

# Full wwPDB X-ray Structure Validation Report (i)

#### Jan 31, 2024 - 02:25 PM EST

PDB ID	:	8FMG
Title	:	Structure of CBASS Cap5 from Pseudomonas syringae as an activated
		tetramer with the cyclic dinucleotide 3'2'-c-diAMP ligand (3 tetramers in the AU)
Authors	:	Rechkoblit, O.; Kreitler, D.F.; Aggarwal, A.K.
Deposited on	:	2022-12-23
Resolution	:	1.79 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 (i) 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 (i)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
$\mathrm{EDS}$	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY \, DIFFRACTION$ 

The reported resolution of this entry is 1.79 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.



Motria	Whole archive	Similar resolution
Metric	$(\# {\rm Entries})$	$(\# { m Entries},  { m resolution}  { m range}({ m \AA}))$
$R_{free}$	130704	5950(1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 <=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	А	388	2% <b>8</b> 9%	5%	5%
1	В	388	83%	7% •	9%
1	С	388	3% 86%	8%	5%
1	D	388	<sup>2%</sup> 85%	6%	9%



Mol	Chain	Length	Quality of chain	
1	Е	388	3% 	6% 5%
1	F	388	3%	6% 9%
1	G	388	% 	9% 5%
1	Н	388	87%	• 8%
1	K	388	2% <b>9</b> 2%	• 5%
1	L	388	% <b>8</b> 5%	6% 8%
1	М	388	3% 90%	5% 5%
1	N	388	86%	5%• 9%



# 2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 69460 atoms, of which 32951 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.

Mol	Chain	Residues			Atom	s			ZeroOcc	AltConf	Trace
1	Δ	260	Total	С	Η	Ν	0	S	0	1	0
1	A	309	5714	1817	2826	520	540	11	0	0 4	0
1	р	254	Total	С	Η	Ν	0	S	0	0	0
1	D	- 554	5368	1718	2656	482	502	10	0	0	0
1	С	368	Total	С	Η	Ν	0	S	0	0	0
1	U	300	5600	1784	2764	512	530	10	0	0	0
1	Л	252	Total	С	Η	Ν	0	S	0	0	0
1	D	000	5340	1713	2635	481	501	10	0	0	0
1	F	360	Total	С	Η	Ν	0	S	0	0	0
1	Ľ	509	5597	1791	2754	510	532	10	0	0	0
1	F	353	Total	С	Η	Ν	Ο	S	0	1	0
1	Ľ	000	5412	1730	2677	485	510	10	0	1	0
1	С	368	Total	С	Η	Ν	Ο	$\mathbf{S}$	0	0	0
1	G	500	5640	1793	2795	514	528	10		0	0
1	ц	356	Total	С	Η	Ν	0	$\mathbf{S}$	0	0	0
1	11	550	5431	1737	2685	486	513	10	0	0	
1	K	360	Total	С	Η	Ν	0	$\mathbf{S}$	0	1	0
1	Γ	509	5580	1787	2745	508	530	10	0	T	0
1	T	357	Total	С	Η	Ν	0	$\mathbf{S}$	0	1	0
1		001	5480	1748	2713	491	518	10	0	T	0
1	М	360	Total	С	Η	Ν	0	S	0	0	0
	111	509	5637	1794	2788	514	531	10	0	0	U
1	N	354	Total	С	Н	Ν	0	S	0	2	0
	1 N	004	5382	1727	2661	484	500	10	U		U

• Molecule 1 is a protein called SAVED domain-containing protein.

• Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	Total Zn 1 1	0	0
2	В	1	Total Zn 1 1	0	0



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	С	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0
2	Е	1	Total Zn 1 1	0	0
2	F	1	Total Zn 1 1	0	0
2	G	1	Total Zn 1 1	0	0
2	Н	1	Total Zn 1 1	0	0
2	К	1	Total Zn 1 1	0	0
2	L	1	Total Zn 1 1	0	0
2	М	1	Total Zn 1 1	0	0
2	Ν	1	Total Zn 1 1	0	0

• Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	2	Total Mg 2 2	0	0
3	С	2	Total Mg 2 2	0	0
3	Е	2	Total Mg 2 2	0	0
3	G	2	Total Mg 2 2	0	0
3	Н	1	Total Mg 1 1	0	0
3	K	2	Total Mg 2 2	0	0
3	М	2	Total Mg 2 2	0	0

• Molecule 4 is Cyclic (adenosine-(2'-5')-monophosphate-adenosine-(3'-5')-monophospha te (three-letter code: Y4F) (formula:  $C_{20}H_{24}N_{10}O_{12}P_2$ ) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms						ZeroOcc	AltConf											
4	٨	1	Total	С	Н	Ν	Ο	Р	0	0											
4	A	1	65	20	21	10	12	2	0	0											
4	D	1	Total	С	Η	Ν	Ο	Р	0	0											
4	D	1	65	20	21	10	12	2	0	0											
4	С	1	Total	С	Η	Ν	Ο	Р	0	0											
	U	1	65	20	21	10	12	2	0	0											
4	Л	1	Total	С	Η	Ν	Ο	Р	0	0											
т	D	1	65	20	21	10	12	2	0	0											
4	E	1	Total	С	Η	Ν	Ο	Р	0	0											
	Ц	Ĩ	65	20	21	10	12	2	0	0											
4	F	1	Total	$\mathbf{C}$	Η	Ν	Ο	Р	0	0											
1	Ŧ	Ŧ	Ŧ	Ŧ	1	1	1	*	-	-	-	-	-	65	20	21	10	12	2	<u> </u>	0
4	G	1	Total	С	Η	Ν	Ο	Р	0	0											
1		1	65	20	21	10	12	2	0	0	0										
4	Н	1	Total	С	Η	Ν	Ο	Р	0	0											
-		1	65	20	21	10	12	2	Ŭ												
4	K	1	Total	С	Η	Ν	Ο	Р	0	0											
		1	65	20	21	10	12	2	Ŭ												
4	L	1	Total	С	Η	Ν	Ο	Р	0	0											
1		1	65	20	21	10	12	2	0	0											
4	М	1	Total	С	Η	Ν	Ο	Р	0	0											
- <u>+</u>	141	1	65	20	21	10	12	2	0												
4	N	1	Total	С	Η	Ν	Ο	Р	0	0											
Т	11	1	65	20	21	10	12	2	U												

• Molecule 5 is water.



