



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:10 PM UTC

PDB ID : 7MXG / pdb_00007mxg
Title : PRMT5(M420T mutant):MEP50 complexed with inhibitor PF-06855800
Authors : McTigue, M.; Deng, Y.L.; Liu, W.; Brooun, A.
Deposited on : 2021-05-19
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

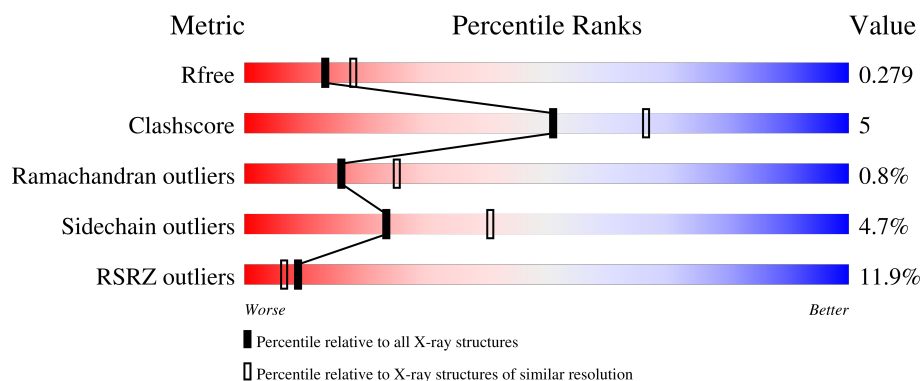
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	637	9% 81% 15% ..
1	C	637	7% 83% 14% ..
2	B	366	12% 67% 14% . 19%
2	D	366	20% 66% 13% . 18%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15557 atoms, of which 32 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 Protein arginine N-methyltransferase 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	625	Total	C	N	O	S	0	1	0
			5068	3241	870	933	24			
1	C	625	Total	C	N	O	S	0	1	0
			5068	3241	870	933	24			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	420	THR	MET	engineered mutation	UNP O14744
C	420	THR	MET	engineered mutation	UNP O14744

- Molecule 2 is a protein called Methylosome protein 50.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	298	Total	C	N	O	S	0	0	0
			2261	1419	387	444	11			
2	D	299	Total	C	N	O	S	0	0	0
			2269	1424	388	445	12			

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-23	MET	-	expression tag	UNP Q9BQA1
B	-22	ALA	-	expression tag	UNP Q9BQA1
B	-21	SER	-	expression tag	UNP Q9BQA1
B	-20	HIS	-	expression tag	UNP Q9BQA1
B	-19	HIS	-	expression tag	UNP Q9BQA1
B	-18	HIS	-	expression tag	UNP Q9BQA1
B	-17	HIS	-	expression tag	UNP Q9BQA1
B	-16	HIS	-	expression tag	UNP Q9BQA1
B	-15	HIS	-	expression tag	UNP Q9BQA1
B	-14	ASP	-	expression tag	UNP Q9BQA1

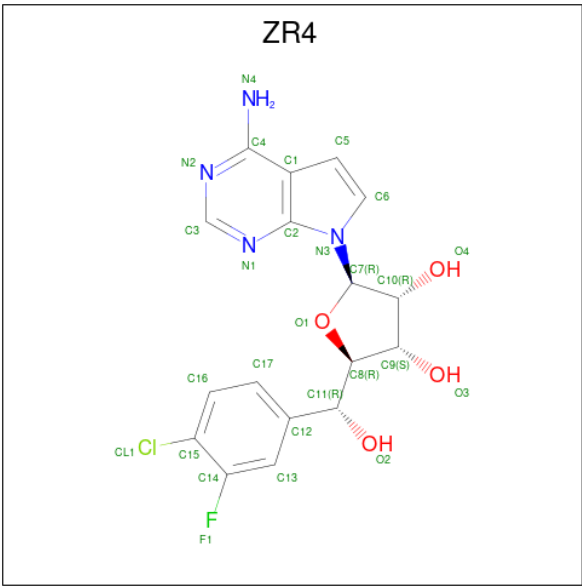
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-13	TYR	-	expression tag	UNP Q9BQA1
B	-12	ASP	-	expression tag	UNP Q9BQA1
B	-11	GLY	-	expression tag	UNP Q9BQA1
B	-10	ALA	-	expression tag	UNP Q9BQA1
B	-9	THR	-	expression tag	UNP Q9BQA1
B	-8	THR	-	expression tag	UNP Q9BQA1
B	-7	GLU	-	expression tag	UNP Q9BQA1
B	-6	ASN	-	expression tag	UNP Q9BQA1
B	-5	LEU	-	expression tag	UNP Q9BQA1
B	-4	TYR	-	expression tag	UNP Q9BQA1
B	-3	PHE	-	expression tag	UNP Q9BQA1
B	-2	GLN	-	expression tag	UNP Q9BQA1
B	-1	GLY	-	expression tag	UNP Q9BQA1
B	0	SER	-	expression tag	UNP Q9BQA1
B	1	LEU	-	expression tag	UNP Q9BQA1
D	-23	MET	-	expression tag	UNP Q9BQA1
D	-22	ALA	-	expression tag	UNP Q9BQA1
D	-21	SER	-	expression tag	UNP Q9BQA1
D	-20	HIS	-	expression tag	UNP Q9BQA1
D	-19	HIS	-	expression tag	UNP Q9BQA1
D	-18	HIS	-	expression tag	UNP Q9BQA1
D	-17	HIS	-	expression tag	UNP Q9BQA1
D	-16	HIS	-	expression tag	UNP Q9BQA1
D	-15	HIS	-	expression tag	UNP Q9BQA1
D	-14	ASP	-	expression tag	UNP Q9BQA1
D	-13	TYR	-	expression tag	UNP Q9BQA1
D	-12	ASP	-	expression tag	UNP Q9BQA1
D	-11	GLY	-	expression tag	UNP Q9BQA1
D	-10	ALA	-	expression tag	UNP Q9BQA1
D	-9	THR	-	expression tag	UNP Q9BQA1
D	-8	THR	-	expression tag	UNP Q9BQA1
D	-7	GLU	-	expression tag	UNP Q9BQA1
D	-6	ASN	-	expression tag	UNP Q9BQA1
D	-5	LEU	-	expression tag	UNP Q9BQA1
D	-4	TYR	-	expression tag	UNP Q9BQA1
D	-3	PHE	-	expression tag	UNP Q9BQA1
D	-2	GLN	-	expression tag	UNP Q9BQA1
D	-1	GLY	-	expression tag	UNP Q9BQA1
D	0	SER	-	expression tag	UNP Q9BQA1
D	1	LEU	-	expression tag	UNP Q9BQA1

