



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 21, 2023 – 07:05 PM JST

PDB ID : 7VIB
Title : Crystal structure of human ACE2 and GX/P2V RBD
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Deposited on : 2021-09-26
Resolution : 3.20 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 : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

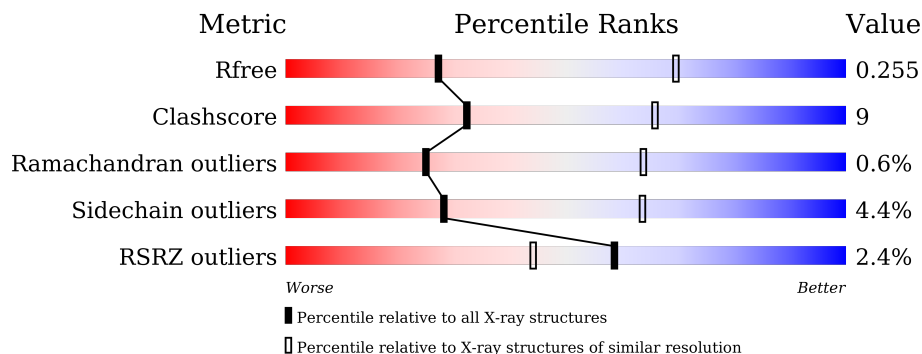
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	597	 2% (Poor fit) 78% (0-1 outliers) 21% (2-3 outliers) • (not modelled)
1	C	597	 % (Poor fit) 75% (0-1 outliers) 25% (2-3 outliers) • (not modelled)
2	B	194	 5% (Poor fit) 71% (0-1 outliers) 26% (2-3 outliers) •• (not modelled)
2	D	194	 5% (Poor fit) 74% (0-1 outliers) 18% (2-3 outliers) • 5% (not modelled)

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12701 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 Angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	597	4877	3120	808	920	29	0	1	0
1	C	597	4877	3120	808	920	29	0	1	0

- Molecule 2 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	188	1486	955	246	277	8	0	0	0
2	D	184	1459	940	241	270	8	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	501	ASN	THR	engineered mutation	UNP A0A6G6A2Q2
D	501	ASN	THR	engineered mutation	UNP A0A6G6A2Q2

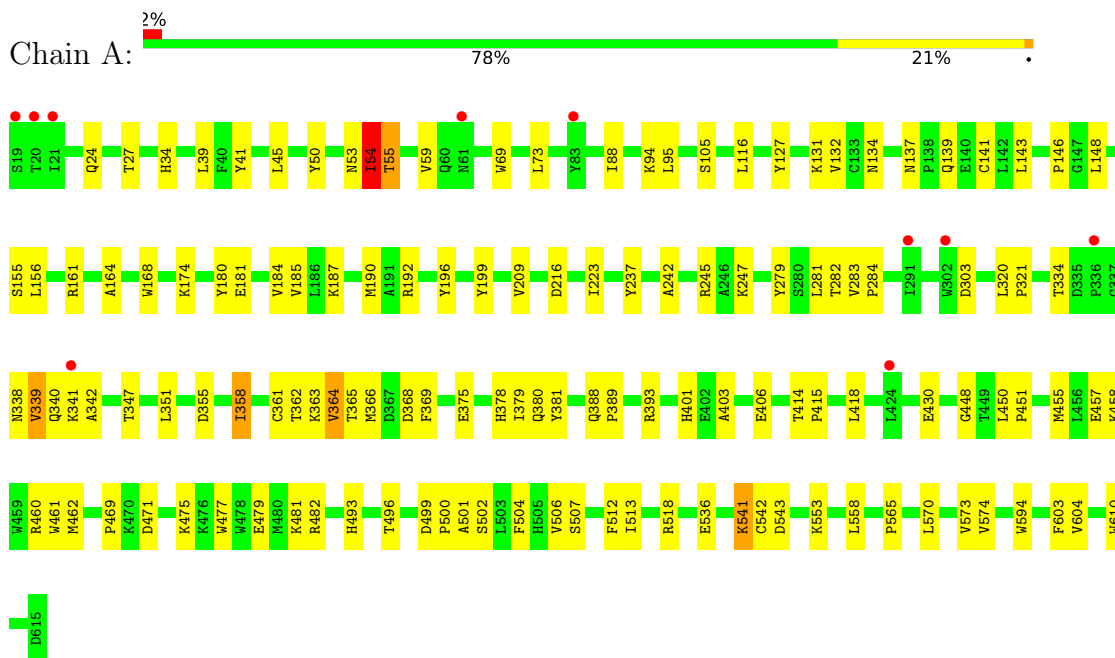
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		