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	230	Total         O           230         230	0	0
5	В	218	Total         O           218         218	0	0
5	С	206	Total         O           206         206	0	0
5	D	141	Total         O           141         141	0	0
5	Е	252	Total         O           252         252	0	0
5	F	162	Total         O           162         162	0	0
5	G	232	Total         O           232         232	0	0
5	Н	212	Total O 212 212	0	0
5	К	233	Total O 233 233	0	0
5	L	223	Total O 223 223	0	0
5	М	202	Total         O           202         202	0	0
5	Ν	163	Total O 163 163	0	0



# 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: SAVED domain-containing protein



# 

# q135 1166 1166 1166 1175 1192 1192 1192 1235 1372 1373 1414 1414 </t

 $\bullet$  Molecule 1: SAVED domain-containing protein







# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	145.19Å 80.52Å 406.84Å	Deperitor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.62^{\circ}$ $90.00^{\circ}$	Depositor
$Bosolution(\AA)$	58.12 - 1.79	Depositor
Resolution (A)	406.82 - 1.79	EDS
% Data completeness	61.0(58.12 - 1.79)	Depositor
(in resolution range)	$61.0 \ (406.82 \text{-} 1.79)$	EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.54 (at 1.80 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
B B.	0.179 , $0.225$	Depositor
It, Itfree	0.180 , $0.225$	DCC
$R_{free}$ test set	12884 reflections $(4.82%)$	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.0	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.41 , $45.3$	EDS
L-test for $twinning^2$	$<  L  > = 0.50, < L^2 > = 0.33$	Xtriage
	0.006 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l	
	0.006 for -1/2*h+3/2*k,1/2*h+1/2*k,-l	
Estimated twinning fraction	0.025  for  1/2 *h-3/2 *k,-1/2 *h-1/2 *k,-1	Xtriage
	0.020 for $1/2$ *h+ $3/2$ *k, $1/2$ *h- $1/2$ *k,-l	
	0.007 for -h,-k,l	
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	69460	wwPDB-VP
Average B, all atoms $(Å^2)$	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.14% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 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: Y4F, ZN, MG  $\,$ 

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).

Mal	Chain	Bond	lengths	Bond	angles
	Ullalli	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	А	0.30	0/2958	0.56	0/4031
1	В	0.29	0/2777	0.55	0/3788
1	С	0.28	0/2905	0.54	0/3961
1	D	0.27	0/2771	0.53	0/3782
1	Ε	0.28	0/2913	0.56	0/3975
1	F	0.28	0/2801	0.56	0/3820
1	G	0.28	0/2914	0.54	0/3971
1	Н	0.28	0/2812	0.54	0/3832
1	Κ	0.29	0/2904	0.55	0/3963
1	L	0.29	0/2833	0.55	0/3861
1	М	0.28	0/2918	0.54	0/3978
1	Ν	0.28	0/2787	0.54	0/3804
All	All	0.28	0/34293	0.55	0/46766

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	2888	2826	2821	14	0



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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2712	2656	2654	20	0
1	C	2836	2764	2763	20	0
1	D	2705	2635	2633	12	0
1	E	2843	2754	2753	15	0
1	F	2735	2677	2674	10	0
1	G	2845	2795	2794	15	0
1	H	2746	2685	2683	10	0
1	K	2835	2745	2743	8	0
1	L	2767	2713	2710	16	0
1	М	2849	2788	2787	9	0
1	N	2721	2661	2657	13	0
2	A	1	0	0	0	0
2	В	1	0	0	0	0
2	С	1	0	0	0	0
2	D	1	0	0	0	0
2	Е	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	Н	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
2	М	1	0	0	0	0
2	Ν	1	0	0	0	0
3	А	2	0	0	0	0
3	С	2	0	0	0	0
3	Е	2	0	0	0	0
3	G	2	0	0	0	0
3	Н	1	0	0	0	0
3	K	2	0	0	0	0
3	М	2	0	0	0	0
4	А	44	21	0	0	0
4	В	44	21	0	0	0
4	С	44	21	0	0	0
4	D	44	21	0	0	0
4	E	44	21	0	0	0
4	F	44	21	0	0	0
4	G	44	21	0	0	0
4	Н	44	21	0	0	0
4	K	44	21	0	0	0
4	L	44	21	0	1	0
4	М	44	21	0	0	0
4	N	44	21	0	1	0



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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	А	230	0	0	4	0
5	В	218	0	0	3	0
5	С	206	0	0	3	0
5	D	141	0	0	0	0
5	Е	252	0	0	3	0
5	F	162	0	0	3	0
5	G	232	0	0	3	0
5	Н	212	0	0	1	0
5	K	233	0	0	1	0
5	L	223	0	0	1	0
5	М	202	0	0	1	0
5	N	163	0	0	0	0
All	All	36509	32951	32672	153	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 2.

