

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

#### Feb 21, 2024 – 09:22 AM EST

PDB ID	:	4Q66
Title	:	Structure of Exomer bound to Arf1
Authors	:	Paczkowski, J.E.; Fromme, J.C.
Deposited on	:	2014-04-21
Resolution	:	3.35  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 (1)) 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 3.35 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.



Motrie	Whole archive	Similar resolution
	$(\# { m Entries})$	$(\# { m Entries},  { m resolution}  { m range}({ m \AA}))$
$R_{free}$	130704	1558 (3.42 - 3.30)
Clashscore	141614	1627 (3.42 - 3.30)
Ramachandran outliers	138981	1599 (3.42 - 3.30)
Sidechain outliers	138945	1598 (3.42 - 3.30)
RSRZ outliers	127900	1507 (3.42 - 3.30)

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	368	2% <b>5</b> 3%		8% •	39%	_		
1	D	368	4%	<u> </u>		5.00	_		
	D	308	5%	6%		54%			
	G	368	49% 4%		8%	43%			
1	J	368	36%	6%	5	7%			
2	В	739	609	6	7% •	31%	-		



Mol	Chain	Length	Quality of chain						
2	Е	739	.% •	66	5%	9%	25%		
2	Н	739	4%	42%	·	54%			
2	Κ	739	2%	e	8%	12% •	20%		
3	С	175	5%	6	8%	9%	23%		
3	F	175	6%		74%	9%	17%		
3	Ι	175	8%	44%	5%	51%			
3	L	175	9%	65	%	13% •	21%		



## 2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 26303 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace	
1	Δ	1 006	Total C N	Ο	$\mathbf{S}$	0	0	0
	A	220	1788 1149 309	323	$\overline{7}$	0	0	0
1	т	159	Total C N	Ο	S	0	0	0
	J	100	1240  801  210	226	3	0		U
1	C	911	Total C N	Ο	S	0	0	0
	G	211	1655  1064  281	304	6	0	0	0
1	1 D	171	Total C N	Ο	S	0	0	0
		1/1	1357  878  230	245	4	0	0	0

• Molecule 1 is a protein called Chs5p.

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	-3	MET	-	initiating methionine	UNP W7PD87
А	-2	ASP	-	expression tag	UNP W7PD87
А	-1	PRO	-	expression tag	UNP W7PD87
А	0	GLU	-	expression tag	UNP W7PD87
А	1	PHE	-	expression tag	UNP W7PD87
J	-3	MET	-	initiating methionine	UNP W7PD87
J	-2	ASP	-	expression tag	UNP W7PD87
J	-1	PRO	-	expression tag	UNP W7PD87
J	0	GLU	-	expression tag	UNP W7PD87
J	1	PHE	-	expression tag	UNP W7PD87
G	-3	MET	-	initiating methionine	UNP W7PD87
G	-2	ASP	-	expression tag	UNP W7PD87
G	-1	PRO	-	expression tag	UNP W7PD87
G	0	GLU	-	expression tag	UNP W7PD87
G	1	PHE	-	expression tag	UNP W7PD87
D	-3	MET	-	initiating methionine	UNP W7PD87
D	-2	ASP	-	expression tag	UNP W7PD87
D	-1	PRO	-	expression tag	UNP W7PD87
D	0	GLU	-	expression tag	UNP W7PD87
D	1	PHE	_	expression tag	UNP W7PD87



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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	K	V 502	Total	С	Ν	Ο	$\mathbf{S}$	0	0	0
	Γ	090	4809	3106	792	888	23	0	0	0
9	F	557	Total	С	Ν	0	S	0	0	0
	Ľ	557	4493	2903	738	830	22	0		0
2	р	507	Total	С	Ν	0	S	0	0	0
	D	507	4108	2656	673	758	21	0	0	0
2	) Ц	338	Total	С	Ν	Ο	S	0	0	0
	338	2711	1747	447	499	18	0	0	U	

• Molecule 2 is a protein called Protein BCH1.

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
К	725	GLY	-	expression tag	UNP Q05029
K	726	THR	-	expression tag	UNP Q05029
K	727	GLU	-	expression tag	UNP Q05029
К	728	ASN	-	expression tag	UNP Q05029
K	729	LEU	-	expression tag	UNP Q05029
K	730	TYR	-	expression tag	UNP Q05029
К	731	PHE	-	expression tag	UNP Q05029
К	732	GLN	-	expression tag	UNP Q05029
К	733	GLY	-	expression tag	UNP Q05029
K	734	HIS	-	expression tag	UNP Q05029
К	735	HIS	-	expression tag	UNP Q05029
K	736	HIS	-	expression tag	UNP Q05029
K	737	HIS	-	expression tag	UNP Q05029
К	738	HIS	-	expression tag	UNP Q05029
K	739	HIS	-	expression tag	UNP Q05029
Е	725	GLY	-	expression tag	UNP Q05029
Е	726	THR	-	expression tag	UNP Q05029
E	727	GLU	-	expression tag	UNP Q05029
Е	728	ASN	-	expression tag	UNP Q05029
Е	729	LEU	-	expression tag	UNP Q05029
E	730	TYR	-	expression tag	UNP Q05029
Е	731	PHE	-	expression tag	UNP Q05029
Е	732	GLN	-	expression tag	UNP Q05029
E	733	GLY	-	expression tag	UNP Q05029
Е	734	HIS	-	expression tag	UNP Q05029
Е	735	HIS	-	expression tag	UNP Q05029
Е	736	HIS	-	expression tag	UNP Q05029
Е	737	HIS	-	expression tag	UNP Q05029
Е	738	HIS	-	expression tag	UNP Q05029
E	739	HIS	-	expression tag	UNP Q05029



