



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2023 – 09:57 AM EDT

PDB ID : 7MXG  
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](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.

The types of validation reports are described at

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

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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 : 2.35.1  
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) : 2.35.1

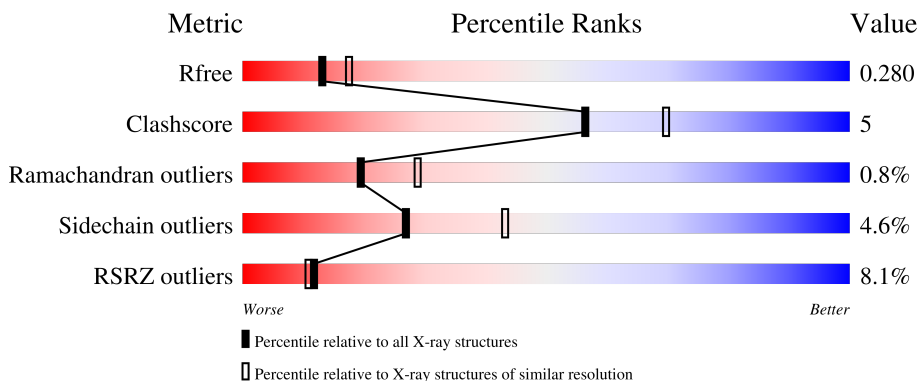
# 1 Overall quality at a glance i

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))
$R_{free}$	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (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  $\geq 3$ , 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	637	<div style="display: flex; align-items: center;"> <div style="width: 7%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 82%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 15%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">7%      82%      15%    ..</p>
1	C	637	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 85%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 13%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">5%      85%      13%    ..</p>
2	B	366	<div style="display: flex; align-items: center;"> <div style="width: 9%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 68%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 13%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 19%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">9%      68%      13%    •    19%</p>
2	D	366	<div style="display: flex; align-items: center;"> <div style="width: 11%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 67%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 14%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 18%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">11%      67%      14%    •    18%</p>

## 2 Entry composition [i](#)

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
			Total	C	N	O	S			
1	A	625	5068	3241	870	933	24	0	1	0
1	C	625	5068	3241	870	933	24	0	1	0

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
			Total	C	N	O	S			
2	B	298	2261	1419	387	444	11	0	0	0
2	D	299	2269	1424	388	445	12	0	0	0

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

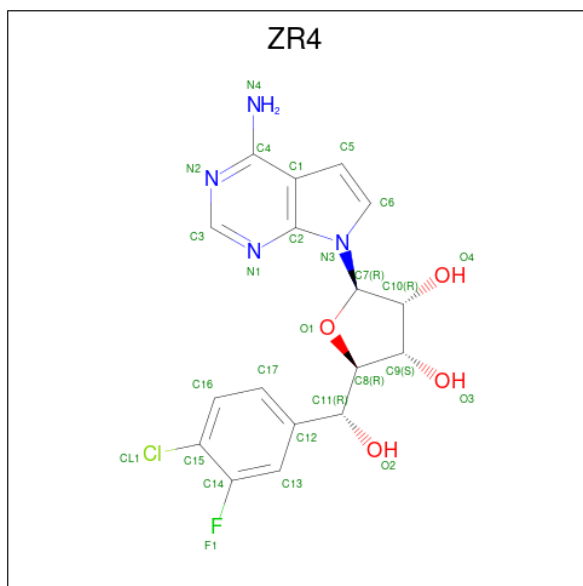
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-13	TYR	-	expression tag	UNP Q9BQA1
B	-12	ASP	-	expression tag	UNP Q9BQA1
B	-11	GLY	-	expression tag	UNP Q9BQA1
B	-10	ALA	-	expression tag	UNP Q9BQA1
B	-9	THR	-	expression tag	UNP Q9BQA1
B	-8	THR	-	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 (three-letter code: ZR4) (formula: C<sub>17</sub>H<sub>16</sub>ClFN<sub>4</sub>O<sub>4</sub>) (labeled as "Ligand

of Interest" by depositor).