All (153) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:F:166:ILE:HD11	1:F:197:GLN:HG3	1.60	0.83
1:D:166:ILE:HD11	1:D:197:GLN:HG3	1.73	0.70
1:A:159:LEU:HD11	1:A:236:LEU:HD22	1.76	0.67
1:B:365:ASP:OD2	5:B:501:HOH:O	2.14	0.65
1:N:166:ILE:HD11	1:N:197:GLN:HG3	1.79	0.64
1:L:166:ILE:HD11	1:L:197:GLN:HG3	1.80	0.63
1:M:267:ASP:O	5:M:501:HOH:O	2.15	0.63
1:N:43:TYR:HB2	1:N:49:MET:HG2	1.83	0.61
1:D:235:ARG:NH2	1:D:348:GLU:OE1	2.33	0.60
1:G:354:THR:HG23	1:G:355:THR:HG23	1.85	0.58
1:H:166:ILE:HD11	1:H:197:GLN:HG3	1.85	0.58
1:L:115:GLU:OE1	1:L:118:ARG:NH1	2.36	0.58
1:C:17:ASN:OD1	1:C:78:ASN:ND2	2.37	0.57
1:B:116:ARG:NH2	5:B:504:HOH:O	2.38	0.57
1:D:229:ILE:HD12	1:D:235:ARG:HD2	1.87	0.56
1:L:166:ILE:HD11	1:L:197:GLN:CG	2.35	0.56
1:A:92:ASP:OD1	5:A:501:HOH:O	2.18	0.56
1:F:194:LEU:HD21	5:F:601:HOH:O	2.06	0.56
1:H:304:TYR:O	5:H:501:HOH:O	2.18	0.55
1:F:34:LEU:HD11	1:F:94:ILE:HD11	1.89	0.54
1:B:195:GLU:HG3	5:B:614:HOH:O	2.08	0.54



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		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:G:320:LEU:HD21	1:G:349:PHE:CD2	2.42	0.54
1:A:88:PRO:HB2	1:C:88:PRO:HB2	1.90	0.54
1:L:39:LEU:HD13	1:L:55:ALA:HB2	1.88	0.54
1:L:194:LEU:HD11	1:L:229:ILE:HG22	1.91	0.53
1:D:115:GLU:OE2	1:D:118:ARG:NH1	2.41	0.53
1:C:116:ARG:NH1	5:C:503:HOH:O	2.33	0.53
1:L:281:PRO:HG2	1:L:284:ASP:OD2	2.09	0.52
1:B:35:CYS:SG	1:B:37:THR:OG1	2.62	0.52
1:K:354:THR:O	5:K:501:HOH:O	2.19	0.52
1:F:116:ARG:NH2	5:F:506:HOH:O	2.42	0.51
1:B:214:VAL:HG21	1:B:246:LEU:HD21	1.92	0.51
1:C:22:ARG:NH1	5:C:501:HOH:O	2.28	0.51
1:L:35:CYS:SG	1:L:37:THR:HG23	2.50	0.51
1:D:166:ILE:HD11	1:D:197:GLN:CG	2.38	0.51
1:E:27:GLN:CG	1:F:44:ARG:HH22	2.24	0.50
1:A:105:ASP:OD2	5:A:502:HOH:O	2.19	0.50
1:A:159:LEU:CD1	1:A:236:LEU:HD22	2.39	0.50
1:F:125:ASP:OD1	1:F:125:ASP:C	2.49	0.50
1:N:138:HIS:NE2	1:N:142:ILE:HD12	2.26	0.50
1:B:125:ASP:OD1	1:B:125:ASP:C	2.50	0.49
1:D:41:PHE:CE1	1:E:322:ILE:HD11	2.47	0.49
1:H:150:LEU:HA	1:H:246:LEU:HD12	1.94	0.49
1:G:328:GLU:OE2	1:G:357:HIS:HB3	2.13	0.49
1:N:159:LEU:HD11	1:N:236[B]:LEU:HD12	1.94	0.48
1:C:328:GLU:OE2	1:C:357:HIS:HB3	2.13	0.48
1:C:333:ASP:HB3	1:C:334:PRO:CD	2.44	0.47
1:N:125:ASP:OD1	1:N:125:ASP:C	2.53	0.47
1:C:220:PRO:HB2	1:C:378:LEU:HD12	1.96	0.47
1:G:377:THR:OG1	1:G:378:LEU:N	2.47	0.47
1:B:135:GLN:O	1:B:169:ALA:HA	2.14	0.47
1:E:201:ARG:HB2	1:E:201:ARG:NH1	2.30	0.47
1:H:150:LEU:CA	1:H:246:LEU:HD12	2.45	0.47
1:E:59:PRO:HD3	1:E:65:PRO:O	2.15	0.46
1:L:125:ASP:OD1	1:L:125:ASP:C	2.53	0.46
1:A:33:GLU:OE1	1:A:110:HIS:ND1	2.40	0.46
1:E:328:GLU:OE2	1:E:357:HIS:HB3	2.16	0.46
4:L:402:Y4F:N3	5:L:505:HOH:O	2.36	0.46
1:M:334:PRO:CB	1:M:362:LEU:HD13	2.46	0.46
1:N:378:LEU:HD21	1:N:380:LEU:HD21	1.97	0.46
1:C:205:TYR:HB3	1:C:209:PRO:HB3	1.98	0.45
1:E:27:GLN:HG2	1:F:44:ARG:HH22	1.81	0.45