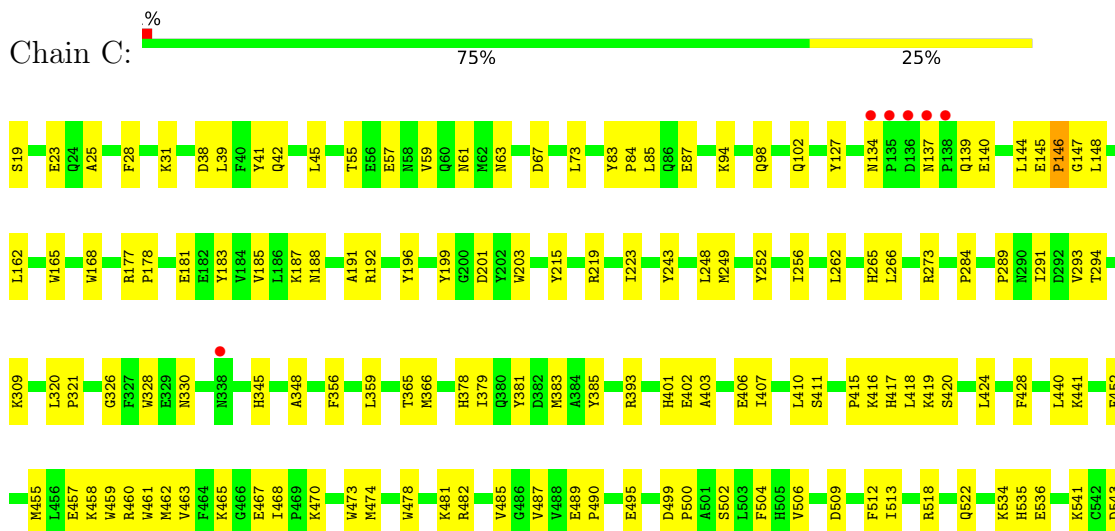
3 Residue-property plots

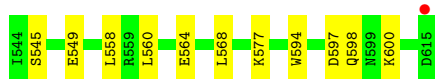
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

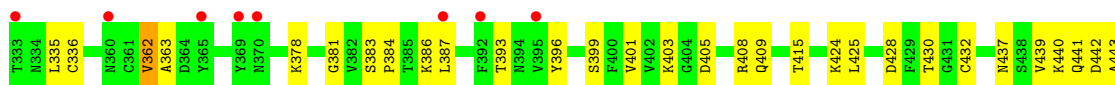


- Molecule 1: Angiotensin-converting enzyme 2

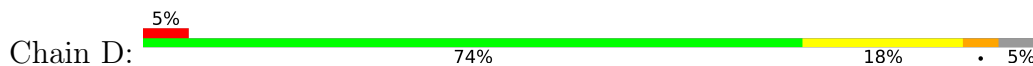




• Molecule 2: Spike glycoprotein



• Molecule 2: Spike glycoprotein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.67Å 120.15Å 107.89Å 90.00° 96.61° 90.00°	Depositor
Resolution (Å)	47.29 – 3.20 48.94 – 3.20	Depositor EDS
% Data completeness (in resolution range)	75.6 (47.29-3.20) 84.2 (48.94-3.20)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 3.19Å)	Xtrriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.204 , 0.258 0.210 , 0.255	Depositor DCC
R_{free} test set	2000 reflections (6.49%)	wwPDB-VP
Wilson B-factor (Å ²)	62.2	Xtrriage
Anisotropy	0.086	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 9.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	12701	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% 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:
ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.62	1/5018 (0.0%)	0.72	0/6818
1	C	0.62	0/5018	0.71	0/6818
2	B	0.77	1/1526 (0.1%)	0.74	0/2074
2	D	0.96	2/1498 (0.1%)	0.85	0/2033
All	All	0.69	4/13060 (0.0%)	0.74	0/17743

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	478	THR	C-N	5.76	1.45	1.34
1	A	358	ILE	C-N	-5.40	1.21	1.34
2	D	430	THR	C-N	-5.24	1.23	1.33
2	B	430	THR	C-N	-5.13	1.23	1.33

