



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:49 AM UTC

PDB ID : 7VIB / pdb_00007vib
Title : Crystal structure of human ACE2 and GX/P2V RBD
Authors : Guo, Y.; Cao, W.; Jia, N.; Wang, W.; Yuan, S.; Wang, Y.
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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
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

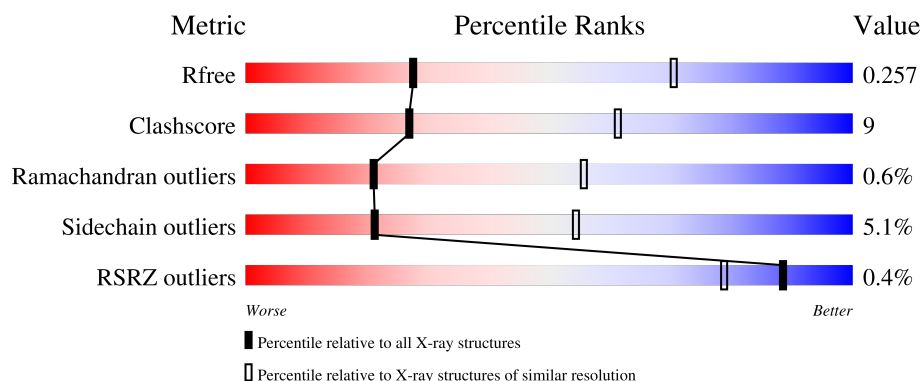
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (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	 76% 22% .
1	C	597	 73% 26% .
2	B	194	 67% 28% . .
2	D	194	 66% 21% 7% . 5%

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
1	A	597	Total	C	N	O	S	0	1	0
			4877	3120	808	920	29			
1	C	597	Total	C	N	O	S	0	1	0
			4877	3120	808	920	29			

- Molecule 2 is a protein called Spike glycoprotein.

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

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

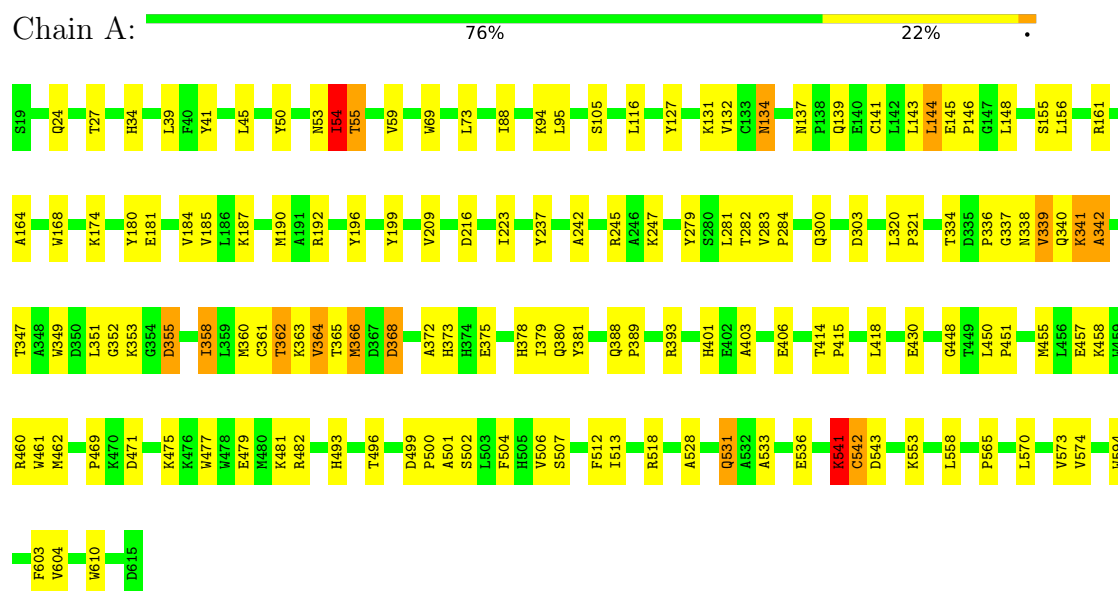
- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