- Molecule 3 is 7-[(5R)-5-C-(4-chloro-3-fluorophenyl)-beta-D-ribofuranosyl]-7H-pyrrolo[2,3-d]pyrimidin-4-amine (CCD ID: ZR4) (formula: C₁₇H₁₆ClFN₄O₄) (labeled as "Ligand of

Interest" by depositor).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
			Total	C	Cl	F	H	N	O		
3	A	1	43	17	1	1	16	4	4	16	0
3	C	1	43	17	1	1	16	4	4	16	0

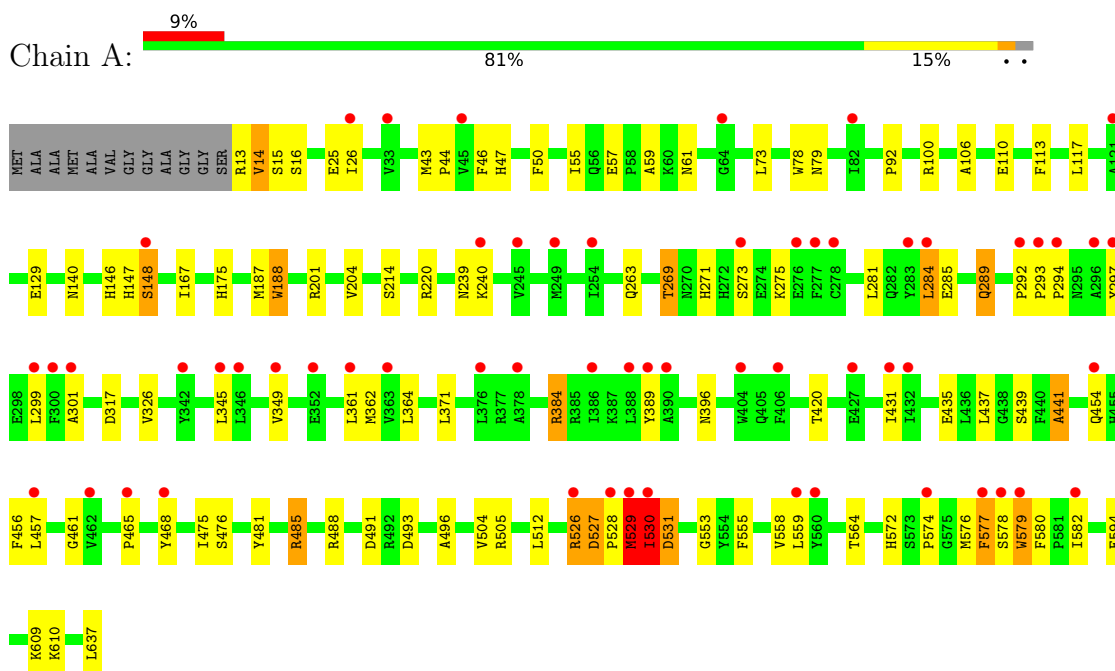
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	256	Total	O	0	0
			256	256		
4	B	85	Total	O	0	0
			85	85		
4	C	348	Total	O	0	0
			348	348		
4	D	116	Total	O	0	0
			116	116		

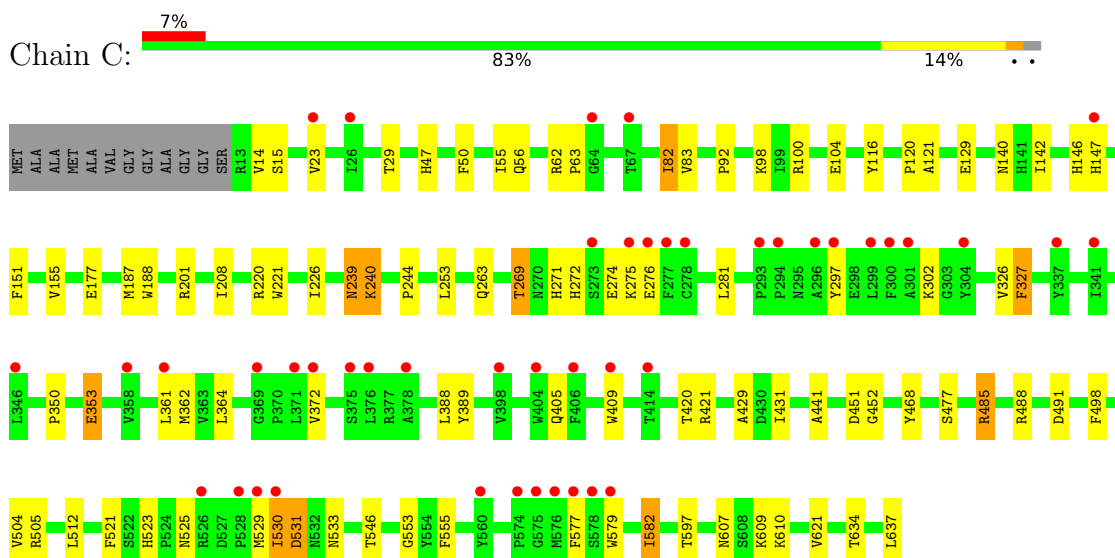
3 Residue-property plots [i](#)

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.

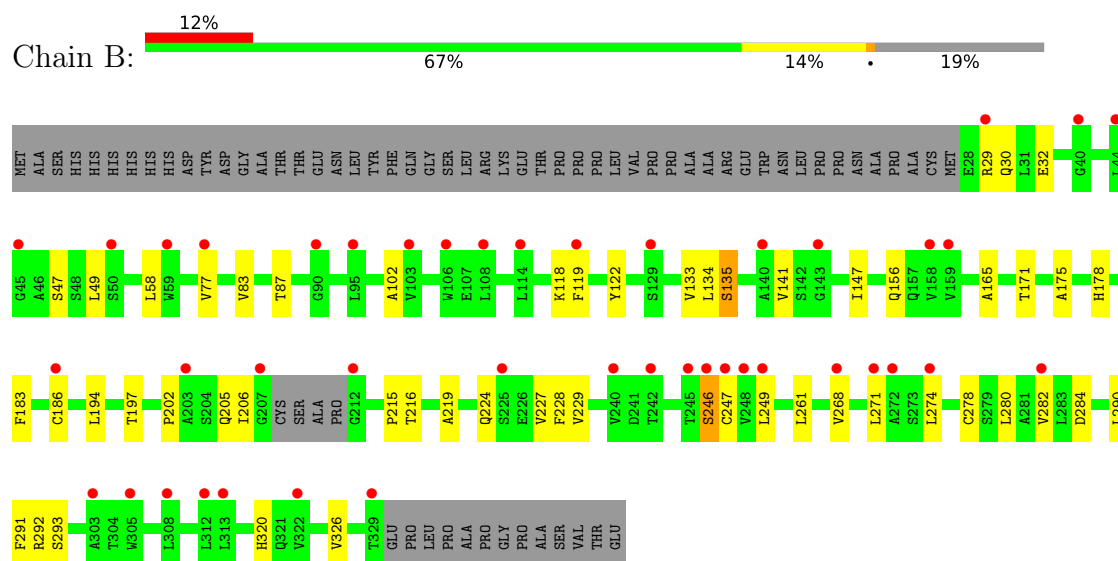
• Molecule 1: Protein arginine N-methyltransferase 5