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4877	0	4650	79	0
1	C	4877	0	4650	103	0
2	B	1486	0	1418	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1459	0	1392	14	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
All	All	12701	0	12110	218	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (218) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:440:LYS:HG3	2:B:441:GLN:HG3	1.60	0.84
1:C:41:TYR:HE1	1:C:45:LEU:HD22	1.45	0.80
1:A:458:LYS:HG2	1:A:462:MET:HE2	1.63	0.79
1:C:460:ARG:NH2	1:C:506:VAL:HA	2.01	0.75
1:A:460:ARG:HH21	1:A:506:VAL:HA	1.51	0.74
1:A:320:LEU:HD13	1:A:380:GLN:HG2	1.70	0.73
1:C:98:GLN:O	1:C:102:GLN:NE2	2.22	0.72
1:C:85:LEU:HD22	1:C:94:LYS:HG3	1.73	0.70
1:A:381:TYR:CD1	1:A:558:LEU:HD22	2.27	0.70
1:C:406:GLU:HG3	1:C:518:ARG:HD3	1.72	0.69
1:C:19:SER:N	1:C:23:GLU:OE1	2.26	0.68
1:C:326:GLY:O	1:C:330:ASN:ND2	2.26	0.68
1:C:294:THR:HG23	1:C:365:THR:HA	1.74	0.68
1:C:145:GLU:HB3	1:C:146:PRO:HD3	1.74	0.67
1:A:381:TYR:HD1	1:A:558:LEU:HD22	1.61	0.65
1:C:252:TYR:CE2	1:C:266:LEU:HD22	2.31	0.65
1:C:560:LEU:HD13	1:C:564:GLU:HG3	1.78	0.65
1:C:41:TYR:CE1	1:C:45:LEU:HD22	2.31	0.64
1:C:402:GLU:HB3	1:C:518:ARG:HG3	1.80	0.63
1:C:203:TRP:HZ3	1:C:460:ARG:HD3	1.65	0.62
1:A:174:LYS:NZ	1:A:496:THR:OG1	2.34	0.61
1:C:144:LEU:HA	1:C:148:LEU:HB2	1.83	0.61
1:C:84:PRO:HG2	1:C:87:GLU:HB2	1.83	0.61
1:C:265:HIS:ND1	1:C:490:PRO:HG3	2.15	0.60
2:B:396:TYR:HB2	2:B:514:SER:HB2	1.82	0.60
1:A:334:THR:O	1:A:361:CYS:HA	2.00	0.59
1:A:245:ARG:NH2	1:A:603:PHE:O	2.36	0.59
1:C:455:MET:CE	1:C:481:LYS:HD2	2.33	0.59
1:C:57:GLU:O	1:C:61:ASN:ND2	2.35	0.59
2:D:344:ALA:HB3	2:D:347:PHE:HE1	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:448:GLY:O	1:A:451:PRO:HD2	2.03	0.59
1:A:88:ILE:HB	1:A:94:LYS:HG3	1.84	0.58
2:B:437:ASN:OD1	2:B:439:VAL:HG23	2.04	0.58
1:C:455:MET:HE2	1:C:481:LYS:HD2	1.85	0.57
1:C:381:TYR:CD1	1:C:558:LEU:HD22	2.39	0.57
1:A:41:TYR:CE2	1:A:45:LEU:HD22	2.40	0.57
1:A:406:GLU:HG3	1:A:518:ARG:NH1	2.20	0.56
1:C:478:TRP:CE3	1:C:481:LYS:HG3	2.41	0.56
2:B:401:VAL:HG22	2:B:509:ARG:HG2	1.88	0.56
1:A:381:TYR:HE1	1:A:558:LEU:HA	1.70	0.56
1:C:25:ALA:HA	1:C:28:PHE:HB3	1.87	0.56
1:C:381:TYR:HD2	1:C:401:HIS:CD2	2.24	0.55
2:D:401:VAL:HG22	2:D:509:ARG:HG2	1.87	0.55
1:C:378:HIS:ND1	1:C:401:HIS:HB3	2.21	0.55
1:C:402:GLU:CB	1:C:518:ARG:HG3	2.36	0.55
2:D:461:LEU:HD22	2:D:465:GLU:HB3	1.89	0.55
1:C:468:ILE:HG22	1:C:473:TRP:HD1	1.72	0.55
1:C:378:HIS:HD1	1:C:401:HIS:HB3	1.72	0.55
1:A:457:GLU:OE2	1:A:512:PHE:N	2.38	0.54
1:A:460:ARG:NH2	1:A:506:VAL:HA	2.19	0.54
1:C:458:LYS:O	1:C:462:MET:HG3	2.08	0.54
2:B:442:ASP:O	2:B:448:ASN:ND2	2.39	0.53
1:C:411:SER:HB3	1:C:543:ASP:HA	1.90	0.53
1:C:183:TYR:OH	1:C:509:ASP:OD1	2.21	0.53
2:B:384:PRO:HA	2:B:387:LEU:HD12	1.91	0.53
1:A:131:LYS:HB3	1:A:143:LEU:HD23	1.91	0.53
1:C:177:ARG:NH2	1:C:470:LYS:O	2.42	0.53
2:B:449:TYR:O	2:B:494:ARG:HD3	2.09	0.52
1:A:137:ASN:OD1	1:A:139:GLN:HB3	2.09	0.52
1:A:406:GLU:HG3	1:A:518:ARG:HH11	1.74	0.52
1:A:475:LYS:HE2	1:A:479:GLU:OE2	2.10	0.52
2:B:449:TYR:HB3	2:B:494:ARG:HD3	1.92	0.52
1:C:39:LEU:O	1:C:42:GLN:HB2	2.10	0.52
1:C:419:LYS:HD3	1:C:428:PHE:HB3	1.91	0.52
1:A:542:CYS:SG	1:A:543:ASP:N	2.84	0.51
1:A:570:LEU:O	1:A:574:VAL:HG22	2.10	0.51
1:A:455:MET:HE3	1:A:481:LYS:HE2	1.93	0.51
1:C:381:TYR:HE1	1:C:558:LEU:HA	1.76	0.51