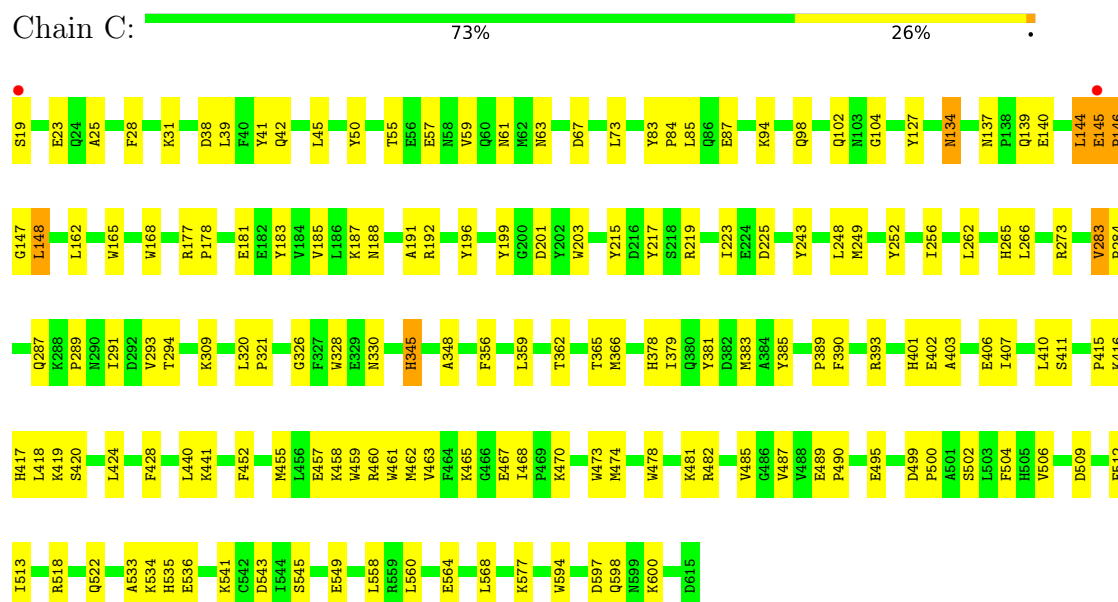
3 Residue-property plots

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.

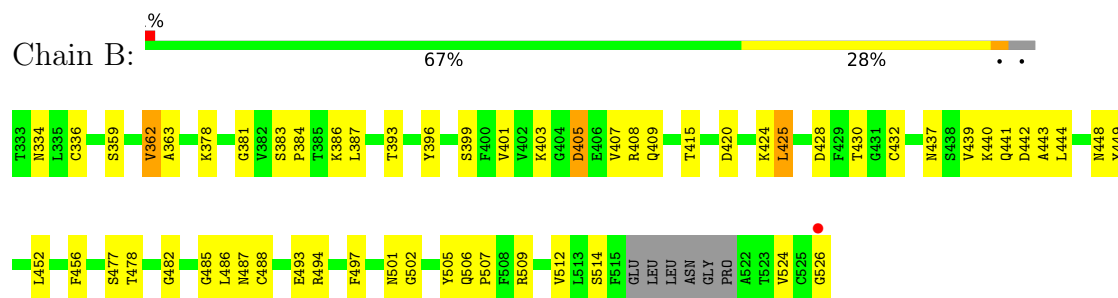
• Molecule 1: Angiotensin-converting enzyme 2



