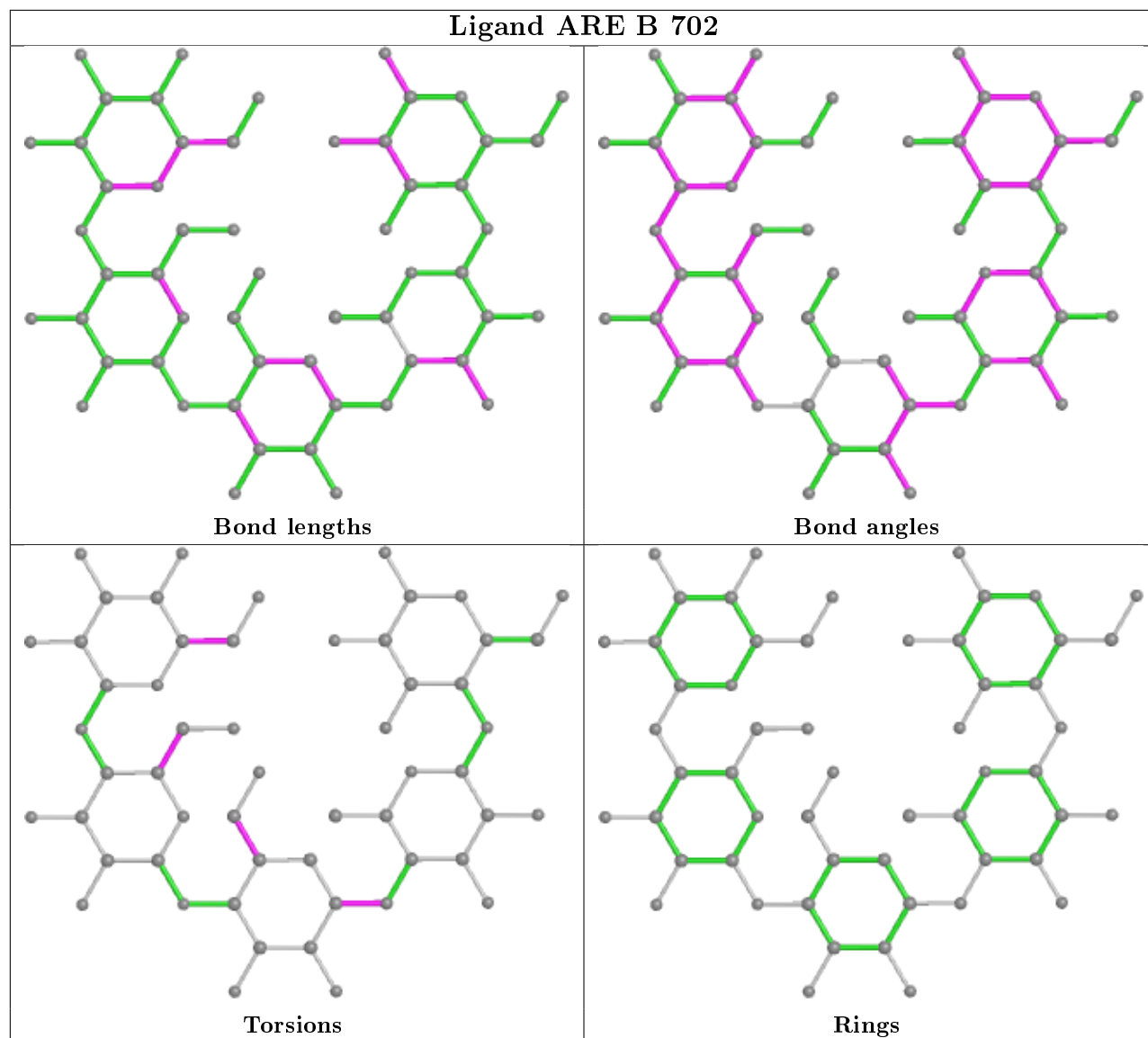
Mol	Chain	Res	Type	Atoms
3	B	702	ARE	C4A-C5A-C6A-O6A