1:A:55:THR:O	1:A:59:VAL:HG23	2.11	0.51
2:D:339:GLY:O	2:D:343:ASN:HB2	2.11	0.51
1:C:249:MET:HG2	1:C:256:ILE:HB	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:424:LEU:HD23	1:C:428:PHE:CD1	2.47	0.50
2:B:452:LEU:HD23	2:B:494:ARG:HG2	1.92	0.50
1:A:381:TYR:CE1	1:A:558:LEU:HA	2.47	0.50
2:B:362:VAL:HG23	2:B:526:GLY:HA2	1.94	0.50
1:C:549:GLU:CD	1:C:549:GLU:H	2.15	0.49
1:A:41:TYR:O	1:A:45:LEU:HB2	2.11	0.49
1:C:597:ASP:OD1	1:C:600:LYS:NZ	2.37	0.49
1:C:177:ARG:NH1	1:C:495:GLU:O	2.46	0.49
1:C:379:ILE:O	1:C:383:MET:HG3	2.12	0.49
1:A:132:VAL:HG22	1:A:148:LEU:HD11	1.95	0.49
1:C:165:TRP:CZ3	1:C:490:PRO:HD2	2.48	0.49
1:C:181:GLU:O	1:C:185:VAL:HG23	2.12	0.49
1:C:485:VAL:HG12	1:C:487:VAL:HG23	1.95	0.49
1:C:459:TRP:O	1:C:463:VAL:HG23	2.13	0.48
1:A:553:LYS:HE3	1:A:573:VAL:O	2.13	0.48
1:A:50:TYR:CE1	1:A:59:VAL:HG22	2.49	0.48
1:A:155:SER:O	1:A:161:ARG:HD2	2.14	0.48
1:A:223:ILE:HG12	1:A:461:TRP:CZ3	2.49	0.48
1:C:564:GLU:OE1	1:C:568:LEU:HD23	2.14	0.48
1:A:457:GLU:HG3	1:A:513:ILE:HB	1.94	0.48
1:C:168:TRP:NE1	1:C:502:SER:HB2	2.29	0.48
1:A:403:ALA:HB2	1:A:518:ARG:HG3	1.96	0.48
2:B:502:GLY:O	2:B:506:GLN:HG3	2.13	0.48
1:A:477:TRP:CE3	1:A:500:PRO:HG3	2.48	0.47
1:C:203:TRP:CZ3	1:C:460:ARG:HD3	2.46	0.47
1:A:127:TYR:CZ	1:A:504:PHE:HB2	2.50	0.47
1:A:501:ALA:HB1	1:A:507:SER:HB3	1.95	0.47
1:C:137:ASN:HB3	1:C:140:GLU:HB2	1.95	0.47
1:A:415:PRO:HB2	1:A:430:GLU:OE2	2.15	0.47
1:C:215:TYR:CE2	1:C:568:LEU:HD13	2.50	0.47
1:C:381:TYR:HD1	1:C:558:LEU:HD22	1.79	0.47
1:A:279:TYR:O	1:A:283:VAL:N	2.48	0.47
1:A:24:GLN:OE1	2:B:487:ASN:ND2	2.47	0.46
1:A:284:PRO:HB3	1:A:594:TRP:CH2	2.50	0.46
1:A:358:ILE:HG13	1:A:379:ILE:HG13	1.96	0.46
1:C:403:ALA:O	1:C:407:ILE:HG23	2.15	0.46
2:D:342:PHE:CZ	2:D:434:ILE:HD12	2.50	0.46
1:C:215:TYR:CE1	1:C:577:LYS:HD3	2.50	0.46
1:C:168:TRP:HE1	1:C:502:SER:HB2	1.79	0.46
2:D:490:TYR:CD1	2:D:491:PRO:HD2	2.51	0.46
1:A:181:GLU:O	1:A:185:VAL:HG23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:VAL:HG12	1:A:216:ASP:HA	1.98	0.46
2:B:452:LEU:CD2	2:B:494:ARG:HG2	2.45	0.45
1:C:320:LEU:HB3	1:C:321:PRO:HD2	1.98	0.45
1:A:116:LEU:HD11	1:A:187:LYS:HE2	1.99	0.45
2:B:443:ALA:O	2:B:444:LEU:HD23	2.15	0.45
2:B:439:VAL:HG13	2:B:443:ALA:HB3	1.99	0.45
1:C:127:TYR:CZ	1:C:504:PHE:HB2	2.52	0.45
1:A:192:ARG:HA	1:A:196:TYR:O	2.16	0.45
1:C:482:ARG:NH2	1:C:489:GLU:OE2	2.50	0.45
1:A:389:PRO:O	1:A:393:ARG:HG3	2.16	0.45
1:C:223:ILE:HG12	1:C:461:TRP:CZ3	2.52	0.45
1:C:457:GLU:HG3	1:C:513:ILE:HB	1.97	0.45
2:D:369:TYR:HD1	2:D:369:TYR:HA	1.54	0.45
1:A:237:TYR:CE1	1:A:451:PRO:HG2	2.52	0.44
1:C:55:THR:O	1:C:59:VAL:HG23	2.17	0.44
1:C:291:ILE:HD12	1:C:415:PRO:HG3	1.98	0.44
1:C:424:LEU:HD23	1:C:428:PHE:CG	2.52	0.44
1:A:69:TRP:CZ2	1:A:73:LEU:HD11	2.52	0.44
1:C:273:ARG:HG3	1:C:452:PHE:CE2	2.52	0.44
1:C:356:PHE:CE2	1:C:383:MET:HG2	2.52	0.44
1:C:381:TYR:CE1	1:C:558:LEU:HA	2.52	0.44
1:C:385:TYR:O	1:C:393:ARG:HG2	2.18	0.44
1:A:34:HIS:HD2	2:B:493:GLU:HG3	1.81	0.44
1:A:180:TYR:O	1:A:184:VAL:HG23	2.18	0.44
1:C:460:ARG:HH21	1:C:506:VAL:HA	1.81	0.44
1:A:381:TYR:HD2	1:A:401:HIS:CD2	2.36	0.44
1:A:168:TRP:CD1	1:A:502:SER:HB2	2.52	0.44
1:A:541:LYS:HB3	1:A:541:LYS:HE3	1.34	0.44
1:A:53:ASN:O	1:A:54:ILE:C	2.57	0.44
2:B:485:GLY:O	2:B:488:CYS:N	2.47	0.44
1:C:73:LEU:HD23	1:C:73:LEU:HA	1.78	0.44
1:C:293:VAL:HG22	1:C:366:MET:SD	2.58	0.44