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

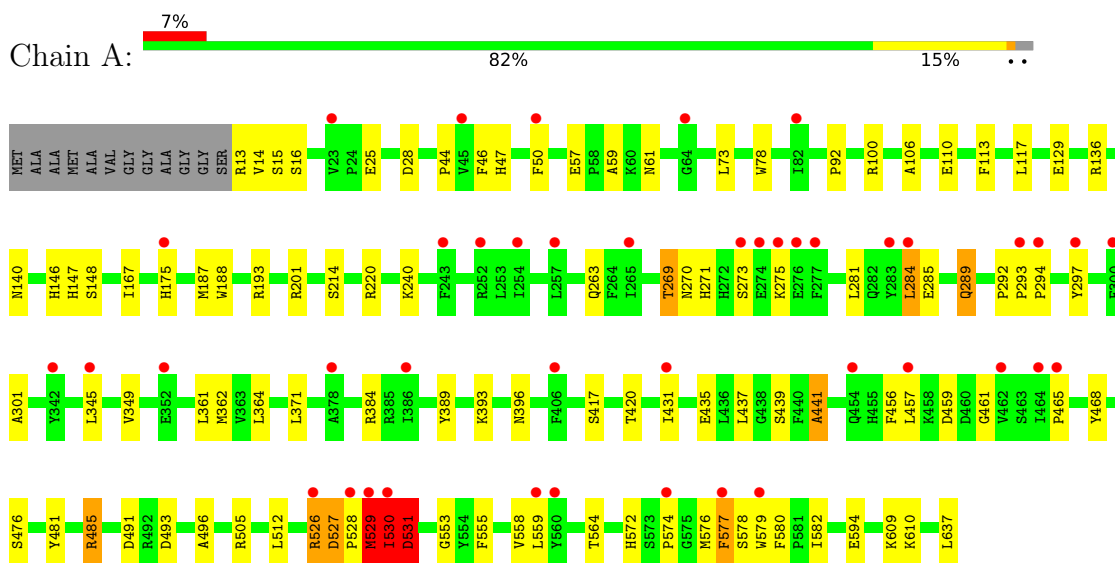
- Molecule 4 is water.

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		

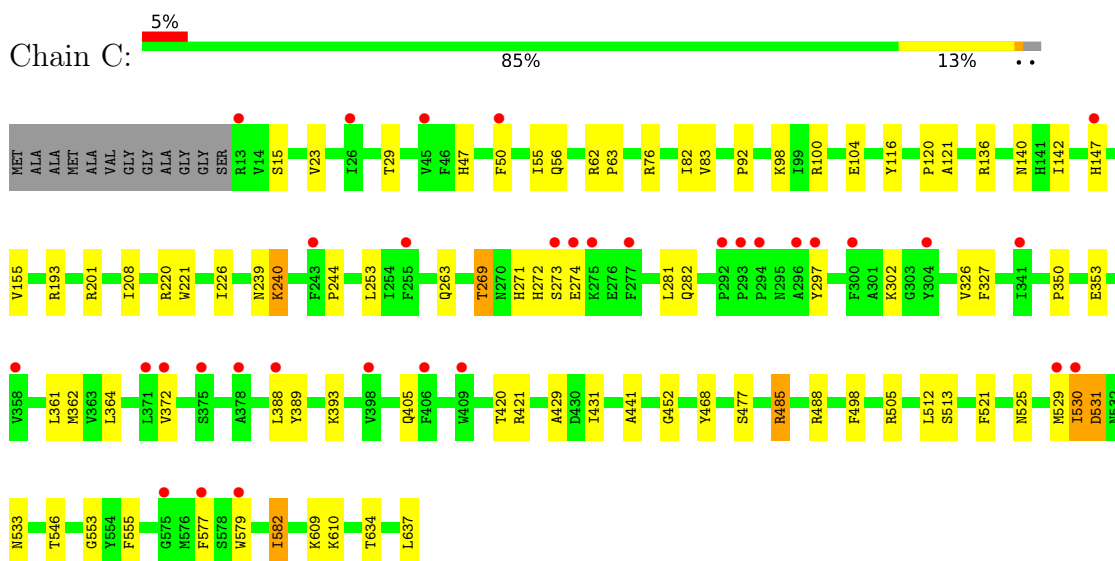
### 3 Residue-property plots [i](#)

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.