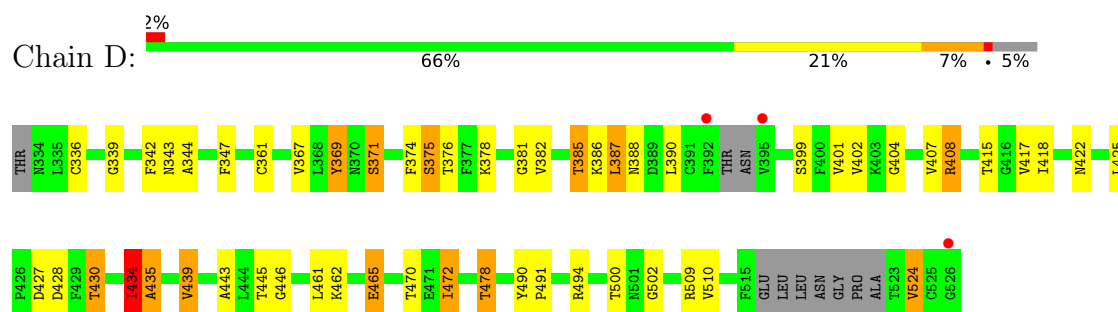
• Molecule 1: Angiotensin-converting enzyme 2



- 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 47.29 – 3.20	Depositor EDS
% Data completeness (in resolution range)	75.6 (47.29-3.20) 84.2 (47.29-3.20)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.204 , 0.258 0.209 , 0.257	Depositor DCC
R_{free} test set	2000 reflections (5.85%)	wwPDB-VP
Wilson B-factor (Å ²)	62.2	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 21.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	12701	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage'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	0.70	6/5018 (0.1%)	0.85	17/6818 (0.2%)
1	C	0.68	2/5018 (0.0%)	0.80	10/6818 (0.1%)
2	B	1.03	7/1526 (0.5%)	0.98	6/2074 (0.3%)
2	D	1.46	8/1498 (0.5%)	1.21	14/2033 (0.7%)
All	All	0.86	23/13060 (0.2%)	0.90	47/17743 (0.3%)

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	430	THR	C-N	-9.43	1.23	1.33
2	D	478	THR	C-N	8.63	1.45	1.33
1	A	358	ILE	C-N	-8.30	1.21	1.33
2	D	381	GLY	C-N	7.99	1.44	1.33
2	D	434	ILE	C-N	7.32	1.42	1.33
2	B	482	GLY	C-N	7.19	1.44	1.33
1	A	542	CYS	CA-C	-7.03	1.43	1.53
2	B	430	THR	C-N	-6.63	1.23	1.33
1	C	283	VAL	CA-C	-6.56	1.46	1.52
2	B	486	LEU	C-N	6.45	1.42	1.33
2	D	478	THR	CA-C	-6.44	1.47	1.52
2	B	334	ASN	C-N	6.40	1.42	1.33
1	A	355	ASP	CA-C	-6.11	1.45	1.52
1	A	541	LYS	C-N	-6.06	1.25	1.33
2	B	420	ASP	CA-C	-5.62	1.45	1.52
1	A	528	ALA	CA-C	-5.50	1.45	1.52
2	D	502	GLY	CA-C	-5.22	1.47	1.52
1	C	345	HIS	C-N	5.19	1.39	1.33
2	D	371	SER	CA-C	-5.09	1.46	1.52
2	B	359	SER	C-N	5.09	1.39	1.33
1	A	533	ALA	CA-C	-5.07	1.46	1.52
2	B	405	ASP	CA-C	-5.07	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	386	LYS	CA-C	-5.07	1.46	1.52