1:C:478:TRP:CZ3	1:C:481:LYS:HG3	2.52	0.44
2:D:439:VAL:O	2:D:443:ALA:HB3	2.18	0.44
1:A:418:LEU:HA	1:A:418:LEU:HD23	1.82	0.43
1:A:381:TYR:CD2	1:A:401:HIS:CD2	3.06	0.43
1:C:191:ALA:O	1:C:196:TYR:HB2	2.18	0.43
1:C:215:TYR:CE2	1:C:568:LEU:HB2	2.53	0.43
2:B:501:ASN:HB2	2:B:506:GLN:HG3	2.01	0.43
1:C:289:PRO:HB2	1:C:428:PHE:CE1	2.53	0.43
2:D:472:ILE:H	2:D:472:ILE:HG12	1.22	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:LYS:HB2	1:A:282:THR:HG22	2.00	0.43
1:A:493:HIS:ND1	1:A:499:ASP:OD2	2.51	0.43
1:A:50:TYR:CD1	1:A:59:VAL:HG22	2.53	0.43
2:B:336:CYS:HB2	2:B:363:ALA:HB2	1.99	0.43
1:C:162:LEU:CD1	1:C:490:PRO:HG2	2.48	0.43
1:C:201:ASP:CG	1:C:219:ARG:HE	2.21	0.43
1:A:105:SER:HA	1:A:190:MET:HG3	2.00	0.43
1:A:321:PRO:O	1:A:380:GLN:NE2	2.47	0.43
1:A:27:THR:HG23	2:B:456:PHE:CE1	2.54	0.43
1:A:209:VAL:HG11	1:A:565:PRO:HB3	2.01	0.43
2:B:336:CYS:HB2	2:B:363:ALA:CB	2.49	0.43
1:C:177:ARG:N	1:C:178:PRO:HD2	2.34	0.43
1:A:341:LYS:HB3	1:A:341:LYS:HE3	1.73	0.43
1:C:187:LYS:HB3	1:C:199:TYR:CD2	2.54	0.43
1:C:188:ASN:O	1:C:192:ARG:HG3	2.19	0.43
1:C:419:LYS:HE2	1:C:428:PHE:O	2.18	0.43
1:C:457:GLU:OE2	1:C:512:PHE:N	2.41	0.43
1:A:375:GLU:O	1:A:378:HIS:HB2	2.18	0.43
2:D:425:LEU:HD23	2:D:425:LEU:HA	1.80	0.43
1:C:418:LEU:CB	1:C:424:LEU:HD13	2.48	0.42
1:A:469:PRO:HB2	1:A:471:ASP:OD1	2.20	0.42
1:C:366:MET:SD	1:C:441:LYS:NZ	2.87	0.42
1:C:465:LYS:HD2	1:C:467:GLU:OE2	2.19	0.42
1:A:148:LEU:HD22	1:A:164:ALA:HB1	2.00	0.42
1:A:242:ALA:HB2	1:A:604:VAL:HA	2.01	0.42
1:A:131:LYS:HD3	1:A:141:CYS:HB3	2.02	0.42
1:C:38:ASP:O	1:C:42:GLN:HG2	2.20	0.42
1:C:248:LEU:HD12	1:C:262:LEU:HD22	2.01	0.42
2:D:418:ILE:HA	2:D:422:ASN:HD22	1.84	0.42
1:C:309:LYS:HD2	1:C:328:TRP:CH2	2.54	0.42
1:C:25:ALA:HB2	1:C:83:TYR:CD2	2.54	0.41
1:C:460:ARG:HH22	1:C:506:VAL:HA	1.80	0.41
1:C:289:PRO:HB2	1:C:428:PHE:HE1	1.84	0.41
1:A:39:LEU:HD23	1:A:39:LEU:HA	1.91	0.41
1:C:63:ASN:O	1:C:67:ASP:N	2.48	0.41
1:C:181:GLU:HG2	1:C:473:TRP:CH2	2.55	0.41
1:C:378:HIS:CE1	1:C:401:HIS:HB3	2.55	0.41
2:D:376:THR:HB	2:D:435:ALA:HB3	2.02	0.41
2:D:387:LEU:HD12	2:D:387:LEU:HA	1.90	0.41
1:A:134:ASN:HD21	1:A:137:ASN:HB3	1.85	0.41
1:A:388:GLN:OE1	1:A:389:PRO:HD2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:459:TRP:CH2	1:C:500:PRO:HG2	2.55	0.41
1:C:543:ASP:C	1:C:545:SER:H	2.23	0.41
2:B:425:LEU:HD21	2:B:512:VAL:HG11	2.03	0.41
1:A:187:LYS:HD2	1:A:199:TYR:CE2	2.56	0.41
1:C:594:TRP:CH2	1:C:598:GLN:HG3	2.56	0.41
1:A:414:THR:HG21	1:A:542:CYS:O	2.21	0.41
1:C:45:LEU:HD12	1:C:45:LEU:HA	1.90	0.41
1:C:410:LEU:HG	1:C:522:GLN:HE21	1.85	0.41
1:C:416:LYS:HE3	1:C:416:LYS:HB2	1.93	0.41
2:D:376:THR:HG23	2:D:378:LYS:HE3	2.03	0.41
1:A:156:LEU:HD22	1:A:281:LEU:HD11	2.03	0.41
1:A:482:ARG:NH1	1:A:610:TRP:O	2.53	0.41
1:A:95:LEU:HD23	1:A:95:LEU:HA	1.86	0.40
2:B:497:PHE:CD2	2:B:507:PRO:HB3	2.55	0.40
1:C:348:ALA:HB1	1:C:379:ILE:HG12	2.04	0.40
1:C:417:HIS:O	1:C:420:SER:HB3	2.22	0.40
1:C:474:MET:CE	1:C:499:ASP:H	2.34	0.40
1:A:450:LEU:HA	1:A:450:LEU:HD23	1.82	0.40
1:A:351:LEU:HB2	1:A:355:ASP:HB3	2.03	0.40
2:B:408:ARG:HG3	2:B:409:GLN:HG3	2.04	0.40
1:A:501:ALA:HA	1:A:506:VAL:HB	2.03	0.40
2:B:501:ASN:ND2	2:B:505:TYR:O	2.54	0.40
1:C:243:TYR:CE2	1:C:440:LEU:HD11	2.57	0.40
1:C:465:LYS:HB2	1:C:465:LYS:HE3	1.78	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [\(i\)](#)