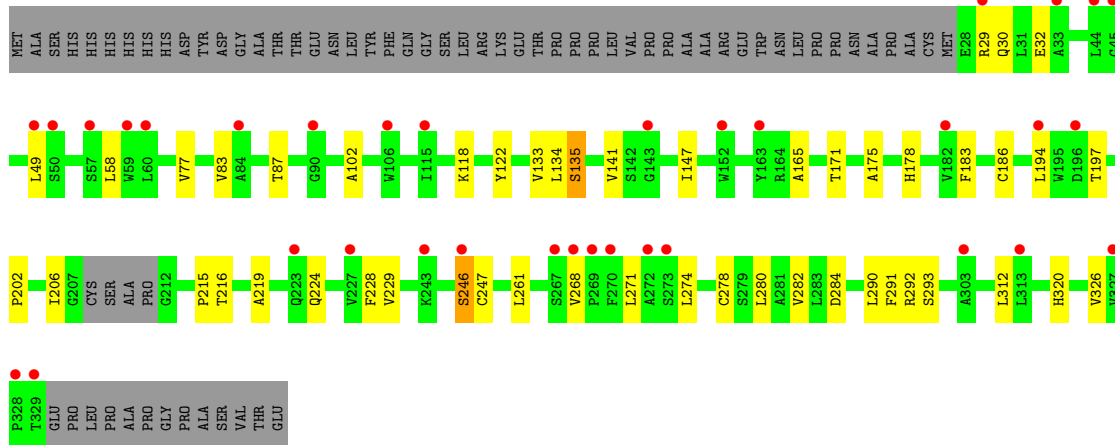
- Molecule 1: Protein arginine N-methyltransferase 5



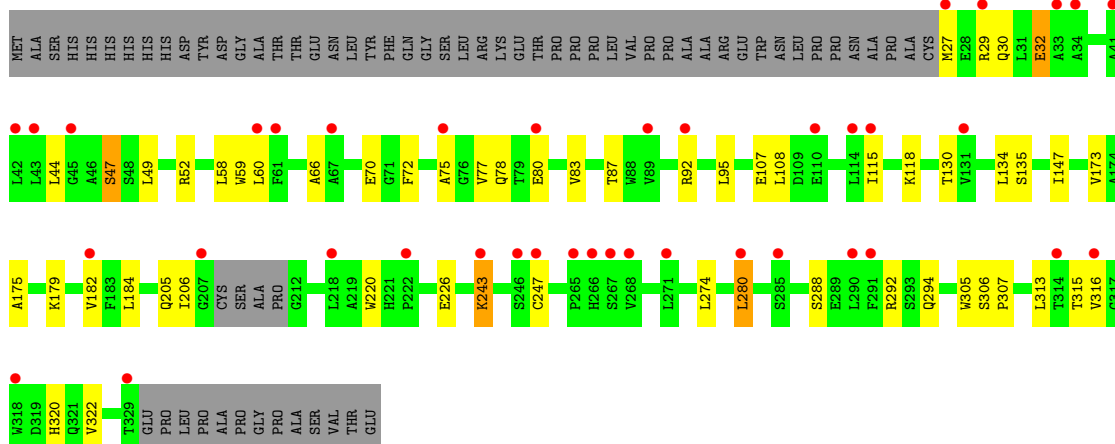
- Molecule 1: Protein arginine N-methyltransferase 5