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	as pagem	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:349:PHE:HE1	1:B:353:LEU:HD11	1.80	0.45
1:L:137:GLN:O	1:L:141:THR:HG23	2.16	0.45
1:B:183:TRP:CE3	1:B:224:MET:HG3	2.52	0.45
1:H:96:ARG:HA	1:H:101:TYR:O	2.16	0.45
1:L:135:GLN:O	1:L:169:ALA:HA	2.17	0.45
1:H:125:ASP:OD1	1:H:125:ASP:C	2.55	0.45
1:B:94:ILE:O	1:B:96:ARG:NE	2.41	0.45
1:M:110:HIS:CE1	1:M:114:LEU:HD11	2.51	0.45
1:K:115[A]:GLU:OE1	1:K:118:ARG:NH1	2.49	0.45
1:G:110:HIS:CE1	1:G:114:LEU:HD11	2.52	0.44
1:M:334:PRO:HB2	1:M:362:LEU:HD13	1.98	0.44
1:C:282:VAL:HG23	1:C:294:ILE:CD1	2.47	0.44
1:K:297:LEU:HD22	1:K:320:LEU:HD13	2.00	0.44
1:N:340:ALA:HA	4:N:402:Y4F:O4'	2.17	0.44
1:D:130:ILE:HD11	1:D:209:PRO:HG2	2.00	0.44
1:F:163:ASP:OD2	1:F:200:ARG:NH1	2.37	0.44
1:G:258:PHE:HB3	1:G:297:LEU:HD11	2.00	0.44
1:C:224:MET:HE2	1:C:378:LEU:HD13	1.99	0.44
1:C:26:THR:O	1:D:29:ALA:HA	2.18	0.43
1:H:135:GLN:O	1:H:169:ALA:HA	2.18	0.43
1:C:104:ASN:ND2	5:C:513:HOH:O	2.46	0.43
1:G:326:GLN:O	1:G:330:LEU:HD13	2.18	0.43
1:E:76:HIS:O	5:E:501:HOH:O	2.21	0.43
1:M:333:ASP:HB3	1:M:334:PRO:CD	2.48	0.43
1:A:201:ARG:CZ	1:D:192:TYR:HE1	2.31	0.43
1:F:130:ILE:HD11	1:F:209:PRO:HG2	2.01	0.43
1:L:123:THR:N	1:L:124:PRO:CD	2.81	0.43
1:A:17:ASN:ND2	1:A:78:ASN:OD1	2.52	0.43
1:B:138:HIS:CE1	1:B:142:ILE:HD13	2.54	0.43
1:G:190:VAL:HG11	1:G:224:MET:HG2	2.00	0.43
5:A:574:HOH:O	1:B:160:THR:HG21	2.19	0.43
1:K:27:GLN:OE1	1:L:44:ARG:NH1	2.50	0.43
1:A:116:ARG:NH2	5:A:506:HOH:O	2.36	0.43
1:D:135:GLN:O	1:D:169:ALA:HA	2.18	0.43
1:F:192:TYR:HB2	1:G:200:ARG:CG	2.49	0.43
1:F:365:ASP:OD1	5:F:501:HOH:O	2.21	0.43
1:K:282:VAL:HG23	1:K:294:ILE:HD13	2.01	0.43
1:M:342:PRO:HD2	1:M:345:LEU:HD12	2.01	0.43
1:A:200:ARG:HG2	1:D:192:TYR:HB2	2.01	0.43
1:C:377:THR:OG1	1:C:378:LEU:N	2.51	0.42
1:B:150:LEU:HA	1:B:246:LEU:HD13	2.02	0.42



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		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:110:HIS:CE1	1:C:114:LEU:HD11	2.54	0.42
1:A:328:GLU:HB3	1:A:359[A]:HIS:CE1	2.54	0.42
1:A:145:ILE:HD11	1:A:216:LEU:HB2	2.00	0.42
1:G:269:PRO:HB2	1:G:289:LEU:HD21	2.01	0.42
1:N:258:PHE:HB3	1:N:297:LEU:HD11	2.02	0.42
1:H:178:ARG:NH2	1:H:218:ASP:OD2	2.47	0.42
1:N:130:ILE:HD11	1:N:209:PRO:HG2	2.01	0.42
1:N:235:ARG:HG3	1:N:236[B]:LEU:N	2.33	0.42
1:E:205:TYR:HB3	1:E:209:PRO:HB3	2.01	0.42
1:G:27:GLN:OE1	1:H:44:ARG:NH2	2.50	0.42
1:G:45:ALA:HB3	5:G:546:HOH:O	2.19	0.42
1:F:178:ARG:HH21	1:F:377:THR:HG21	1.83	0.42
1:G:15:ASN:N	5:G:527:HOH:O	2.52	0.42
1:C:157:GLU:OE1	1:C:310:ARG:NH2	2.40	0.41
1:E:377:THR:OG1	1:E:378:LEU:N	2.53	0.41
1:K:27:GLN:HG3	1:L:44:ARG:HH22	1.85	0.41
1:B:235:ARG:HD2	1:B:235:ARG:C	2.40	0.41
1:C:224:MET:CE	1:C:378:LEU:HD13	2.51	0.41
1:H:130:ILE:HD11	1:H:209:PRO:HG2	2.01	0.41
1:N:235:ARG:HG3	1:N:236[A]:LEU:N	2.33	0.41
1:E:240:PHE:CE2	1:E:245:LEU:HD23	2.55	0.41
1:G:290:PRO:O	5:G:501:HOH:O	2.21	0.41
1:M:354:THR:O	1:M:354:THR:HG22	2.20	0.41
1:A:120:ALA:O	1:B:116:ARG:NH1	2.54	0.41
1:B:34:LEU:HD12	1:B:86:LEU:HD22	2.02	0.41
1:B:342:PRO:HD2	1:B:345:LEU:HD22	2.02	0.41
1:E:183:TRP:CE3	1:E:378:LEU:HD21	2.55	0.41
1:F:342:PRO:HD2	1:F:345:LEU:HD22	2.02	0.41
1:M:205:TYR:HB3	1:M:209:PRO:HB3	2.02	0.41
1:D:43:TYR:HB2	1:D:49:MET:HG2	2.02	0.41
1:B:160:THR:HG22	1:C:44:ARG:CZ	2.51	0.41
1:C:183:TRP:CH2	1:C:220:PRO:HG2	2.56	0.41
1:K:27:GLN:OE1	1:L:44:ARG:NH2	2.54	0.41
1:K:159:LEU:HD11	1:K:236:LEU:HD22	2.02	0.41
1:M:26:THR:O	1:N:29:ALA:HA	2.20	0.41
1:C:354:THR:HG23	1:C:355:THR:N	2.36	0.41
1:L:309:ASN:OD1	1:L:311:ARG:HB2	2.21	0.40
1:C:94:ILE:HA	1:C:101:TYR:CD2	2.56	0.40
1:E:135:GLN:O	1:E:169:ALA:HA	2.21	0.40
1:A:130:ILE:HB	1:A:211:LEU:HD23	2.02	0.40
1:B:349:PHE:CE1	1:B:353:LEU:HD11	2.56	0.40