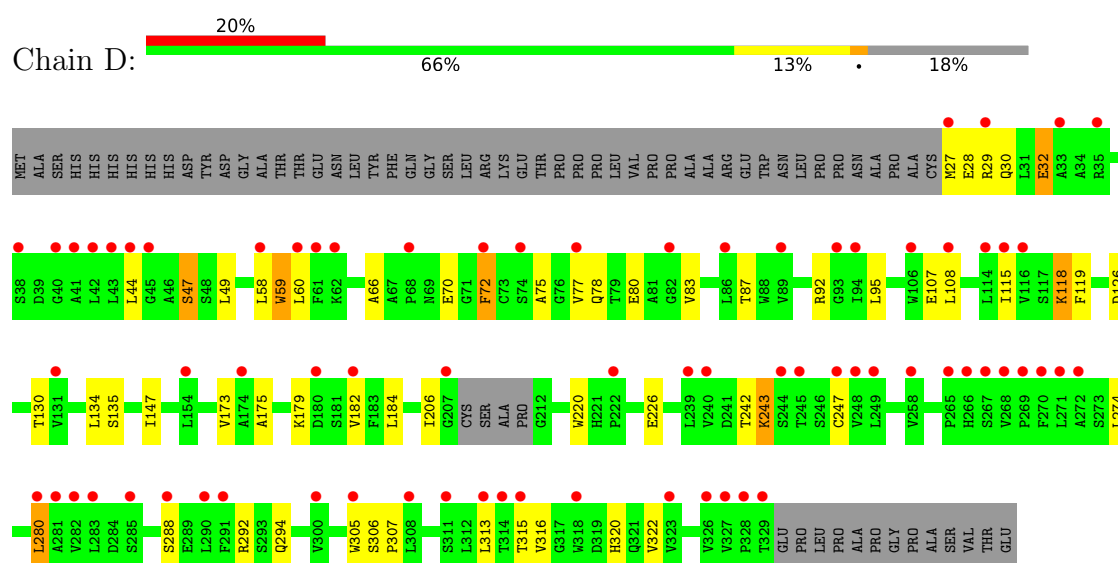
• Molecule 1: Protein arginine N-methyltransferase 5



● Molecule 2: Methylosome protein 50



● Molecule 2: Methylosome protein 50



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	98.41Å 138.45Å 178.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	109.39 – 2.40 109.39 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (109.39-2.40) 99.8 (109.39-2.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.68 (at 2.40Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.227 , 0.282 0.224 , 0.279	Depositor DCC
R_{free} test set	4716 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	45.5	Xtriage
Anisotropy	0.923	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 65.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15557	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 35.94 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.3984e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZR4

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	0.75	0/5210	1.05	9/7088 (0.1%)
1	C	0.76	1/5210 (0.0%)	1.09	13/7088 (0.2%)
2	B	0.71	0/2313	1.06	1/3157 (0.0%)
2	D	0.76	0/2321	1.16	6/3167 (0.2%)
All	All	0.75	1/15054 (0.0%)	1.08	29/20500 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	276	GLU	CA-C	5.38	1.59	1.52

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	126	ASP	CA-CB-CG	6.99	119.59	112.60
1	C	529	MET	CA-C-N	6.97	134.52	121.97
1	C	529	MET	C-N-CA	6.97	134.52	121.97
2	B	119	PHE	CA-CB-CG	5.90	119.70	113.80
2	D	119	PHE	CA-CB-CG	5.57	119.37	113.80
1	C	327	PHE	CA-CB-CG	-5.52	108.28	113.80
1	A	188	TRP	CA-C-N	5.46	127.87	120.44
1	A	188	TRP	C-N-CA	5.46	127.87	120.44
2	D	72	PHE	CA-CB-CG	5.36	119.16	113.80
2	D	28	GLU	CA-C-N	5.36	128.20	120.38
2	D	28	GLU	C-N-CA	5.36	128.20	120.38
1	C	607	ASN	CA-CB-CG	5.34	117.94	112.60
1	C	146	HIS	CA-C-N	5.30	131.67	121.54
1	C	146	HIS	C-N-CA	5.30	131.67	121.54
1	A	55	ILE	N-CA-C	5.28	115.79	111.62
1	A	239	ASN	CA-CB-CG	5.24	117.84	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	148	SER	CA-C-N	5.24	130.69	122.21
1	A	148	SER	C-N-CA	5.24	130.69	122.21
1	C	239	ASN	CA-CB-CG	5.22	117.82	112.60
1	C	151	PHE	CA-CB-CG	-5.22	108.58	113.80
1	A	204	VAL	N-CA-C	5.20	115.79	108.36
1	C	409	TRP	N-CA-C	5.19	116.75	111.14
2	D	59	TRP	N-CA-C	5.15	116.72	107.80
1	A	79	ASN	CA-CB-CG	5.10	117.70	112.60
1	C	82	ILE	N-CA-C	5.06	115.26	108.17
1	A	317	ASP	CA-CB-CG	5.04	117.64	112.60
1	C	451	ASP	CA-CB-CG	5.03	117.63	112.60
1	C	353	GLU	CA-C-N	5.02	127.70	120.38
1	C	353	GLU	C-N-CA	5.02	127.70	120.38

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	5068	0	4958	59	0
1	C	5068	0	4958	46	0
2	B	2261	0	2180	24	0
2	D	2269	0	2189	29	0
3	A	27	16	0	0	0
3	C	27	16	0	2	0
4	A	256	0	0	0	0
4	B	85	0	0	0	0
4	C	348	0	0	1	0
4	D	116	0	0	1	0
All	All	15525	32	14285	152	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 5.