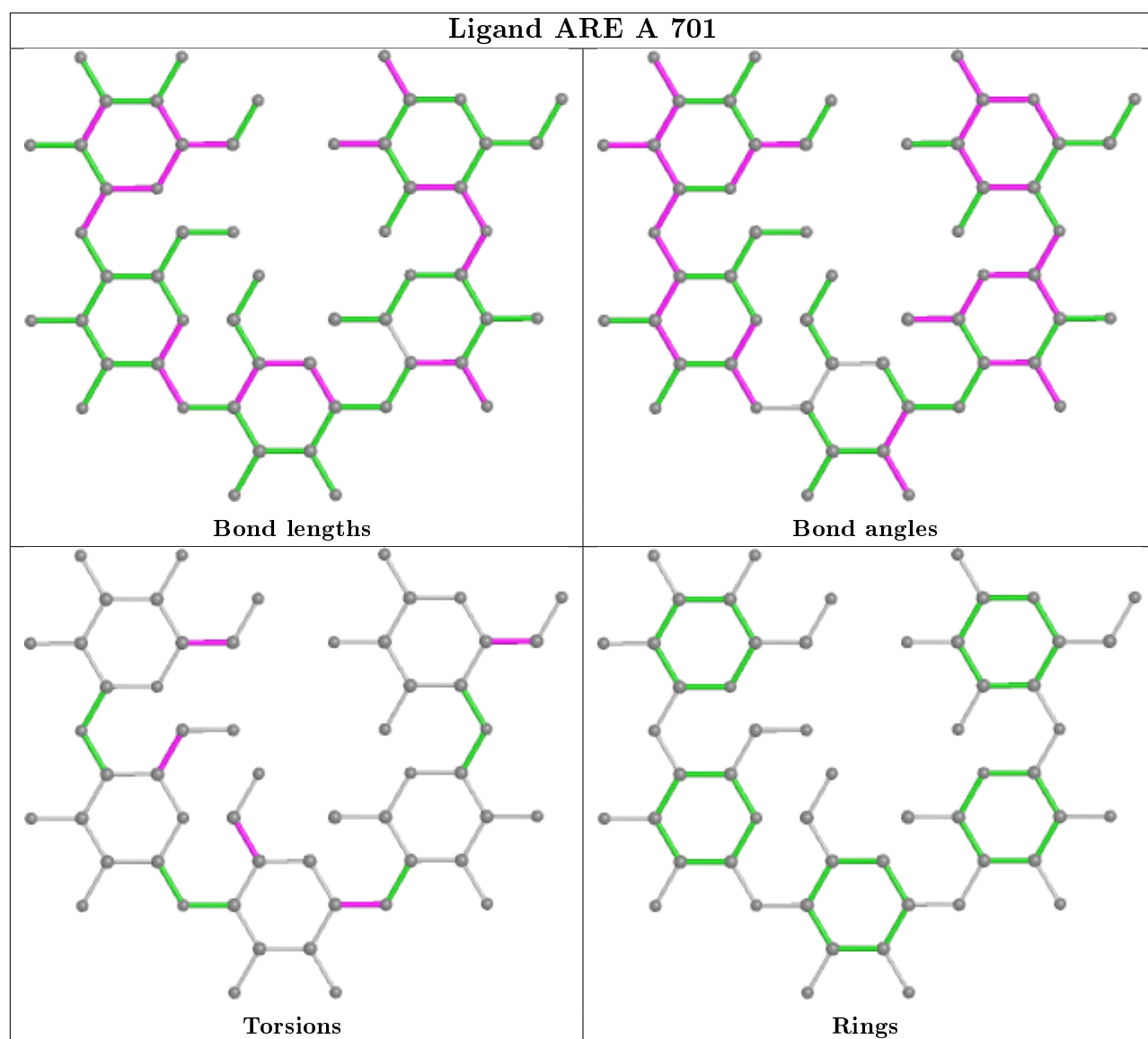
There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	702	ARE	2	0
3	A	701	ARE	7	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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	585/585 (100%)	-0.73	2 (0%) 94 93	8, 23, 47, 77	0
1	B	585/585 (100%)	-0.63	3 (0%) 91 88	9, 23, 48, 90	0
All	All	1170/1170 (100%)	-0.68	5 (0%) 92 91	8, 23, 48, 90	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	548	SER	3.7
1	B	279	SER	3.3
1	A	279	SER	3.1
1	B	277	LYS	2.9
1	B	272	ASP	2.9