Atom-1	Atom-2	Interatomic	Clash
		distance (A)	overlap (A)
1:C:351:ALA:O	1:C:354:THR:HG22	2.22	0.40
1:E:37:THR:HG22	5:E:540:HOH:O	2.21	0.40
1:E:267:ASP:OD2	5:E:502:HOH:O	2.22	0.40
1:E:333:ASP:HB3	1:E:334:PRO:HD2	2.03	0.40
1:F:219:ILE:O	1:F:223:MET:HG3	2.21	0.40
1:B:123:THR:N	1:B:124:PRO:CD	2.85	0.40
1:G:163:ASP:OD2	1:G:165:GLY:N	2.50	0.40
1:L:240:PHE:HA	1:L:246:LEU:HD23	2.03	0.40
1:N:17:ASN:OD1	1:N:18:ASP:N	2.55	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	Perce	entiles
1	А	371/388~(96%)	356~(96%)	15~(4%)	0	100	100
1	В	350/388~(90%)	337~(96%)	13 (4%)	0	100	100
1	С	366/388~(94%)	355~(97%)	11 (3%)	0	100	100
1	D	349/388~(90%)	337~(97%)	12 (3%)	0	100	100
1	Ε	367/388~(95%)	351 (96%)	16 (4%)	0	100	100
1	F	350/388~(90%)	342~(98%)	8 (2%)	0	100	100
1	G	366/388~(94%)	353~(96%)	13~(4%)	0	100	100
1	Н	352/388~(91%)	340~(97%)	12 (3%)	0	100	100
1	Κ	368/388~(95%)	350~(95%)	18~(5%)	0	100	100
1	L	354/388~(91%)	348~(98%)	6(2%)	0	100	100
1	М	367/388~(95%)	355~(97%)	12 (3%)	0	100	100
1	Ν	352/388~(91%)	338 (96%)	14 (4%)	0	100	100
All	All	4312/4656~(93%)	4162 (96%)	150 (4%)	0	100	100



There are no Ramachandran outliers to report.

#### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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	Perce	ntiles
1	А	304/317~(96%)	300~(99%)	4 (1%)	69	62
1	В	283/317~(89%)	274 (97%)	9~(3%)	39	25
1	С	296/317~(93%)	292~(99%)	4 (1%)	67	59
1	D	281/317~(89%)	275~(98%)	6(2%)	53	42
1	Ε	295/317~(93%)	292~(99%)	3 (1%)	76	71
1	F	288/317~(91%)	281 (98%)	7 (2%)	49	36
1	G	298/317~(94%)	290~(97%)	8 (3%)	44	31
1	Н	288/317~(91%)	286~(99%)	2(1%)	84	81
1	Κ	292/317~(92%)	290~(99%)	2(1%)	84	81
1	L	292/317~(92%)	289~(99%)	3 (1%)	76	71
1	М	298/317~(94%)	292~(98%)	6 (2%)	55	44
1	Ν	282/317~(89%)	278~(99%)	4 (1%)	67	59
All	All	3497/3804~(92%)	3439 (98%)	58 (2%)	60	51

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	61	SER
1	А	201	ARG
1	А	218	ASP
1	А	349	PHE
1	В	95	ASP
1	В	96	ARG
1	В	142	ILE
1	В	143	ASN
1	В	195	GLU
1	В	267	ASP
1	В	349	PHE



Mol	Chain	Res	Type
1	В	372	ASP
1	В	377	THR
1	С	218	ASP
1	С	317	ARG
1	С	333	ASP
1	С	359	HIS
1	D	14	PHE
1	D	16	THR
1	D	21	LYS
1	D	125	ASP
1	D	349	PHE
1	D	372	ASP
1	Е	218	ASP
1	Е	231	ASP
1	Е	354	THR
1	F	14	PHE
1	F	58	LEU
1	F	92	ASP
1	F	125	ASP
1	F	349	PHE
1	F	372	ASP
1	F	375	THR
1	G	61	SER
1	G	201	ARG
1	G	218	ASP
1	G	232	ARG
1	G	236	LEU
1	G	267	ASP
1	G	317	ARG
1	G	356	GLN
1	Н	19	GLU
1	Н	349	PHE
1	K	201	ARG
1	K	218	ASP
1	L	125	ASP
1	L	143	ASN
1	L	349	PHE
1	М	61	SER
1	М	128	ARG
1	М	218	ASP
1	М	232	ARG
1	М	317	ARG



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Mol	Chain	Res	Type
1	М	321	GLN
1	Ν	125	ASP
1	Ν	235	ARG
1	N	293	ARG
1	Ν	349	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	С	78	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 monosaccharides in this entry.

## 5.6 Ligand geometry (i)

Of 37 ligands modelled in this entry, 25 are monoatomic - leaving 12 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mal	Turne	Chain	Dec	Tiple	Bo	ond leng	$_{\rm ths}$	B	ond ang	les
WIOI	туре	Unam	nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	Y4F	G	404	-	43,50,50	0.75	1 (2%)	50,78,78	1.03	2 (4%)
4	Y4F	D	402	-	43,50,50	0.76	1 (2%)	50,78,78	0.99	3 (6%)



Mal	Tuno	Chain	Dog	Tink	Bo	ond leng	ths	B	ond ang	les
WIOI	Type	Ullalli	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z  > 2
4	Y4F	L	402	-	43,50,50	0.72	1 (2%)	50,78,78	1.11	3 (6%)
4	Y4F	К	404	-	43,50,50	0.73	1 (2%)	50,78,78	1.03	2 (4%)
4	Y4F	В	402	-	43,50,50	0.77	1 (2%)	50,78,78	0.97	2 (4%)
4	Y4F	Н	403	-	43,50,50	0.74	1 (2%)	50,78,78	1.04	3 (6%)
4	Y4F	А	404	-	43,50,50	0.77	1 (2%)	50,78,78	1.12	3 (6%)
4	Y4F	Ν	402	-	43,50,50	0.77	1 (2%)	50,78,78	1.02	3 (6%)
4	Y4F	F	402	-	43,50,50	0.78	1 (2%)	50,78,78	1.05	3 (6%)
4	Y4F	Е	404	-	43,50,50	0.76	1 (2%)	50,78,78	1.05	<mark>3 (6%)</mark>
4	Y4F	С	404	-	43,50,50	0.74	1 (2%)	50,78,78	0.98	2 (4%)
4	Y4F	М	404	-	43,50,50	0.75	1 (2%)	50,78,78	0.98	2 (4%)