All (152) 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:194:LEU:HB2	2:B:206:ILE:HD11	1.46	0.95
1:A:129:GLU:HG3	1:A:187[B]:MET:HE1	1.52	0.90
1:C:140:ASN:HB3	4:C:1048:HOH:O	1.70	0.89
1:C:269:THR:HG22	1:C:271:HIS:CE1	2.08	0.89
1:A:147:HIS:CD2	1:A:201:ARG:HH12	1.95	0.84
2:D:226:GLU:HG3	2:D:243:LYS:HZ2	1.47	0.79
1:C:142:ILE:O	1:C:147:HIS:CE1	2.43	0.71
1:A:364:LEU:HB3	1:A:420:THR:HG21	1.74	0.69
1:C:129:GLU:HG3	1:C:187[B]:MET:HE1	1.76	0.68
2:D:29:ARG:HD2	2:D:320:HIS:HB2	1.75	0.66
2:D:32:GLU:HG2	2:D:83:VAL:O	1.96	0.65
2:D:66:ALA:HB1	2:D:72:PHE:HB3	1.79	0.65
1:C:441:ALA:HB2	1:C:555:PHE:HB2	1.79	0.64
2:D:30:GLN:HG2	2:D:49:LEU:HD12	1.80	0.63
1:A:269:THR:HG22	1:A:271:HIS:NE2	2.13	0.63
1:A:441:ALA:HB2	1:A:555:PHE:HB2	1.80	0.62
2:B:284:ASP:HB3	2:B:290:LEU:HD11	1.81	0.62
2:D:226:GLU:HB2	2:D:243:LYS:HZ3	1.63	0.62
1:A:26:ILE:HD12	1:A:43:MET:HE1	1.82	0.60
1:A:285:GLU:O	1:A:289:GLN:HG2	2.02	0.60
1:C:610:LYS:HD2	1:C:634:THR:HB	1.84	0.59
2:D:305:TRP:CD2	2:D:313:LEU:HD13	2.38	0.58
1:A:361:LEU:HD11	1:A:431:ILE:HD12	1.83	0.58
1:A:92:PRO:O	1:A:100:ARG:HG3	2.02	0.58
1:C:421:ARG:HG2	1:C:452:GLY:HA3	1.84	0.58
1:C:100:ARG:O	1:C:104:GLU:HG3	2.03	0.57
2:B:58:LEU:HB2	2:B:77:VAL:HG12	1.86	0.57
1:C:239:ASN:HB2	1:C:240:LYS:HE3	1.86	0.57
2:B:282:VAL:HB	2:B:291:PHE:HB3	1.86	0.56
2:B:32:GLU:HG2	2:B:83:VAL:O	2.04	0.56
1:C:23:VAL:HG22	1:C:29:THR:HG21	1.86	0.56
1:C:364:LEU:HB3	1:C:420:THR:HG21	1.87	0.56
2:D:305:TRP:CE2	2:D:313:LEU:HD13	2.41	0.56
1:A:106:ALA:O	1:A:110:GLU:HG3	2.06	0.55
2:B:102:ALA:HB2	2:B:122:TYR:CD2	2.42	0.54
1:A:15:SER:HB3	1:A:263:GLN:HG2	1.89	0.54
1:A:371:LEU:HD11	1:A:435:GLU:HB2	1.90	0.54
1:A:147:HIS:CD2	1:A:201:ARG:NH1	2.73	0.54
1:A:609:LYS:O	1:A:637:LEU:HB2	2.08	0.53
2:B:134:LEU:HD23	2:B:175:ALA:HB1	1.90	0.52
1:A:530:ILE:HG22	1:A:531:ASP:H	1.75	0.52
1:C:553:GLY:HA3	1:C:582:ILE:HG22	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:345:LEU:HB3	1:A:384:ARG:HG3	1.92	0.52
1:C:372:VAL:HG13	1:C:388:LEU:HD13	1.92	0.52
1:C:297:TYR:HE2	1:C:505:ARG:NH1	2.08	0.52
2:B:134:LEU:HD23	2:B:175:ALA:CB	2.40	0.51
1:A:530:ILE:CG2	1:A:531:ASP:N	2.74	0.50
2:D:70:GLU:CD	2:D:70:GLU:H	2.19	0.50
1:C:83:VAL:HG22	1:C:121:ALA:HB3	1.93	0.50
1:C:187[B]:MET:HE2	1:C:188:TRP:HD1	1.75	0.50
1:C:525:ASN:HD21	1:C:530:ILE:HG12	1.76	0.50
1:A:362:MET:SD	1:A:456:PHE:CE1	3.05	0.50
1:C:92:PRO:O	1:C:100:ARG:HG3	2.11	0.50
1:C:147:HIS:HB3	1:C:201:ARG:NH2	2.26	0.50
1:A:530:ILE:CG2	1:A:531:ASP:H	2.25	0.50
2:D:60:LEU:HB3	2:D:75:ALA:HB3	1.93	0.50
2:D:32:GLU:HG3	4:D:414:HOH:O	2.12	0.49
1:C:82:ILE:O	1:C:120:PRO:HD2	2.12	0.49
1:A:47:HIS:HB3	1:A:50:PHE:HB2	1.95	0.49
1:A:579:TRP:H	1:A:579:TRP:CD1	2.28	0.49
1:A:16:SER:CB	1:A:281:LEU:HD11	2.43	0.48
2:D:226:GLU:HB2	2:D:243:LYS:NZ	2.27	0.48
2:B:280:LEU:O	2:B:292:ARG:HD2	2.13	0.48
1:C:50:PHE:CE1	1:C:62:ARG:NH1	2.81	0.48
1:A:14:VAL:HG21	1:A:284:LEU:HD22	1.96	0.48
1:C:56:GLN:HE22	1:C:98:LYS:HZ3	1.60	0.48
1:C:362:MET:HG2	1:C:389:TYR:HB2	1.94	0.48
2:D:130:THR:HG23	2:D:173:VAL:HG22	1.96	0.48
2:B:261:LEU:HD22	2:B:271:LEU:HD21	1.96	0.47
1:C:420:THR:HG23	3:C:701:ZR4:N2	2.29	0.47
1:C:361:LEU:HD11	1:C:431:ILE:HD12	1.95	0.47
2:D:179:LYS:HB2	2:D:182:VAL:HB	1.96	0.47
1:A:269:THR:HG22	1:A:271:HIS:CE1	2.49	0.47
1:C:47:HIS:HB3	1:C:50:PHE:HB2	1.97	0.47
1:C:297:TYR:CE2	1:C:505:ARG:NH1	2.82	0.46
1:A:577:PHE:CD1	1:A:577:PHE:N	2.78	0.46
1:A:187[B]:MET:CE	1:A:188:TRP:HD1	2.28	0.46
2:B:219:ALA:HB3	2:B:229:VAL:HG23	1.98	0.46
1:A:558:VAL:HA	1:A:564:THR:HG22	1.97	0.46