5.3.1 Protein backbone [\(i\)](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	596/597 (100%)	553 (93%)	37 (6%)	6 (1%)	15 54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	596/597 (100%)	547 (92%)	46 (8%)	3 (0%)	29 67
2	B	184/194 (95%)	170 (92%)	13 (7%)	1 (0%)	29 67
2	D	178/194 (92%)	162 (91%)	16 (9%)	0	100 100
All	All	1554/1582 (98%)	1432 (92%)	112 (7%)	10 (1%)	25 64

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	ILE
1	C	146	PRO
1	A	146	PRO
1	A	342	ALA
1	A	338	ASN
1	A	364	VAL
1	C	284	PRO
2	B	381	GLY
1	C	147	GLY
1	A	339	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	528/527 (100%)	513 (97%)	15 (3%)	43 74
1	C	528/527 (100%)	519 (98%)	9 (2%)	60 83
2	B	162/167 (97%)	148 (91%)	14 (9%)	10 38
2	D	159/167 (95%)	136 (86%)	23 (14%)	3 15
All	All	1377/1388 (99%)	1316 (96%)	61 (4%)	28 64

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	ILE

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Mol	Chain	Res	Type
1	A	55	THR
1	A	303	ASP
1	A	339	VAL
1	A	340	GLN
1	A	347	THR
1	A	362	THR
1	A	363	LYS
1	A	364	VAL
1	A	365	THR
1	A	366	MET
1	A	368	ASP
1	A	369	PHE
1	A	536	GLU
1	A	541	LYS
2	B	335	LEU
2	B	362	VAL
2	B	378	LYS
2	B	383	SER
2	B	386	LYS
2	B	393	THR
2	B	399	SER
2	B	403	LYS
2	B	405	ASP
2	B	415	THR
2	B	424	LYS
2	B	428	ASP
2	B	432	CYS
2	B	478	THR
1	C	31	LYS
1	C	134	ASN
1	C	139	GLN
1	C	345	HIS
1	C	359	LEU
1	C	534	LYS
1	C	535	HIS
1	C	536	GLU
1	C	541	LYS
2	D	367	VAL
2	D	369	TYR
2	D	371	SER
2	D	375	SER
2	D	382	VAL