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	373	HIS	N-CA-C	-11.32	98.07	112.90
1	C	287	GLN	N-CA-C	-10.12	98.67	112.94
1	A	341	LYS	N-CA-C	9.50	123.04	110.88
1	C	50	TYR	N-CA-C	-8.51	101.36	112.68
1	A	372	ALA	N-CA-C	-8.47	101.77	114.64
1	A	366	MET	N-CA-C	-8.34	103.23	113.41
1	C	362	THR	N-CA-C	8.06	121.98	109.96
1	A	336	PRO	N-CA-C	-7.68	102.48	113.47
2	D	404	GLY	N-CA-C	7.61	122.12	112.83
1	A	531	GLN	N-CA-C	-7.57	104.28	113.97
1	A	144	LEU	N-CA-C	-7.54	102.41	111.69
1	A	533	ALA	N-CA-C	-7.40	103.34	112.88
2	D	371	SER	N-CA-C	-7.31	102.63	112.94
1	A	134	ASN	N-CA-C	7.00	118.89	110.07
1	C	145	GLU	CA-C-N	-7.00	111.08	119.84
1	C	145	GLU	C-N-CA	-7.00	111.08	119.84
2	D	462	LYS	CA-C-N	-6.93	112.62	119.76
2	D	462	LYS	C-N-CA	-6.93	112.62	119.76
1	A	300	GLN	N-CA-C	-6.70	104.69	112.92
2	D	524	VAL	N-CA-C	6.47	115.65	106.53
1	C	533	ALA	N-CA-C	-6.45	105.04	113.17
2	D	375	SER	N-CA-C	-6.42	105.19	114.12
1	A	368	ASP	N-CA-C	-6.41	105.38	113.72
1	A	145	GLU	CA-C-N	-6.41	111.83	119.84
1	A	145	GLU	C-N-CA	-6.41	111.83	119.84
2	D	361	CYS	N-CA-C	6.21	118.75	108.99
2	D	336	CYS	N-CA-C	6.17	117.47	109.64
1	A	342	ALA	N-CA-C	6.12	123.83	110.80
2	D	435	ALA	N-CA-C	6.07	118.30	109.07
2	B	477	SER	N-CA-C	-6.07	105.46	112.92
2	B	334	ASN	CA-C-N	-5.98	113.74	122.65
2	B	334	ASN	C-N-CA	-5.98	113.74	122.65
2	B	420	ASP	N-CA-C	-5.93	106.08	113.55
1	C	148	LEU	N-CA-C	-5.77	104.96	112.23
2	D	408	ARG	N-CA-C	-5.67	106.52	113.50
1	C	144	LEU	N-CA-C	-5.62	105.30	111.82
2	B	425	LEU	CA-C-N	-5.61	114.97	120.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	425	LEU	C-N-CA	-5.61	114.97	120.52
1	A	362	THR	N-CA-C	5.60	117.86	108.96
1	C	134	ASN	CA-C-N	-5.48	112.98	119.84
1	C	134	ASN	C-N-CA	-5.48	112.98	119.84
1	A	349	TRP	N-CA-C	5.48	117.33	108.34
2	D	374	PHE	N-CA-C	-5.37	100.91	109.23
2	D	386	LYS	N-CA-C	-5.28	106.14	112.59
2	D	385	THR	N-CA-C	5.21	120.28	113.30
2	D	446	GLY	N-CA-C	-5.11	101.06	113.18
1	A	337	GLY	CA-C-O	-5.09	114.64	122.52

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	4877	0	4650	82	0
1	C	4877	0	4650	109	0
2	B	1486	0	1418	25	0
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	227	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 (227) 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	1.66	0.76
1:C:460:ARG:NH2	1:C:506:VAL:HA	2.01	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:462:MET:HE3	1:C:468:ILE:HD11	1.71	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:455:MET:HE1	1:A:481:LYS:HE2	1.76	0.66
1:C:455:MET:HE2	1:C:481:LYS:HD2	1.77	0.65
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:549:GLU:CD	1:C:549:GLU:H	2.15	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:A:455:MET:HE1	1:A:481:LYS:CE	2.36	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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:459:TRP:O	1:C:463:VAL:HG23	2.13	0.48
1:A:53:ASN:O	1:A:54:ILE:C	2.57	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:C:201:ASP:CG	1:C:219:ARG:HE	2.21	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:C:217:TYR:OH	1:C:225:ASP:OD2	2.30	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
1:C:543:ASP:C	1:C:545:SER:H	2.23	0.46
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:360:MET:HE2	1:A:360:MET:HB2	1.82	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
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:549:GLU:CD	1:C:549:GLU:N	2.77	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
1:C:389:PRO:O	1:C:390:PHE:C	2.62	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:102:GLN:C	1:C:104:GLY:N	2.79	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:C:440:LEU:HD23	1:C:440:LEU:C	2.45	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
1:C:459:TRP:CH2	1:C:500:PRO:HG2	2.55	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:A:352:GLY:O	1:A:353:LYS:C	2.63	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	12	45
1	C	596/597 (100%)	547 (92%)	46 (8%)	3 (0%)	24	59
2	B	184/194 (95%)	170 (92%)	13 (7%)	1 (0%)	24	59
2	D	178/194 (92%)	162 (91%)	16 (9%)	0	100	100
All	All	1554/1582 (98%)	1432 (92%)	112 (7%)	10 (1%)	21	56