1:A:476:SER:HB2	1:A:512:LEU:HD21	1.98	0.46
1:C:56:GLN:NE2	1:C:98:LYS:NZ	2.63	0.46
1:A:269:THR:CG2	1:A:271:HIS:CE1	2.99	0.45
2:D:280:LEU:HD22	2:D:315:THR:HG21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:29:ARG:HA	2:D:320:HIS:ND1	2.32	0.45
2:B:87:THR:HG21	2:B:133:VAL:HG23	1.99	0.45
1:C:221:TRP:HB3	1:C:226:ILE:HD11	1.98	0.45
1:A:187[B]:MET:HE2	1:A:188:TRP:HD1	1.82	0.45
2:D:184:LEU:HG	2:D:220:TRP:CZ2	2.52	0.45
1:A:362:MET:SD	1:A:456:PHE:CD1	3.10	0.44
1:A:437:LEU:HD21	1:A:468:TYR:CD2	2.52	0.44
1:A:527:ASP:HA	1:A:528:PRO:HD3	1.92	0.44
2:B:175:ALA:HA	2:B:183:PHE:CB	2.48	0.44
1:A:396:ASN:HB3	1:C:116:TYR:CG	2.53	0.44
1:A:362:MET:HG2	1:A:389:TYR:HB2	2.00	0.44
2:B:206:ILE:HG21	2:B:228:PHE:HZ	1.83	0.44
1:A:73:LEU:HB2	1:A:78:TRP:CE2	2.54	0.43
1:A:465:PRO:HB3	1:A:559:LEU:HD23	1.99	0.43
2:B:280:LEU:HB3	2:B:293:SER:HB3	2.00	0.43
1:C:15:SER:OG	1:C:263:GLN:NE2	2.44	0.43
1:A:129:GLU:HG3	1:A:187[B]:MET:CE	2.37	0.43
1:C:350:PRO:HG2	1:C:353:GLU:HG3	2.01	0.43
1:A:44:PRO:HB2	1:A:46:PHE:O	2.18	0.43
1:A:297:TYR:OH	1:A:574:PRO:HA	2.18	0.43
1:A:439:SER:OG	1:A:580:PHE:O	2.29	0.43
1:A:488:ARG:HH22	1:C:491:ASP:CG	2.27	0.43
2:D:108:LEU:HD23	2:D:115:ILE:HG12	2.01	0.43
1:C:468:TYR:OH	1:C:523:HIS:NE2	2.46	0.43
1:A:57:GLU:HG2	1:A:61:ASN:HD21	1.83	0.42
1:C:208:ILE:HD12	1:C:253:LEU:HD21	2.00	0.42
1:A:553:GLY:HA3	1:A:582:ILE:HG22	2.00	0.42
2:D:58:LEU:HB2	2:D:77:VAL:HG12	2.00	0.42
1:A:167:ILE:HD11	2:B:165:ALA:HB2	2.01	0.42
2:D:44:LEU:HB2	2:D:59:TRP:HB2	2.01	0.42
2:D:306:SER:HA	2:D:307:PRO:HD3	1.95	0.42
2:B:135:SER:OG	2:B:178:HIS:HA	2.19	0.42
1:A:493:ASP:HB3	1:A:496:ALA:HB2	2.01	0.42
1:A:528:PRO:O	1:A:529:MET:HB3	2.20	0.42
1:A:293:PRO:HA	1:A:294:PRO:HD3	1.97	0.41
1:A:301:ALA:HB1	1:A:505:ARG:HG2	2.02	0.41
1:C:512:LEU:HD13	1:C:546:THR:HG21	2.02	0.41
1:A:349:VAL:O	1:A:384:ARG:NH1	2.53	0.41
2:B:87:THR:CG2	2:B:133:VAL:HG23	2.50	0.41
1:C:327:PHE:HB2	3:C:701:ZR4:CL1	2.57	0.41
2:D:27:MET:SD	2:D:320:HIS:HE1	2.42	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:30:GLN:HB2	2:D:47:SER:O	2.20	0.41
1:A:491:ASP:OD2	1:C:488:ARG:NH2	2.50	0.41
2:D:27:MET:HE2	2:D:59:TRP:CE2	2.55	0.41
2:D:134:LEU:HD23	2:D:175:ALA:HB1	2.01	0.41
1:A:491:ASP:CG	1:C:488:ARG:HH22	2.28	0.41
2:B:30:GLN:HG2	2:B:49:LEU:HD12	2.00	0.41
1:A:113:PHE:CE2	1:A:117:LEU:HD11	2.55	0.41
2:B:186:CYS:HB2	2:B:215:PRO:HB2	2.02	0.41
1:C:609:LYS:O	1:C:637:LEU:HB2	2.21	0.41
1:A:526:ARG:H	1:A:526:ARG:HD2	1.86	0.41
1:C:269:THR:CG2	1:C:271:HIS:CE1	2.94	0.41
1:A:292:PRO:HA	1:A:293:PRO:HD2	1.96	0.41
2:D:316:VAL:HG12	2:D:322:VAL:HG22	2.02	0.41
2:B:197:THR:HA	2:B:202:PRO:HB3	2.04	0.40
1:C:362:MET:SD	1:C:429:ALA:HB2	2.61	0.40
1:C:485:ARG:HG3	1:C:498:PHE:HZ	1.85	0.40
1:A:572:HIS:HE1	1:A:576:MET:O	2.04	0.40
1:C:244:PRO:HB3	1:C:272:HIS:CE1	2.56	0.40
1:C:531:ASP:OD1	1:C:533:ASN:HB2	2.21	0.40
1:A:59:ALA:HB2	2:B:278:CYS:SG	2.61	0.40
1:A:457:LEU:HG	1:A:461:GLY:HA3	2.02	0.40
2:B:171:THR:HG21	2:B:216:THR:HA	2.03	0.40
2:D:87:THR:HG22	2:D:95:LEU:HB3	2.03	0.40
2:D:118:LYS:HA	2:D:118:LYS:NZ	2.37	0.40
1:A:481:TYR:CE2	1:A:485:ARG:HD2	2.57	0.40
2:B:29:ARG:HG3	2:B:320:HIS:HB2	2.04	0.40
1:C:468:TYR:CE1	1:C:521:PHE:HB2	2.57	0.40
2:D:92:ARG:HA	2:D:108:LEU:HD12	2.02	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	624/637 (98%)	594 (95%)	24 (4%)	6 (1%)	12	20
1	C	624/637 (98%)	600 (96%)	20 (3%)	4 (1%)	21	32
2	B	294/366 (80%)	279 (95%)	12 (4%)	3 (1%)	12	20
2	D	295/366 (81%)	279 (95%)	14 (5%)	2 (1%)	18	28
All	All	1837/2006 (92%)	1752 (95%)	70 (4%)	15 (1%)	16	25