- 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, $\alpha$ , $\beta$ , $\gamma$	98.41Å 138.45Å 178.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	109.39 – 2.40 109.39 – 2.39	Depositor EDS
% Data completeness (in resolution range)	99.8 (109.39-2.40) 99.8 (109.39-2.39)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.68 (at 2.40Å)	Xtrriage
Refinement program	BUSTER 2.11.7	Depositor
R, $R_{free}$	0.227 , 0.282 0.224 , 0.280	Depositor DCC
$R_{free}$ test set	4716 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.5	Xtrriage
Anisotropy	0.923	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 60.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	15557	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtrriage'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.*

<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 [i](#)

### 5.1 Standard geometry [i](#)

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	0.42	0/5210	0.59	0/7088
1	C	0.44	0/5210	0.62	1/7088 (0.0%)
2	B	0.38	0/2313	0.62	0/3157
2	D	0.41	0/2321	0.67	0/3167
All	All	0.42	0/15054	0.62	1/20500 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	529	MET	C-N-CA	5.13	134.52	121.70

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	5068	0	4958	56	0
1	C	5068	0	4958	40	0
2	B	2261	0	2180	24	0
2	D	2269	0	2189	28	0
3	A	27	16	0	0	0
3	C	27	16	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	144	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 (144) 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: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
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: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:A:187[B]:MET:HE1	1:A:188:TRP:HD1	1.68	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:129:GLU:HG3	1:A:187[B]:MET:CE	2.37	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
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
1:A:129:GLU:HG3	1:A:187[B]:MET:HE1	1.92	0.51
2:B:134:LEU:HD23	2:B:175:ALA:CB	2.40	0.51
1:A:187[B]:MET:HE1	1:A:188:TRP:CD1	2.45	0.51
1:A:530:ILE:CG2	1:A:531:ASP:N	2.74	0.50
1:C:83:VAL:HG22	1:C:121:ALA:HB3	1.93	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:70:GLU:CD	2:D:70:GLU:H	2.19	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
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
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: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
2:D:108:LEU:HD23	2:D:115:ILE:HG12	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:134:LEU:HD23	2:D:175:ALA:HB1	2.01	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%)	15	23
1	C	624/637 (98%)	600 (96%)	20 (3%)	4 (1%)	25	36
2	B	294/366 (80%)	279 (95%)	12 (4%)	3 (1%)	15	23
2	D	295/366 (81%)	279 (95%)	14 (5%)	2 (1%)	22	32
All	All	1837/2006 (92%)	1752 (95%)	70 (4%)	15 (1%)	19	29

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 [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	559/562 (100%)	529 (95%)	30 (5%)	22	36
1	C	559/562 (100%)	538 (96%)	21 (4%)	33	51
2	B	254/310 (82%)	245 (96%)	9 (4%)	36	55
2	D	255/310 (82%)	240 (94%)	15 (6%)	19	32
All	All	1627/1744 (93%)	1552 (95%)	75 (5%)	27	43

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ARG
1	A	25	GLU
1	A	28	ASP
1	A	136	ARG
1	A	140	ASN
1	A	146	HIS
1	A	175	HIS
1	A	193	ARG
1	A	214	SER
1	A	220	ARG
1	A	240	LYS
1	A	269	THR
1	A	270	ASN
1	A	273	SER
1	A	275	LYS
1	A	284	LEU
1	A	289	GLN
1	A	393	LYS
1	A	417	SER
1	A	459	ASP
1	A	485	ARG
1	A	526	ARG
1	A	529	MET
1	A	530	ILE
1	A	531	ASP
1	A	577	PHE
1	A	578	SER
1	A	579	TRP
1	A	594	GLU
1	A	610	LYS
2	B	118	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	B	135	SER
2	B	141	VAL
2	B	224	GLN
2	B	246	SER
2	B	268	VAL
2	B	274	LEU
2	B	312	LEU
2	B	326	VAL
1	C	55	ILE
1	C	76	ARG
1	C	136	ARG
1	C	155	VAL
1	C	193	ARG
1	C	220	ARG
1	C	240	LYS
1	C	269	THR
1	C	273	SER
1	C	274	GLU
1	C	281	LEU
1	C	282	GLN
1	C	302	LYS
1	C	326	VAL
1	C	393	LYS
1	C	405	GLN
1	C	485	ARG
1	C	513	SER
1	C	577	PHE
1	C	579	TRP
1	C	582	ILE
2	D	32	GLU
2	D	47	SER
2	D	52	ARG
2	D	78	GLN
2	D	80	GLU
2	D	107	GLU
2	D	135	SER
2	D	205	GLN
2	D	206	ILE
2	D	247	CYS
2	D	274	LEU
2	D	280	LEU
2	D	288	SER