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 ⓘ

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%)	512 (97%)	16 (3%)	36	66
1	C	528/527 (100%)	518 (98%)	10 (2%)	50	73
2	B	162/167 (97%)	147 (91%)	15 (9%)	8	33
2	D	159/167 (95%)	130 (82%)	29 (18%)	2	9
All	All	1377/1388 (99%)	1307 (95%)	70 (5%)	21	54

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	ILE
1	A	55	THR
1	A	144	LEU
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

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Mol	Chain	Res	Type
1	A	368	ASP
1	A	531	GLN
1	A	536	GLU
1	A	541	LYS
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	407	VAL
2	B	415	THR
2	B	424	LYS
2	B	428	ASP
2	B	432	CYS
2	B	478	THR
2	B	524	VAL
1	C	31	LYS
1	C	134	ASN
1	C	139	GLN
1	C	283	VAL
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
2	D	385	THR
2	D	387	LEU
2	D	388	ASN
2	D	390	LEU
2	D	399	SER
2	D	402	VAL
2	D	407	VAL
2	D	408	ARG

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Mol	Chain	Res	Type
2	D	415	THR
2	D	417	VAL
2	D	427	ASP
2	D	428	ASP
2	D	430	THR
2	D	434	ILE
2	D	439	VAL
2	D	445	THR
2	D	465	GLU
2	D	470	THR
2	D	472	ILE
2	D	478	THR
2	D	494	ARG
2	D	500	THR
2	D	510	VAL
2	D	524	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	ASN
1	A	61	ASN
1	A	81	GLN
1	A	195	HIS
1	A	221	GLN
1	A	239	HIS
1	A	531	GLN
1	A	535	HIS
1	A	540	HIS
1	A	572	ASN
1	A	599	ASN
2	B	370	ASN
2	B	388	ASN
2	B	483	GLN
1	C	58	ASN
1	C	98	GLN
1	C	134	ASN
1	C	154	ASN
1	C	325	GLN
1	C	526	GLN
1	C	531	GLN
1	C	540	HIS

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Mol	Chain	Res	Type
2	D	370	ASN
2	D	441	GLN
2	D	501	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 [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	597/597 (100%)	0.03	0 100 100	38, 57, 89, 112	1 (0%)
1	C	597/597 (100%)	-0.10	2 (0%) 90 81	36, 51, 85, 120	1 (0%)
2	B	188/194 (96%)	0.20	1 (0%) 87 76	44, 58, 106, 121	0
2	D	184/194 (94%)	0.40	3 (1%) 70 51	48, 64, 100, 112	0
All	All	1566/1582 (98%)	0.04	6 (0%) 88 79	36, 56, 96, 121	2 (0%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	526	GLY	3.1
2	D	392	PHE	3.1
2	D	395	VAL	2.4
1	C	145	GLU	2.1
1	C	19	SER	2.1
2	D	526	GLY	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 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,