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	147	ILE
1	C	530	ILE
2	D	147	ILE
2	D	243	LYS
1	A	148	SER
1	A	529	MET
1	A	530	ILE
2	B	247	CYS
1	A	531	ASP
1	C	477	SER
1	A	441	ALA
2	B	246	SER
1	C	531	ASP
1	A	527	ASP
1	C	63	PRO

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	559/562 (100%)	530 (95%)	29 (5%)	21	36
1	C	559/562 (100%)	539 (96%)	20 (4%)	31	52
2	B	254/310 (82%)	241 (95%)	13 (5%)	21	37
2	D	255/310 (82%)	240 (94%)	15 (6%)	18	31
All	All	1627/1744 (93%)	1550 (95%)	77 (5%)	23	41

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ARG
1	A	14	VAL
1	A	25	GLU
1	A	140	ASN
1	A	146	HIS
1	A	175	HIS
1	A	214	SER
1	A	220	ARG
1	A	240	LYS
1	A	269	THR
1	A	273	SER
1	A	275	LYS
1	A	284	LEU
1	A	289	GLN
1	A	299	LEU
1	A	326	VAL
1	A	384	ARG
1	A	454	GLN
1	A	475	ILE
1	A	485	ARG
1	A	504	VAL
1	A	526	ARG
1	A	529	MET
1	A	530	ILE
1	A	577	PHE
1	A	578	SER
1	A	579	TRP
1	A	594	GLU
1	A	610	LYS
2	B	47	SER
2	B	118	LYS
2	B	135	SER
2	B	141	VAL
2	B	156	GLN
2	B	205	GLN
2	B	224	GLN
2	B	227	VAL
2	B	246	SER
2	B	249	LEU
2	B	268	VAL
2	B	274	LEU
2	B	326	VAL

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Mol	Chain	Res	Type
1	C	14	VAL
1	C	55	ILE
1	C	155	VAL
1	C	177	GLU
1	C	220	ARG
1	C	240	LYS
1	C	269	THR
1	C	274	GLU
1	C	275	LYS
1	C	281	LEU
1	C	302	LYS
1	C	326	VAL
1	C	405	GLN
1	C	485	ARG
1	C	504	VAL
1	C	577	PHE
1	C	579	TRP
1	C	582	ILE
1	C	597	THR
1	C	621	VAL
2	D	32	GLU
2	D	47	SER
2	D	78	GLN
2	D	80	GLU
2	D	107	GLU
2	D	118	LYS
2	D	135	SER
2	D	206	ILE
2	D	242	THR
2	D	247	CYS
2	D	274	LEU
2	D	280	LEU
2	D	288	SER
2	D	292	ARG
2	D	294	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	ASN
1	A	66	GLN
1	A	141	HIS

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Mol	Chain	Res	Type
1	A	146	HIS
1	A	147	HIS
1	A	251	GLN
1	A	270	ASN
1	A	339	GLN
1	A	572	HIS
1	A	588	GLN
2	B	178	HIS
2	B	224	GLN
2	B	254	HIS
2	B	256	GLN
2	B	266	HIS
2	B	320	HIS
1	C	56	GLN
1	C	61	ASN
1	C	128	GLN
1	C	263	GLN
1	C	282	GLN
1	C	290	ASN
1	C	309	GLN
1	C	339	GLN
1	C	511	GLN
1	C	525	ASN
1	C	588	GLN
2	D	190	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

2 ligands are modelled in this entry.

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	ZR4	C	701	-	30,30,30	0.20	0	41,45,45	0.53	0
3	ZR4	A	701	-	30,30,30	0.25	0	41,45,45	0.58	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ZR4	C	701	-	-	0/12/28/28	0/4/4/4
3	ZR4	A	701	-	-	0/12/28/28	0/4/4/4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