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Mol	Chain	Res	Type
2	D	292	ARG
2	D	294	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	ASN
1	A	147	HIS
1	A	270	ASN
1	A	322	GLN
1	A	339	GLN
1	A	572	HIS
1	C	56	GLN
1	C	61	ASN
1	C	263	GLN
1	C	322	GLN
1	C	525	ASN
1	C	588	GLN
2	D	178	HIS

### 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 [i](#)

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	A	701	-	27,30,30	0.84	1 (3%)	35,45,45	0.81	1 (2%)
3	ZR4	C	701	-	27,30,30	0.85	1 (3%)	35,45,45	0.77	1 (2%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ZR4	A	701	-	-	0/8/28/28	0/4/4/4
3	ZR4	C	701	-	-	0/8/28/28	0/4/4/4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	701	ZR4	C4-C1	-3.64	1.41	1.45
3	C	701	ZR4	C4-C1	-3.62	1.41	1.45

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	701	ZR4	C1-C4-N2	-2.66	119.16	121.93
3	C	701	ZR4	C1-C4-N2	-2.58	119.25	121.93

There are no chirality outliers.

There are no torsion outliers.

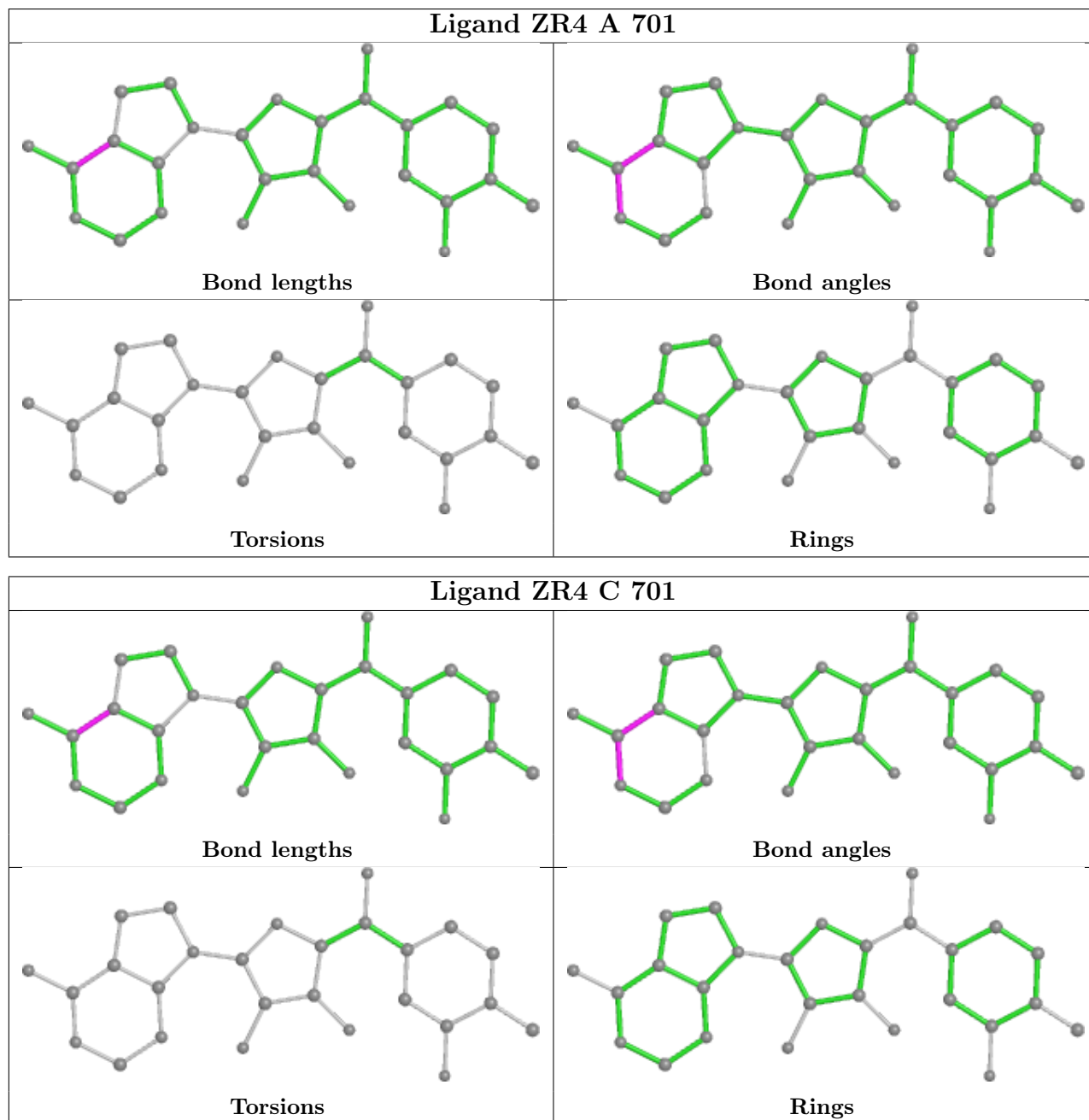
There are no ring outliers.