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

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

### 6.3 Carbohydrates [i](#)

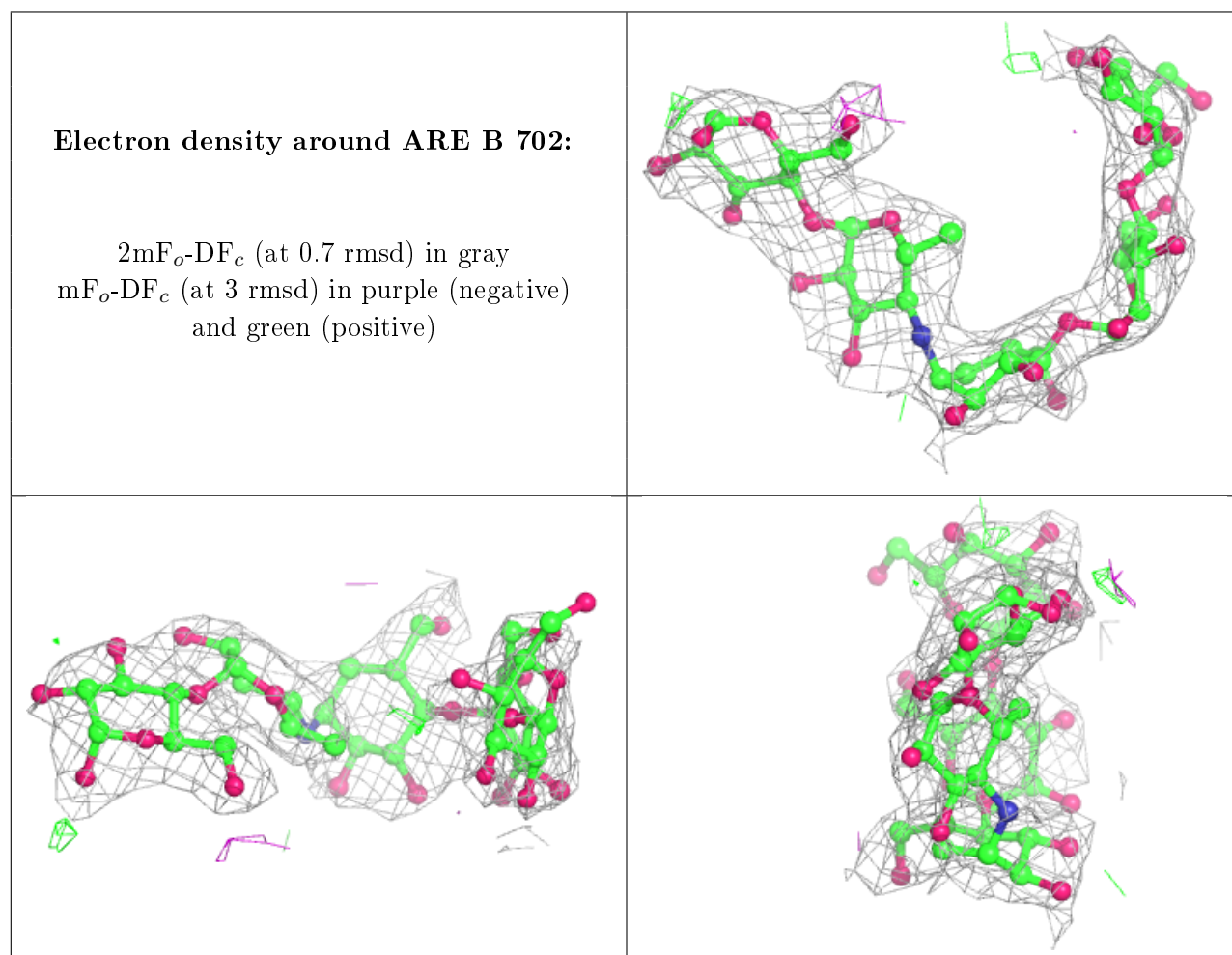
There are no carbohydrates in this entry.