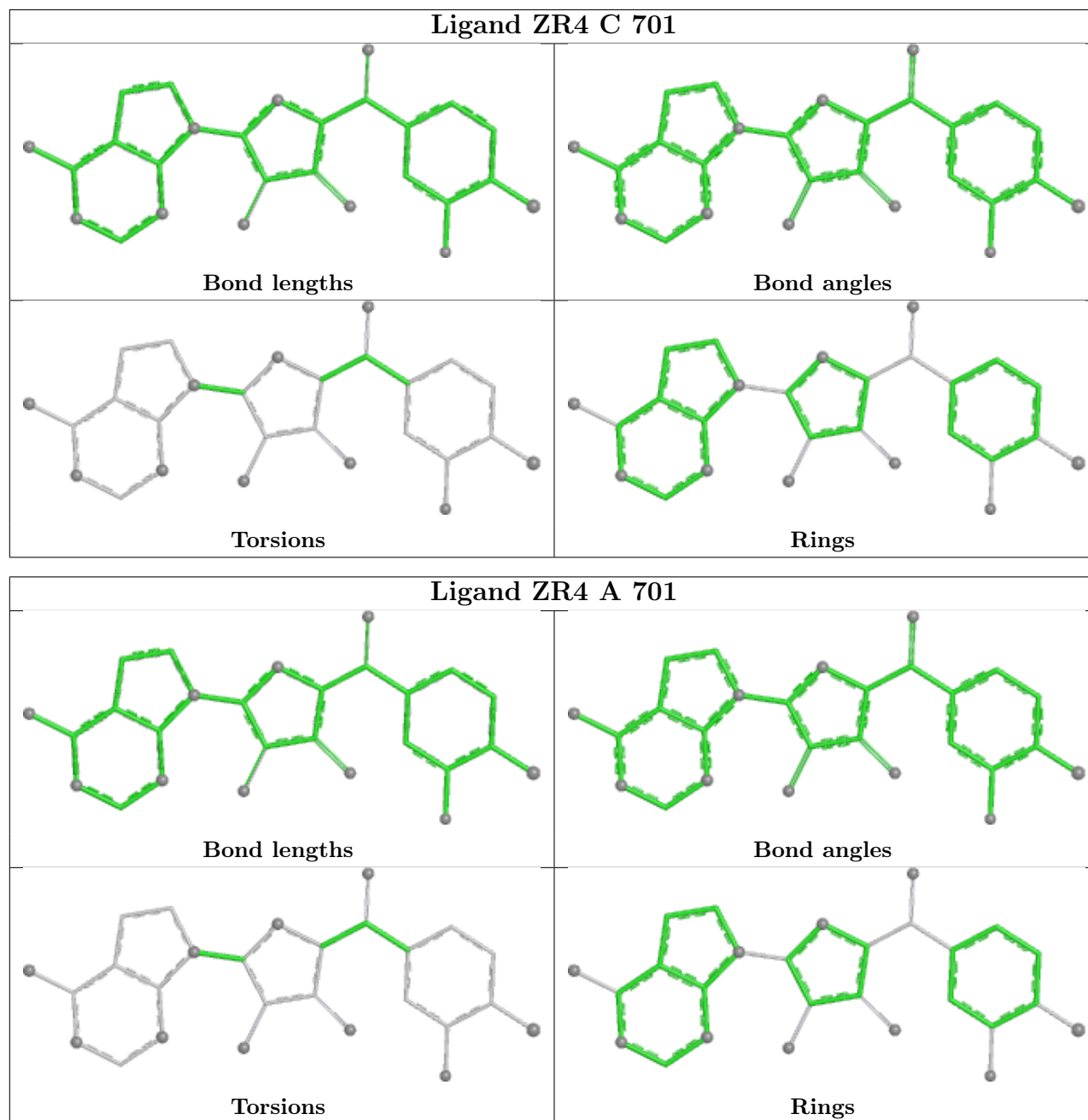
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	701	ZR4	2	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 ⓘ

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	625/637 (98%)	0.80	59 (9%)	14 11	23, 55, 91, 115	1 (0%)
1	C	625/637 (98%)	0.62	45 (7%)	21 18	18, 48, 84, 109	1 (0%)
2	B	298/366 (81%)	1.23	43 (14%)	6 4	51, 66, 85, 99	0
2	D	299/366 (81%)	1.35	73 (24%)	2 1	40, 65, 90, 101	0
All	All	1847/2006 (92%)	0.90	220 (11%)	9 6	18, 58, 88, 115	2 (0%)

All (220) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	297	TYR	6.2
1	A	530	ILE	6.0
2	D	207	GLY	5.9
1	C	530	ILE	5.5
1	A	579	TRP	4.8
2	D	114	LEU	4.6
1	C	296	ALA	4.6
2	B	207	GLY	4.5
2	D	248	VAL	4.4
1	A	297	TYR	4.3
2	D	41	ALA	4.2
1	C	579	TRP	4.1
1	C	299	LEU	4.1
1	C	300	PHE	4.1
1	C	529	MET	4.1
2	D	249	LEU	4.0
1	C	577	PHE	3.9
1	A	277	PHE	3.8
1	A	577	PHE	3.6
2	B	272	ALA	3.6
2	D	323	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
2	B	45	GLY	3.4
1	A	529	MET	3.4
1	C	375	SER	3.4
2	D	62	LYS	3.3
1	A	64	GLY	3.3
2	B	248	VAL	3.3
2	D	115	ILE	3.3
2	D	326	VAL	3.2
1	A	296	ALA	3.2
2	D	106	TRP	3.2
2	B	114	LEU	3.2
2	D	222	PRO	3.2
2	B	303	ALA	3.1
1	A	361	LEU	3.1
2	D	271	LEU	3.1
2	D	247	CYS	3.1
1	C	277	PHE	3.1
1	C	409	TRP	3.1
1	A	300	PHE	3.1
1	A	528	PRO	3.0
2	D	265	PRO	3.0
1	A	432	ILE	3.0
2	B	106	TRP	3.0
2	B	271	LEU	3.0
2	D	45	GLY	3.0
2	D	108	LEU	2.9
2	B	247	CYS	2.9
1	A	376	LEU	2.9
2	D	60	LEU	2.9
1	A	462	VAL	2.9
2	D	27	MET	2.9
1	C	575	GLY	2.8
2	D	290	LEU	2.8
1	A	390	ALA	2.8
2	D	61	PHE	2.8
1	A	273	SER	2.8
2	B	225	SER	2.8
1	C	376	LEU	2.8
2	D	239	LEU	2.8
2	D	291	PHE	2.8
2	D	245	THR	2.8
1	A	301	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
2	D	281	ALA	2.8
1	C	406	PHE	2.8
2	D	131	VAL	2.8
2	D	182	VAL	2.8
2	D	327	VAL	2.8
1	C	574	PRO	2.8
2	D	285	SER	2.7
1	A	559	LEU	2.7
2	D	58	LEU	2.7
1	A	468	TYR	2.7
2	B	140	ALA	2.7
1	A	45	VAL	2.7
2	D	29	ARG	2.7
1	A	363	VAL	2.7
2	B	322	VAL	2.7
2	D	268	VAL	2.7
1	A	82	ILE	2.7
1	A	431	ILE	2.7
1	C	64	GLY	2.7
1	A	346	LEU	2.7
1	A	342	TYR	2.6
1	A	292	PRO	2.6
1	C	578	SER	2.6
2	D	313	LEU	2.6
2	D	272	ALA	2.6
1	C	276	GLU	2.6
1	C	372	VAL	2.6
2	D	315	THR	2.6
1	A	294	PRO	2.6
1	A	465	PRO	2.6
2	D	328	PRO	2.6
1	A	148	SER	2.6
2	D	288	SER	2.6
1	A	406	PHE	2.6
1	A	249	MET	2.6
1	A	349	VAL	2.6
2	D	89	VAL	2.6
2	D	311	SER	2.6
1	C	147	HIS	2.6
1	C	576	MET	2.6
2	B	268	VAL	2.6
2	B	246	SER	2.6