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 [i](#)

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, 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	625/637 (98%)	0.60	43 (6%) 16 15	33, 55, 91, 115	0
1	C	625/637 (98%)	0.51	33 (5%) 26 25	24, 48, 84, 109	0
2	B	298/366 (81%)	0.77	34 (11%) 5 4	51, 66, 85, 99	0
2	D	299/366 (81%)	0.82	39 (13%) 3 3	40, 65, 90, 101	0
All	All	1847/2006 (92%)	0.63	149 (8%) 12 11	24, 58, 88, 115	0

All (149) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	297	TYR	8.0
1	A	277	PHE	7.0
1	C	296	ALA	6.8
1	A	530	ILE	6.5
1	A	273	SER	6.4
1	C	529	MET	6.3
1	A	274	GLU	5.6
1	C	530	ILE	5.6
1	C	274	GLU	5.0
2	D	27	MET	5.0
2	B	268	VAL	4.9
2	B	44	LEU	4.4
1	A	529	MET	4.1
1	A	293	PRO	4.0
2	B	59	TRP	4.0
1	C	273	SER	4.0
1	A	352	GLU	3.7
2	D	41	ALA	3.6
1	A	342	TYR	3.6
2	D	290	LEU	3.6
1	A	462	VAL	3.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	300	PHE	3.6
1	A	297	TYR	3.5
1	C	293	PRO	3.5
2	B	223	GLN	3.5
2	D	75	ALA	3.4
1	C	277	PHE	3.3
2	D	329	THR	3.3
1	A	45	VAL	3.3
2	D	60	LEU	3.3
2	D	114	LEU	3.3
2	B	327	VAL	3.3
2	B	143	GLY	3.2
2	D	291	PHE	3.2
2	D	271	LEU	3.2
2	B	227	VAL	3.1
2	D	318	TRP	3.1
2	D	110	GLU	3.1
1	C	406	PHE	3.1
2	B	243	LYS	3.1
1	C	575	GLY	3.1
2	D	43	LEU	3.1
2	B	246	SER	3.0
1	C	577	PHE	3.0
1	A	294	PRO	3.0
2	D	267	SER	3.0
2	D	89	VAL	2.9
2	D	247	CYS	2.9
1	A	577	PHE	2.9
1	C	275	LYS	2.9
1	A	254	ILE	2.9
2	B	115	ILE	2.9
2	D	222	PRO	2.9
2	B	50	SER	2.9
2	D	316	VAL	2.9
2	D	33	ALA	2.9
1	A	406	PHE	2.8
1	A	579	TRP	2.8
2	D	80	GLU	2.8
2	D	34	ALA	2.8
1	A	265	ILE	2.8
1	C	372	VAL	2.8