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Mol	Chain	Res	Type
2	D	385	THR
2	D	387	LEU
2	D	388	ASN
2	D	399	SER
2	D	402	VAL
2	D	407	VAL
2	D	408	ARG
2	D	415	THR
2	D	427	ASP
2	D	428	ASP
2	D	430	THR
2	D	434	ILE
2	D	445	THR
2	D	465	GLU
2	D	472	ILE
2	D	478	THR
2	D	494	ARG
2	D	500	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	GLN
1	A	531	GLN
1	A	535	HIS
1	C	134	ASN
1	C	526	GLN
1	C	531	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 monosaccharides in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	597/597 (100%)	-0.05	10 (1%) 70 57	41, 57, 89, 112	0
1	C	597/597 (100%)	-0.13	7 (1%) 79 67	36, 51, 85, 120	0
2	B	188/194 (96%)	0.31	10 (5%) 26 14	44, 58, 106, 121	0
2	D	184/194 (94%)	0.28	10 (5%) 25 14	48, 64, 100, 112	0
All	All	1566/1582 (98%)	0.00	37 (2%) 59 44	36, 56, 96, 121	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	370	ASN	4.5
2	B	333	THR	4.0
1	C	137	ASN	4.0
1	C	135	PRO	3.9
2	D	368	LEU	3.9
1	C	136	ASP	3.8
2	D	363	ALA	3.6
1	A	341	LYS	3.2
1	C	134	ASN	3.0
2	D	366	SER	3.0
1	A	336	PRO	2.8
1	A	20	THR	2.8
2	B	392	PHE	2.6
1	A	19	SER	2.6
1	C	138	PRO	2.6
2	D	367	VAL	2.6
2	B	387	LEU	2.6
2	D	362	VAL	2.5
2	D	524	VAL	2.4
2	D	365	TYR	2.4
1	A	291	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	395	VAL	2.4
1	C	615	ASP	2.4
1	A	21	ILE	2.3
1	A	424	LEU	2.3
2	D	369	TYR	2.3
1	A	302	TRP	2.2
1	A	83	TYR	2.2
2	B	360	ASN	2.1
2	B	370	ASN	2.1
2	B	515	PHE	2.1
2	B	365	TYR	2.1
2	B	522	ALA	2.0
1	A	61	ASN	2.0
1	C	338	ASN	2.0
2	D	487	ASN	2.0
2	B	369	TYR	2.0

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 monosaccharides in this entry.

6.4 Ligands [i](#)

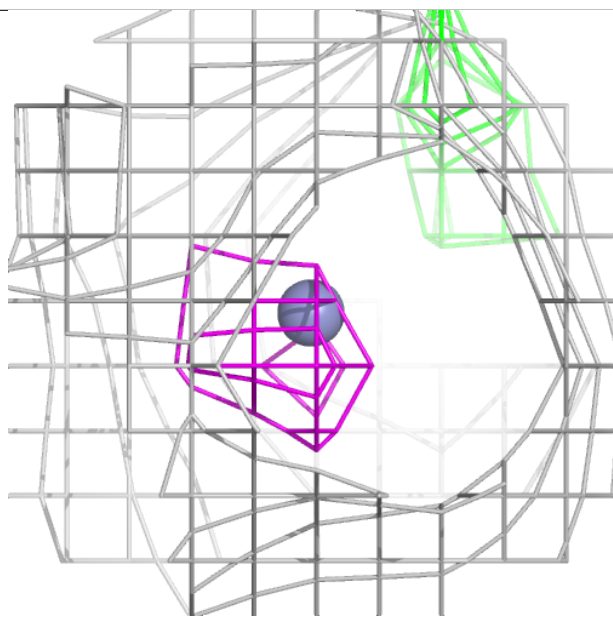
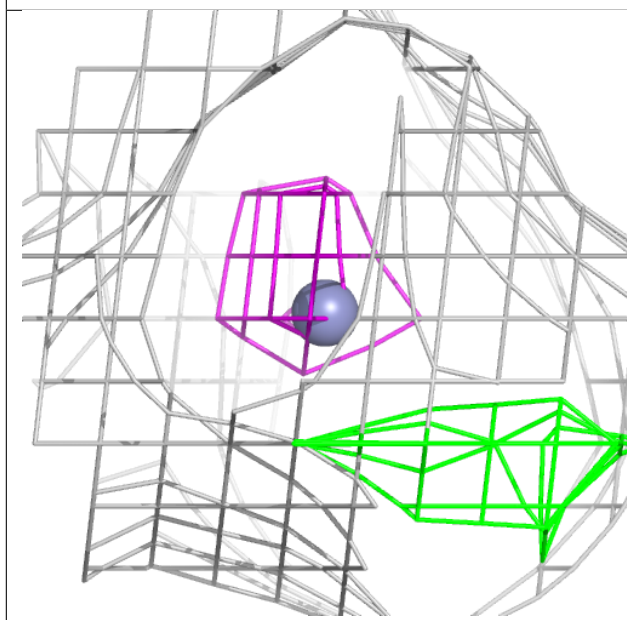
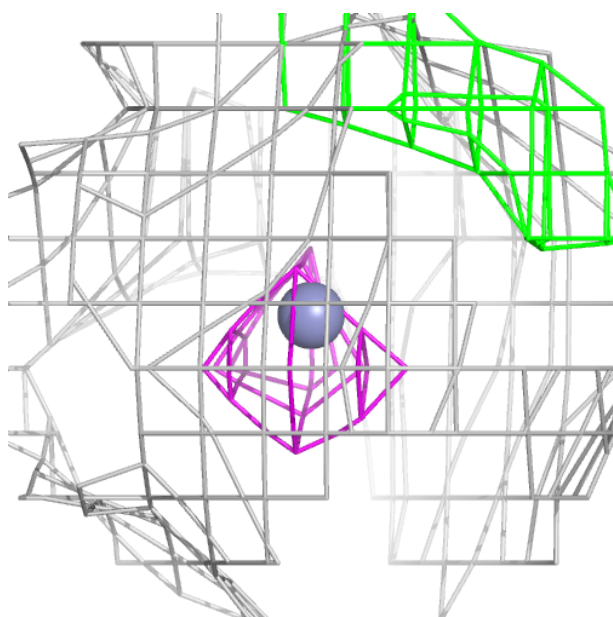
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