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Mol	Chain	Res	Type	RSRZ
2	D	42	LEU	2.5
2	D	44	LEU	2.5
1	C	301	ALA	2.5
2	B	242	THR	2.5
2	D	270	PHE	2.5
2	D	314	THR	2.5
2	B	282	VAL	2.5
1	C	341	ILE	2.5
1	C	528	PRO	2.5
1	C	273	SER	2.5
1	C	304	TYR	2.5
1	A	293	PRO	2.5
2	D	318	TRP	2.5
2	D	283	LEU	2.5
2	D	68	PRO	2.5
1	A	245	VAL	2.4
2	D	72	PHE	2.4
1	A	299	LEU	2.4
1	A	345	LEU	2.4
1	C	346	LEU	2.4
1	C	361	LEU	2.4
2	D	329	THR	2.4
1	A	386	ILE	2.4
2	D	282	VAL	2.4
2	D	94	ILE	2.4
1	A	457	LEU	2.4
1	C	294	PRO	2.4
1	A	240	LYS	2.4
2	D	267	SER	2.4
1	A	26	ILE	2.4
2	B	158	VAL	2.4
1	A	388	LEU	2.4
2	B	40	GLY	2.3
2	D	93	GLY	2.3
1	C	358	VAL	2.3
2	B	103	VAL	2.3
2	D	116	VAL	2.3
2	D	280	LEU	2.3
1	A	526	ARG	2.3
1	C	398	VAL	2.3
1	A	284	LEU	2.3
2	B	186	CYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	389	TYR	2.3
1	C	369	GLY	2.3
2	D	240	VAL	2.3
1	C	275	LYS	2.3
2	B	44	LEU	2.3
2	B	249	LEU	2.3
2	B	308	LEU	2.3
2	B	313	LEU	2.3
2	D	154	LEU	2.3
1	A	560	TYR	2.3
1	A	121	ALA	2.3
2	B	245	THR	2.3
2	D	86	LEU	2.2
2	D	269	PRO	2.2
1	A	276	GLU	2.2
2	D	305	TRP	2.2
2	D	77	VAL	2.2
2	D	300	VAL	2.2
2	D	82	GLY	2.2
1	A	454	GLN	2.2
1	C	404	TRP	2.2
2	B	59	TRP	2.2
1	C	371	LEU	2.2
2	B	159	VAL	2.2
2	B	240	VAL	2.2
1	A	574	PRO	2.2
1	C	293	PRO	2.2
1	C	337	TYR	2.2
1	C	26	ILE	2.2
2	D	308	LEU	2.2
2	B	77	VAL	2.2
2	B	143	GLY	2.2
1	C	278	CYS	2.2
2	D	74	SER	2.2
1	A	283	TYR	2.1
2	B	305	TRP	2.1
2	D	43	LEU	2.1
1	C	23	VAL	2.1
1	A	352	GLU	2.1
2	B	212	GLY	2.1
1	A	578	SER	2.1
1	C	414	THR	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	35	ARG	2.1
1	A	582	ILE	2.1
2	B	108	LEU	2.1
2	B	274	LEU	2.1
1	A	33	VAL	2.1
1	A	404	TRP	2.1
2	B	29	ARG	2.1
1	A	378	ALA	2.1
2	D	244	SER	2.1
1	A	427	GLU	2.1
1	A	254	ILE	2.1
2	B	312	LEU	2.1
1	C	560	TYR	2.1
2	D	40	GLY	2.1
2	B	50	SER	2.1
2	B	203	ALA	2.1
2	D	33	ALA	2.1
2	B	95	LEU	2.1
2	D	180	ASP	2.1
2	B	119	PHE	2.1
1	C	526	ARG	2.1
1	C	67	THR	2.0
2	B	329	THR	2.0
1	A	278	CYS	2.0
1	C	378	ALA	2.0
2	D	174	ALA	2.0
2	D	266	HIS	2.0
2	D	258	VAL	2.0
2	B	90	GLY	2.0
2	B	129	SER	2.0
2	D	38	SER	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 ⓘ

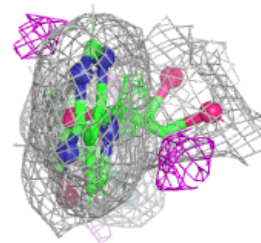
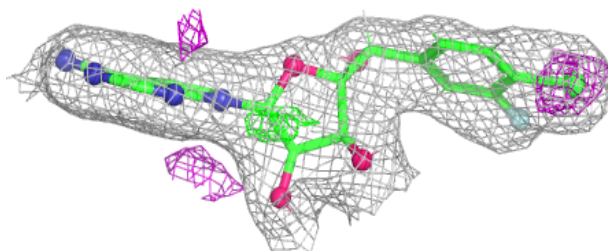
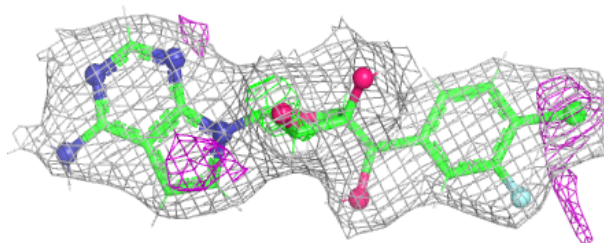
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists 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	ZR4	C	701	27/27	0.91	0.10	38,43,51,54	16
3	ZR4	A	701	27/27	0.92	0.08	35,42,49,52	16

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.

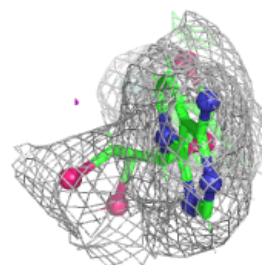
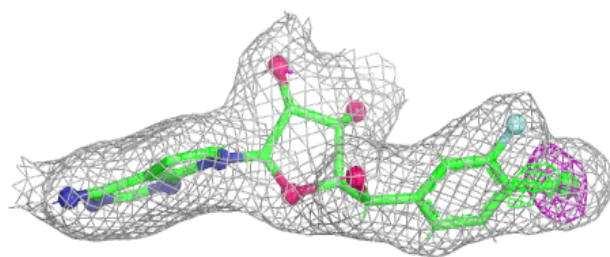
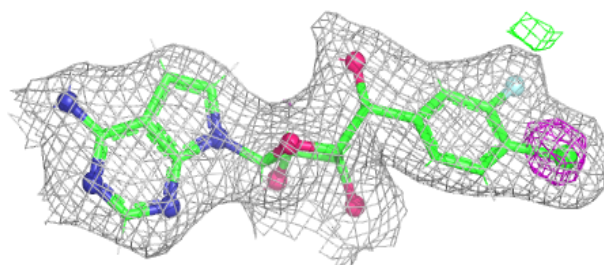
Electron density around ZR4 C 701:

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



Electron density around ZR4 A 701:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.