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
4	Y4F	G	404	-	-	5/22/62/62	0/6/7/7
4	Y4F	D	402	-	-	2/22/62/62	0/6/7/7
4	Y4F	L	402	-	-	4/22/62/62	0/6/7/7
4	Y4F	K	404	-	-	5/22/62/62	0/6/7/7
4	Y4F	В	402	-	-	3/22/62/62	0/6/7/7
4	Y4F	Н	403	-	-	5/22/62/62	0/6/7/7
4	Y4F	А	404	-	-	4/22/62/62	0/6/7/7
4	Y4F	Ν	402	-	-	7/22/62/62	0/6/7/7
4	Y4F	F	402	-	-	4/22/62/62	0/6/7/7
4	Y4F	Е	404	-	-	4/22/62/62	0/6/7/7
4	Y4F	С	404	-	-	5/22/62/62	0/6/7/7
4	Y4F	М	404	-	-	5/22/62/62	0/6/7/7

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
4	G	404	Y4F	C40-N42	3.06	1.37	1.32
4	М	404	Y4F	C40-N42	3.04	1.37	1.32
4	Е	404	Y4F	C40-N42	3.03	1.37	1.32
4	F	402	Y4F	C40-N42	3.01	1.36	1.32



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	А	404	Y4F	C40-N42	2.99	1.36	1.32
4	Н	403	Y4F	C40-N42	2.99	1.36	1.32
4	В	402	Y4F	C40-N42	2.98	1.36	1.32
4	Ν	402	Y4F	C40-N42	2.97	1.36	1.32
4	С	404	Y4F	C40-N42	2.96	1.36	1.32
4	L	402	Y4F	C40-N42	2.95	1.36	1.32
4	D	402	Y4F	C40-N42	2.93	1.36	1.32
4	Κ	404	Y4F	C40-N42	2.83	1.36	1.32

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	G	404	Y4F	N42-C40-N39	-4.19	122.13	128.68
4	Е	404	Y4F	N42-C40-N39	-4.15	122.19	128.68
4	L	402	Y4F	N42-C40-N39	-4.13	122.22	128.68
4	Ν	402	Y4F	N42-C40-N39	-4.12	122.24	128.68
4	Н	403	Y4F	N42-C40-N39	-4.08	122.30	128.68
4	F	402	Y4F	N42-C40-N39	-4.08	122.30	128.68
4	В	402	Y4F	N42-C40-N39	-4.08	122.30	128.68
4	А	404	Y4F	N42-C40-N39	-4.04	122.36	128.68
4	М	404	Y4F	N42-C40-N39	-4.04	122.36	128.68
4	D	402	Y4F	N42-C40-N39	-4.04	122.37	128.68
4	К	404	Y4F	N42-C40-N39	-4.03	122.37	128.68
4	С	404	Y4F	N42-C40-N39	-3.95	122.50	128.68
4	L	402	Y4F	P27-O28-C3'	-3.07	108.25	119.41
4	F	402	Y4F	P27-O28-C3'	-2.75	109.40	119.41
4	А	404	Y4F	O2'-C2'-C3'	2.47	118.18	111.17
4	L	402	Y4F	C5-C6-N01	2.37	123.95	120.35
4	А	404	Y4F	C5-C6-N01	2.36	123.94	120.35
4	Н	403	Y4F	C5-C6-N01	2.36	123.94	120.35
4	М	404	Y4F	C5-C6-N01	2.36	123.94	120.35
4	Ν	402	Y4F	C2'-C3'-C4'	2.35	107.39	103.22
4	F	402	Y4F	C5-C6-N01	2.33	123.90	120.35
4	С	404	Y4F	C5-C6-N01	2.29	123.83	120.35
4	G	404	Y4F	C5-C6-N01	2.29	123.83	120.35
4	Е	404	Y4F	C5-C6-N01	2.28	123.82	120.35
4	K	404	Y4F	C5-C6-N01	2.28	123.82	120.35
4	D	402	Y4F	C5-C6-N01	2.27	123.80	120.35
4	В	402	Y4F	C5-C6-N01	2.22	123.73	120.35
4	Ν	402	Y4F	C5-C6-N01	2.21	123.70	120.35
4	Н	403	Y4F	02'-C2'-C3'	2.20	117.41	111.17
4	Е	404	Y4F	C22-C21-C32	-2.12	98.90	102.89



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Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
4	D	402	Y4F	P27-O28-C3'	-2.09	111.81	119.41

There are no chirality outliers.