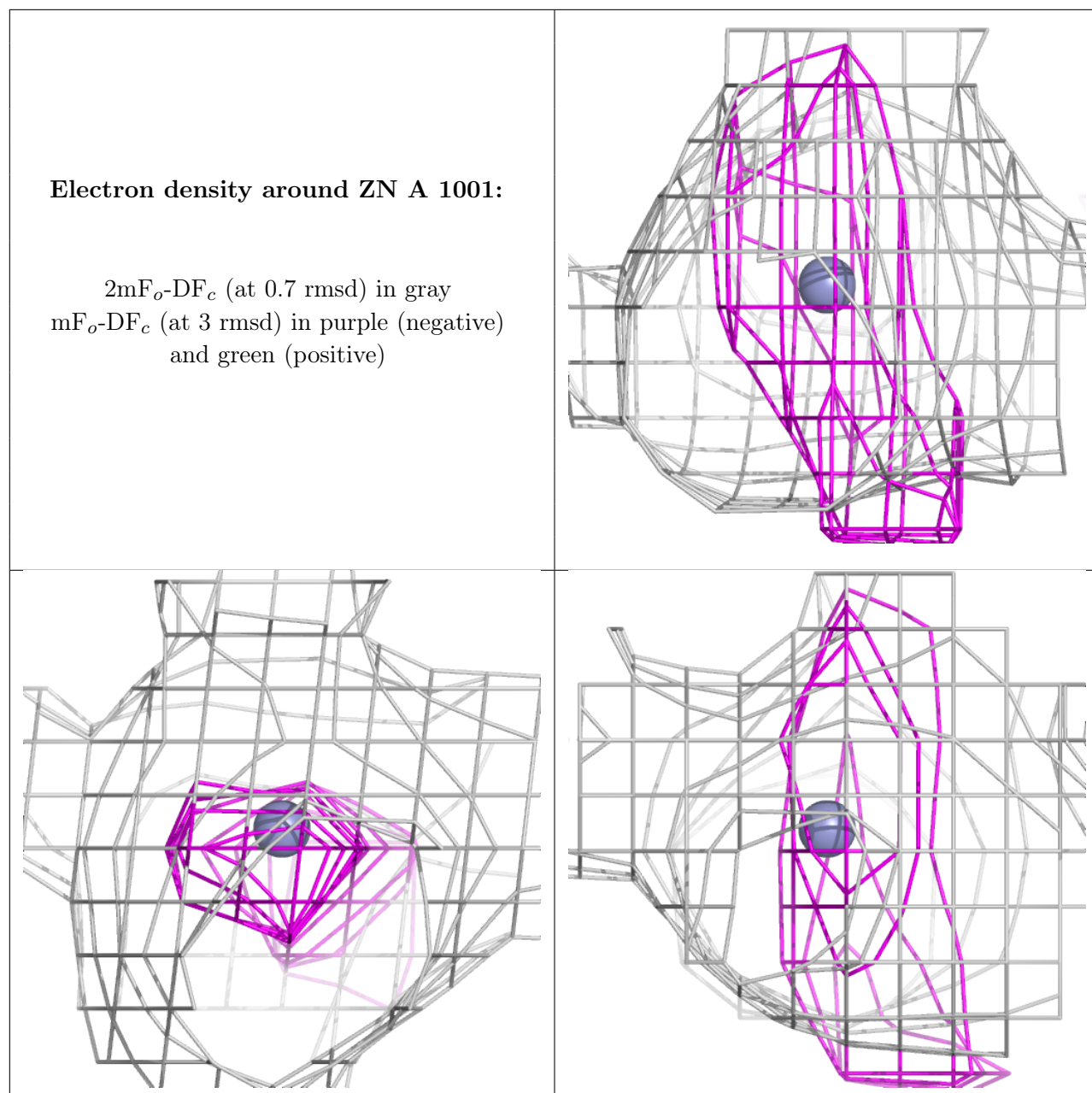
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	ZN	C	1001	1/1	0.89	0.06	68,68,68,68	0
3	ZN	A	1001	1/1	0.98	0.05	84,84,84,84	0

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 ZN C 1001:

$2mF_o-DF_c$ (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.