1	A	345	LEU	2.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	45	VAL	2.8
2	B	29	ARG	2.8
2	D	265	PRO	2.7
2	B	329	THR	2.7
1	A	82	ILE	2.7
1	A	431	ILE	2.7
1	A	378	ALA	2.7
1	A	464	ILE	2.7
1	C	341	ILE	2.7
2	B	182	VAL	2.7
2	D	42	LEU	2.7
1	A	560	TYR	2.7
2	D	61	PHE	2.7
2	D	314	THR	2.7
2	D	243	LYS	2.7
1	A	257	LEU	2.7
1	C	50	PHE	2.6
2	B	270	PHE	2.6
2	B	57	SER	2.6
2	D	92	ARG	2.6
1	A	284	LEU	2.6
1	A	243	PHE	2.6
2	D	131	VAL	2.6
1	C	358	VAL	2.5
1	A	50	PHE	2.5
2	D	45	GLY	2.5
2	D	268	VAL	2.5
2	B	273	SER	2.5
2	D	246	SER	2.5
2	B	60	LEU	2.5
1	C	300	PHE	2.5
1	A	276	GLU	2.5
1	C	398	VAL	2.4
2	B	163	TYR	2.4
1	A	559	LEU	2.4
2	D	285	SER	2.4
2	B	106	TRP	2.4
2	D	29	ARG	2.4
1	C	409	TRP	2.4
1	C	147	HIS	2.4
1	C	294	PRO	2.4
1	C	304	TYR	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	D	280	LEU	2.4
2	B	328	PRO	2.4
2	D	266	HIS	2.3
1	A	275	LYS	2.3
2	D	67	ALA	2.3
1	A	574	PRO	2.3
1	C	292	PRO	2.3
1	A	386	ILE	2.3
2	B	269	PRO	2.3
2	B	313	LEU	2.3
2	B	267	SER	2.3
1	C	255	PHE	2.3
1	C	388	LEU	2.3
2	B	45	GLY	2.3
1	A	252	ARG	2.3
1	C	243	PHE	2.3
1	A	528	PRO	2.3
2	B	303	ALA	2.3
1	A	465	PRO	2.2
1	C	13	ARG	2.2
2	B	194	LEU	2.2
1	A	175	HIS	2.2
1	A	457	LEU	2.2
1	C	371	LEU	2.2
1	A	283	TYR	2.2
1	A	526	ARG	2.2
2	D	207	GLY	2.2
2	D	115	ILE	2.2
1	A	23	VAL	2.1
2	D	182	VAL	2.1
2	B	84	ALA	2.1
2	B	49	LEU	2.1
2	B	196	ASP	2.1
2	B	272	ALA	2.1
1	C	26	ILE	2.1
2	D	218	LEU	2.1
1	A	454	GLN	2.1
2	B	90	GLY	2.1
1	C	375	SER	2.1
1	C	579	TRP	2.1
2	B	152	TRP	2.0
1	A	64	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	378	ALA	2.0
2	B	33	ALA	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](#)