All (53) torsion outliers are listed below:

Mol	Chain	$\mathbf{Res}$	Type	Atoms
4	A	404	Y4F	C3'-O28-P27-O30
4	В	402	Y4F	C3'-O28-P27-O29
4	В	402	Y4F	C3'-O28-P27-O30
4	С	404	Y4F	C3'-O28-P27-O30
4	Е	404	Y4F	C3'-O28-P27-O30
4	G	404	Y4F	C3'-O28-P27-O30
4	Н	403	Y4F	C3'-O28-P27-O30
4	K	404	Y4F	C3'-O28-P27-O30
4	М	404	Y4F	C3'-O28-P27-O30
4	N	402	Y4F	C3'-O28-P27-O30
4	D	402	Y4F	O17-C16-C4'-O4'
4	N	402	Y4F	O17-C16-C4'-O4'
4	В	402	Y4F	C3'-O28-P27-O26
4	N	402	Y4F	C3'-O28-P27-O26
4	К	404	Y4F	C3'-O28-P27-O26
4	С	404	Y4F	C3'-O28-P27-O29
4	Н	403	Y4F	C3'-O28-P27-O29
4	K	404	Y4F	C3'-O28-P27-O29
4	N	402	Y4F	C3'-O28-P27-O29
4	N	402	Y4F	O17-C16-C4'-C3'
4	Е	404	Y4F	C4'-C16-O17-P18
4	G	404	Y4F	C4'-C16-O17-P18
4	Н	403	Y4F	C4'-C16-O17-P18
4	K	404	Y4F	C4'-C16-O17-P18
4	С	404	Y4F	C3'-O28-P27-O26
4	Н	403	Y4F	C3'-O28-P27-O26
4	С	404	Y4F	C4'-C16-O17-P18
4	М	404	Y4F	C4'-C16-O17-P18
4	G	404	Y4F	C3'-O28-P27-O26
4	A	404	Y4F	C4'-C16-O17-P18
4	F	402	Y4F	C4'-C16-O17-P18
4	L	402	Y4F	C4'-C16-O17-P18
4	N	402	Y4F	C2'-C3'-O28-P27
4	М	404	Y4F	C3'-O28-P27-O26
4	A	404	Y4F	C3'-O28-P27-O26
4	D	402	Y4F	C4'-C16-O17-P18



Mol	Chain	Res	Type	Atoms
4	Е	404	Y4F	C3'-O28-P27-O26
4	F	402	Y4F	O17-C16-C4'-O4'
4	F	402	Y4F	C3'-O28-P27-O30
4	G	404	Y4F	C3'-O28-P27-O29
4	L	402	Y4F	C3'-O28-P27-O30
4	М	404	Y4F	C3'-O28-P27-O29
4	А	404	Y4F	O17-C16-C4'-O4'
4	С	404	Y4F	O17-C16-C4'-O4'
4	G	404	Y4F	O17-C16-C4'-O4'
4	Н	403	Y4F	O17-C16-C4'-O4'
4	Κ	404	Y4F	O17-C16-C4'-O4'
4	F	402	Y4F	C3'-O28-P27-O26
4	L	402	Y4F	C3'-O28-P27-O26
4	N	402	Y4F	C4'-C3'-O28-P27
4	Е	404	Y4F	O17-C16-C4'-O4'
4	L	402	Y4F	O17-C16-C4'-O4'
4	М	404	Y4F	O17-C16-C4'-O4'

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There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	402	Y4F	1	0
4	N	402	Y4F	1	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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

















































# 5.7 Other polymers (i)

There are no such residues in this entry.

# 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



# 6 Fit of model and data (i)

# 6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median,  $95^{th}$  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	$\langle RSRZ \rangle$	#RSRZ>2	$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q < 0.9
1	А	369/388~(95%)	0.15	9 (2%) 59 54	16, 27, 60, 125	0
1	В	354/388~(91%)	0.26	17 (4%) 30 25	16, 28, 72, 98	0
1	С	368/388~(94%)	0.17	10 (2%) 54 49	18, 30, 66, 94	0
1	D	353/388~(90%)	0.26	9 (2%) 57 52	22, 35, 68, 94	0
1	Ε	369/388~(95%)	0.12	11 (2%) 50 44	19, 29, 60, 106	0
1	F	353/388~(90%)	0.20	10 (2%) 53 47	20, 32, 62, 93	0
1	G	368/388~(94%)	0.08	4 (1%) 80 78	18, 28, 56, 91	0
1	Н	356/388~(91%)	0.15	13 (3%) 41 36	18, 28, 62, 89	0
1	Κ	369/388~(95%)	0.09	6 (1%) 72 68	19, 29, 64, 92	0
1	L	357/388~(92%)	0.05	5 (1%) 75 72	17, 27, 50, 76	0
1	М	369/388~(95%)	0.18	11 (2%) 50 44	20, 31, 64, 97	0
1	Ν	354/388~(91%)	0.23	16 (4%) 33 27	21, 33, 70, 96	0
All	All	4339/4656~(93%)	0.16	121 (2%) 53 47	16, 30, 64, 125	0

All (121) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	94	ILE	7.8
1	D	14	PHE	6.8
1	А	207	ASP	6.8
1	Н	142	ILE	5.6
1	А	208	SER	5.5
1	В	99	ASP	5.0
1	Н	170	PHE	4.9
1	В	98	ALA	4.9
1	F	14	PHE	4.8
1	Н	139	PHE	4.7
1	Ν	14	PHE	4.5



Mol	Chain	Res	Type	RSRZ
1	Κ	355	THR	4.3
1	Κ	357	HIS	4.3
1	Н	98	ALA	4.1
1	А	205	TYR	4.1
1	Е	14	PHE	4.1
1	М	356	GLN	4.0
1	Ν	94	ILE	3.8
1	Е	355	THR	3.8
1	Е	356	GLN	3.7
1	D	194	LEU	3.6
1	Ν	382	PRO	3.5
1	D	101	TYR	3.5
1	Е	232	ARG	3.5
1	N	101	TYR	3.4
1	С	60	ALA	3.4
1	C	69	ALA	3.4
1	М	14	PHE	3.3
1	Н	368	LYS	3.3
1	С	282	VAL	3.3
1	D	99	ASP	3.2
1	Ν	15	ASN	3.2
1	В	62	PRO	3.2
1	F	304	TYR	3.2
1	В	106	LEU	3.1
1	Н	14	PHE	3.1
1	Н	194	LEU	3.1
1	М	76	HIS	3.1
1	Κ	356	GLN	3.1
1	G	234	LYS	3.0
1	K	322	ILE	3.0
1	L	48	PRO	3.0
1	E	205	TYR	2.9
1	N	16	THR	2.9
1	B	109	LEU	2.9
1	D	170	PHE	2.8
1	А	206	GLY	2.8
1	N	41	PHE	2.8
1	N	106	LEU	2.8
1	А	332	PRO	2.8
1	Н	104	ASN	2.8
1	В	83	LEU	2.7
1	F	194	LEU	2.7