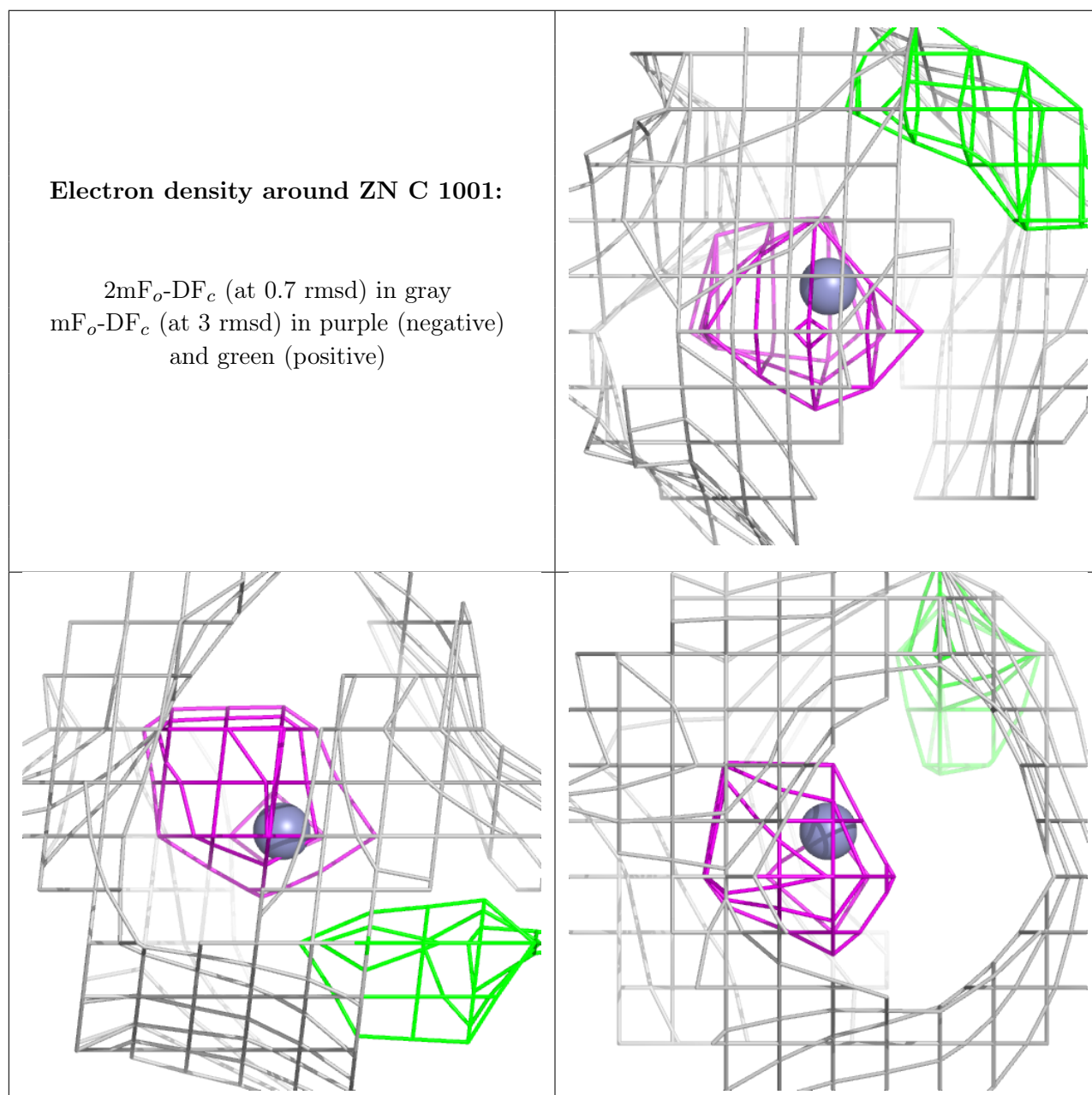
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ZN	C	1001	1/1	0.84	0.12	68,68,68,68	0
3	ZN	A	1001	1/1	0.96	0.16	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.