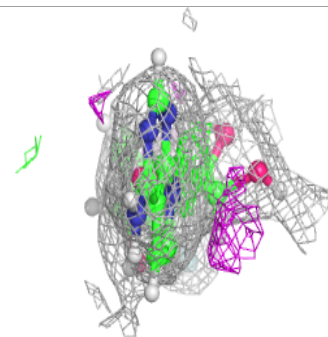
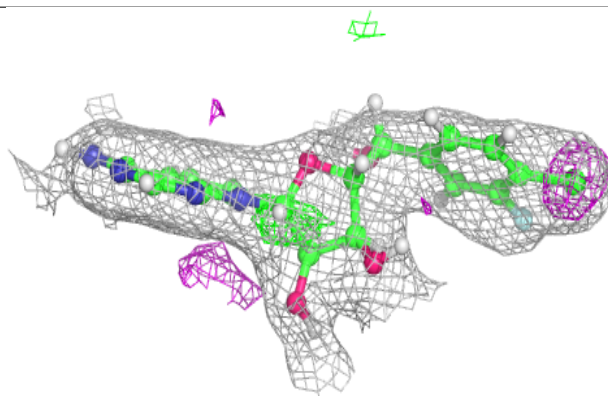
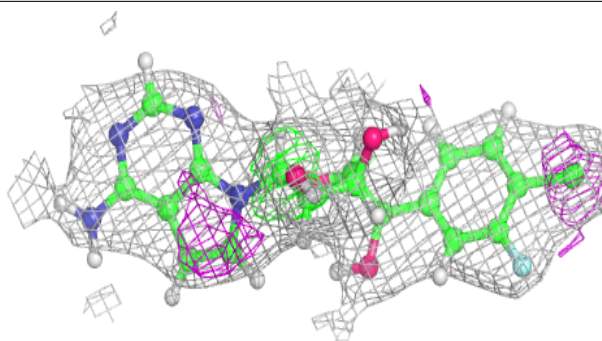
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q < 0.9
3	ZR4	C	701	27/27	0.93	0.17	38,43,51,54	16
3	ZR4	A	701	27/27	0.95	0.15	35,42,49,52	16

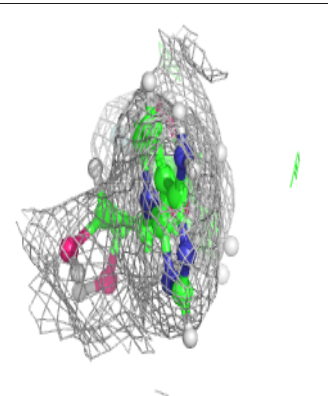
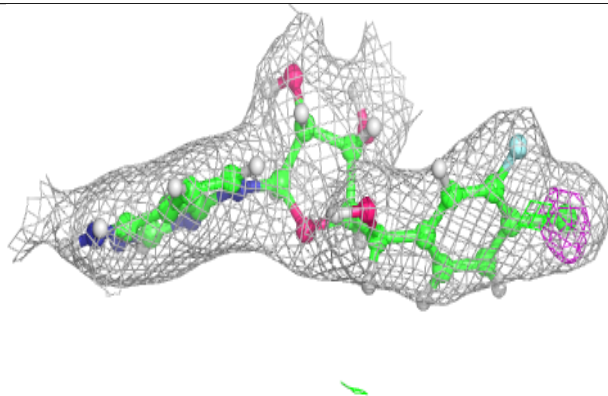
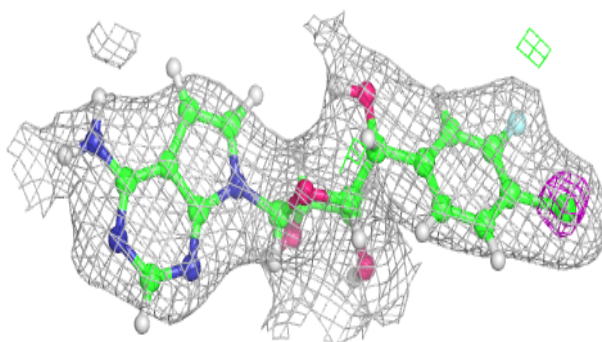
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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