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Mol	Chain	Res	Type	RSRZ
1	F	58	LEU	2.7
1	F	109	LEU	2.7
1	М	322	ILE	2.7
1	М	231	ASP	2.7
1	В	96	ARG	2.6
1	Ν	13	ARG	2.6
1	K	233	SER	2.6
1	F	99	ASP	2.6
1	Н	99	ASP	2.6
1	N	142	ILE	2.6
1	Н	242	ARG	2.6
1	N	109	LEU	2.5
1	G	207	ASP	2.5
1	D	41	PHE	2.5
1	F	168	ILE	2.5
1	N	194	LEU	2.5
1	F	106	LEU	2.5
1	D	192	TYR	2.5
1	С	62	PRO	2.5
1	Н	109	LEU	2.4
1	В	104	ASN	2.4
1	Е	382	PRO	2.4
1	В	111	GLN	2.4
1	Е	231	ASP	2.4
1	М	77	THR	2.4
1	М	58	LEU	2.3
1	F	175	PRO	2.3
1	L	109	LEU	2.3
1	А	68	ARG	2.3
1	Н	192	TYR	2.3
1	М	60	ALA	2.3
1	Е	331	THR	2.3
1	E	68	ARG	2.3
1	Ν	22	ARG	2.3
1	A	75	ALA	2.3
1	М	62	PRO	2.3
1	С	64	GLY	2.3
1	М	71	HIS	2.3
1	G	352	LEU	2.3
1	С	77	THR	2.2
1	В	16	THR	2.2
1	В	79	ASP	2.2



Mol	Chain	Res	Type	RSRZ
1	В	13	ARG	2.2
1	С	203	GLY	2.2
1	С	331	THR	2.2
1	L	198	LEU	2.2
1	F	100	GLY	2.2
1	Е	357	HIS	2.1
1	Е	211	LEU	2.1
1	L	64	GLY	2.1
1	G	357	HIS	2.1
1	С	332	PRO	2.1
1	А	69	ALA	2.1
1	В	25	TRP	2.1
1	D	175	PRO	2.1
1	С	231	ASP	2.1
1	Ν	99	ASP	2.1
1	А	204	THR	2.0
1	Н	12	GLY	2.0
1	М	282	VAL	2.0
1	Ν	54	VAL	2.0
1	В	58	LEU	2.0
1	L	382	PRO	2.0
1	Ν	96	ARG	2.0
1	В	198	LEU	2.0
1	D	95	ASP	2.0
1	В	382	PRO	2.0
1	Κ	382	PRO	2.0

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## 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,  $95^{th}$  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	$B-factors(A^2)$	Q<0.9
3	MG	С	402	1/1	0.90	0.06	38,38,38,38	0
3	MG	Е	403	1/1	0.90	0.13	66,66,66,66	0
3	MG	Е	402	1/1	0.91	0.08	23,23,23,23	0
3	MG	М	402	1/1	0.91	0.07	30,30,30,30	0
4	Y4F	L	402	44/44	0.92	0.15	35,56,70,77	0
4	Y4F	F	402	44/44	0.93	0.15	35,49,73,79	0
3	MG	G	402	1/1	0.94	0.06	27,27,27,27	0
4	Y4F	D	402	44/44	0.94	0.12	31,45,62,69	0
3	MG	М	403	1/1	0.95	0.07	45,45,45,45	0
3	MG	К	402	1/1	0.96	0.05	28,28,28,28	0
3	MG	А	402	1/1	0.96	0.05	28,28,28,28	0
4	Y4F	Н	403	44/44	0.96	0.08	28,36,45,49	0
3	MG	Н	402	1/1	0.96	0.04	33,33,33,33	0
4	Y4F	N	402	44/44	0.96	0.12	24,35,52,63	0
4	Y4F	В	402	44/44	0.97	0.10	20,30,49,53	0
3	MG	С	403	1/1	0.97	0.03	44,44,44,44	0
3	MG	G	403	1/1	0.97	0.10	43,43,43,43	0
4	Y4F	Е	404	44/44	0.98	0.09	14,21,30,36	0
4	Y4F	А	404	44/44	0.98	0.10	11,17,21,26	0
4	Y4F	G	404	44/44	0.98	0.10	13,20,26,27	0
3	MG	А	403	1/1	0.98	0.18	44,44,44,44	0
4	Y4F	K	404	44/44	0.98	0.09	14,20,25,29	0
4	Y4F	С	404	44/44	0.98	0.09	$15,\!22,\!31,\!37$	0
3	MG	K	403	1/1	0.98	0.16	43,43,43,43	0
2	ZN	G	401	1/1	0.99	0.19	29,29,29,29	0
2	ZN	Н	401	1/1	0.99	0.11	30,30,30,30	0
2	ZN	L	401	1/1	0.99	0.11	32,32,32,32	0
2	ZN	N	401	1/1	0.99	0.12	$35,\!35,\!35,\!35$	0
2	ZN	В	401	1/1	0.99	0.11	42,42,42,42	0
2	ZN	D	401	1/1	0.99	0.12	$35,\!35,\!35,\!35$	0
4	Y4F	М	404	44/44	0.99	0.09	17,23,31,34	0
2	ZN	F	401	1/1	0.99	0.16	33,33,33,33	0
2	ZN	Е	401	1/1	1.00	0.13	24,24,24,24	0
2	ZN	K	401	1/1	1.00	0.10	20,20,20,20	0
2	ZN	С	401	1/1	1.00	0.14	26,26,26,26	0
2	ZN	М	401	1/1	1.00	0.12	$23,\!23,\!23,\!23$	0
2	ZN	A	401	1/1	1.00	0.14	26,26,26,26	0

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































# 6.5 Other polymers (i)

There are no such residues in this entry.