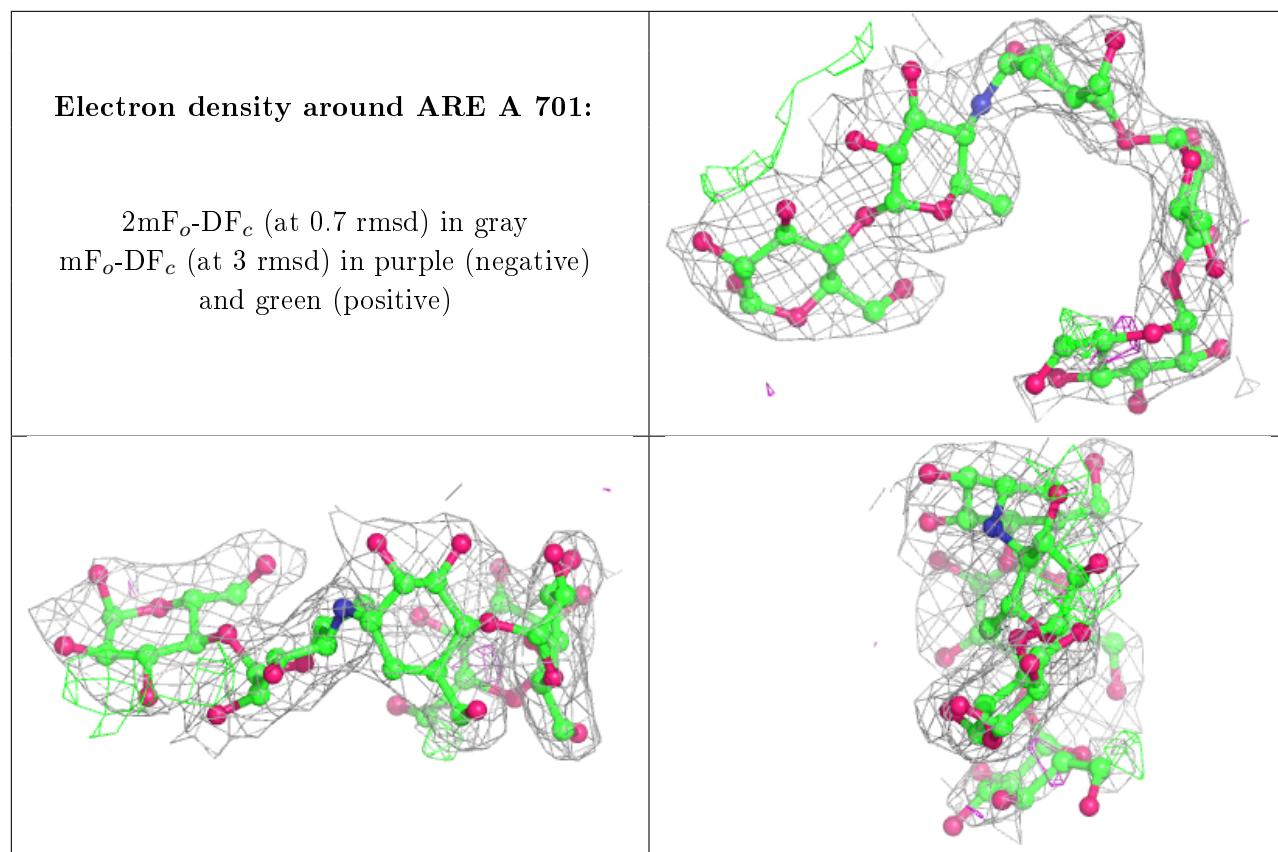
### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	ARE	B	702	55/55	0.94	0.16	24,38,67,71	0
3	ARE	A	701	55/55	0.94	0.17	17,35,76,78	0
2	CA	B	586	1/1	0.99	0.04	28,28,28,28	0
2	CA	A	586	1/1	1.00	0.06	19,19,19,19	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.





## 6.5 Other polymers [i](#)

There are no such residues in this entry.