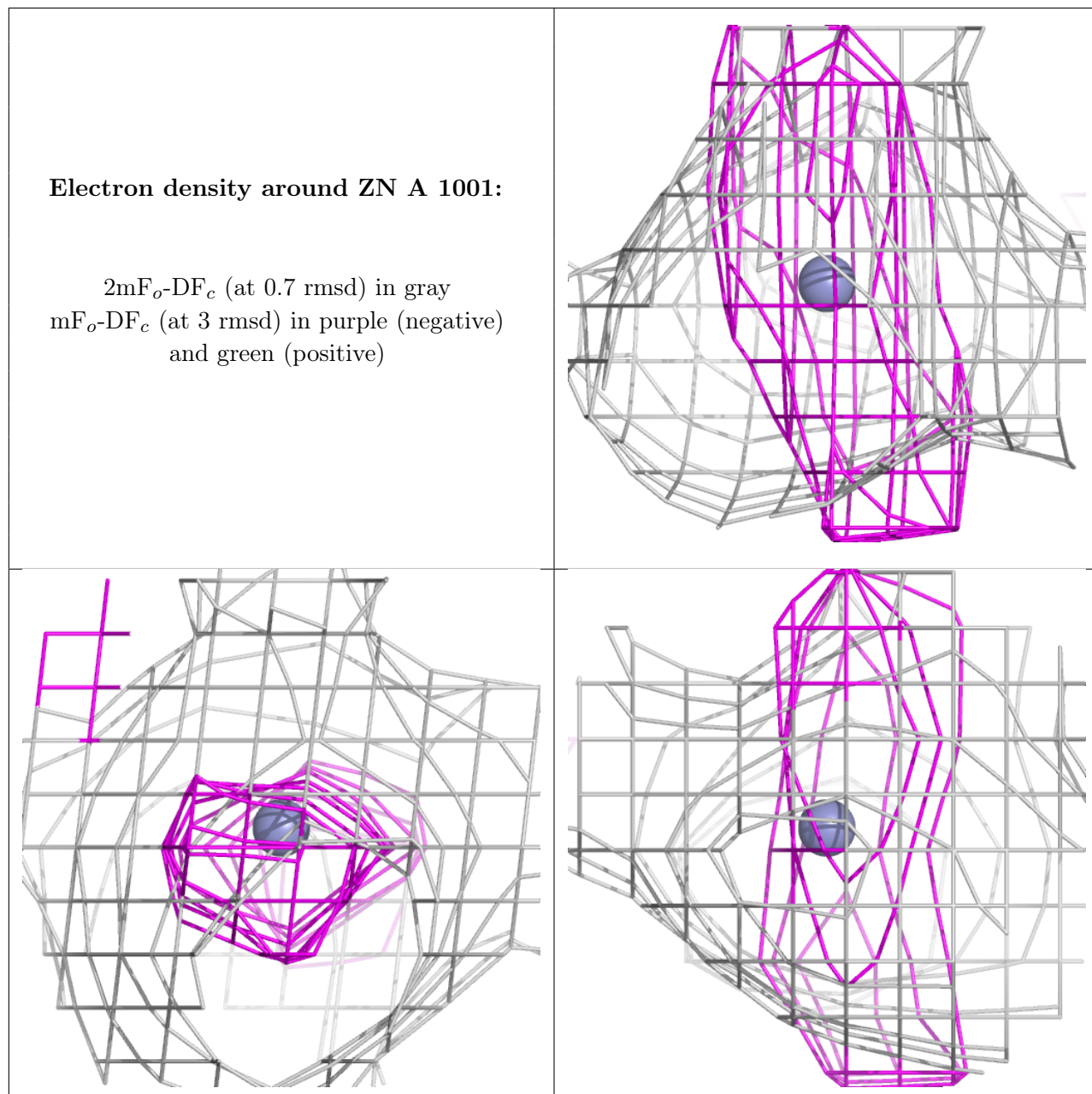
Electron density around ZN C 1001:

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



Electron density around ZN A 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 ⓘ

There are no such residues in this entry.