Chain	Residue	Modelled	Actual	Comment	Reference
В	725	GLY	-	expression tag	UNP Q05029
В	726	THR	-	expression tag	UNP Q05029
В	727	GLU	-	expression tag	UNP Q05029
В	728	ASN	-	expression tag	UNP Q05029
В	729	LEU	-	expression tag	UNP Q05029
В	730	TYR	-	expression tag	UNP Q05029
В	731	PHE	-	expression tag	UNP Q05029
В	732	GLN	-	expression tag	UNP Q05029
В	733	GLY	-	expression tag	UNP Q05029
В	734	HIS	-	expression tag	UNP Q05029
В	735	HIS	-	expression tag	UNP Q05029
В	736	HIS	-	expression tag	UNP Q05029
В	737	HIS	-	expression tag	UNP Q05029
В	738	HIS	-	expression tag	UNP Q05029
В	739	HIS	-	expression tag	UNP Q05029
Н	725	GLY	-	expression tag	UNP Q05029
Н	726	THR	-	expression tag	UNP Q05029
Н	727	GLU	-	expression tag	UNP Q05029
Н	728	ASN	-	expression tag	UNP Q05029
Н	729	LEU	-	expression tag	UNP Q05029
Н	730	TYR	-	expression tag	UNP Q05029
Н	731	PHE	-	expression tag	UNP Q05029
H	732	GLN	-	expression tag	UNP Q05029
Н	733	GLY	-	expression tag	UNP Q05029
Н	734	HIS	-	expression tag	UNP Q05029
H	735	HIS	-	expression tag	UNP Q05029
Н	736	HIS	-	expression tag	UNP Q05029
Н	737	HIS	-	expression tag	UNP Q05029
H	738	HIS	-	expression tag	UNP Q05029
Н	739	HIS	-	expression tag	UNP Q05029

• Molecule 3 is a protein called ADP-ribosylation factor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	F	146	Total	С	Ν	0	S	0	0	0
0	Г	140	1173	745	205	217	6	0	0	0
9	т	120	Total	С	Ν	0	S	0	0	0
0	L	159	1115	711	195	203	6	0		0
2	С	124	Total	С	Ν	0	S	0	0	0
0	C	104	1056	673	177	202	4	0	0	0
2	3 I	86	Total	С	Ν	0	S	0	0	0
5		80	666	426	113	123	4	0	0	0





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Chain	Residue	Modelled	Actual	Comment	Reference
F	7	MET	-	expression tag	UNP P11076
F	8	THR	_	expression tag	UNP P11076
F	9	GLU	_	expression tag	UNP P11076
F	10	ASN	-	expression tag	UNP P11076
F	11	LEU	-	expression tag	UNP P11076
F	12	TYR	-	expression tag	UNP P11076
F	13	PHE	-	expression tag	UNP P11076
F	14	GLN	-	expression tag	UNP P11076
F	15	GLY	-	expression tag	UNP P11076
F	16	SER	-	expression tag	UNP P11076
F	17	GLY	-	expression tag	UNP P11076
F	71	LEU	GLN	engineered mutation	UNP P11076
L	7	MET	-	expression tag	UNP P11076
L	8	THR	-	expression tag	UNP P11076
L	9	GLU	-	expression tag	UNP P11076
L	10	ASN	-	expression tag	UNP P11076
L	11	LEU	-	expression tag	UNP P11076
L	12	TYR	-	expression tag	UNP P11076
L	13	PHE	-	expression tag	UNP P11076
L	14	GLN	-	expression tag	UNP P11076
L	15	GLY	-	expression tag	UNP P11076
L	16	SER	-	expression tag	UNP P11076
L	17	GLY	-	expression tag	UNP P11076
L	71	LEU	GLN	engineered mutation	UNP P11076
С	7	MET	-	expression tag	UNP P11076
C	8	THR	-	expression tag	UNP P11076
C	9	GLU	-	expression tag	UNP P11076
C	10	ASN	-	expression tag	UNP P11076
C	11	LEU	-	expression tag	UNP P11076
C	12	TYR	-	expression tag	UNP P11076
C	13	PHE	-	expression tag	UNP P11076
C	14	GLN	-	expression tag	UNP P11076
C	15	GLY	-	expression tag	UNP P11076
C	16	SER	-	expression tag	UNP P11076
C	17	GLY	-	expression tag	UNP P11076
	71	LEU	GLN	engineered mutation	UNP P11076
	7	MET	-	expression tag	UNP P11076
	8	THR	-	expression tag	UNP P11076
	9	GLU	-	expression tag	UNP P11076
	10	ASN	-	expression tag	UNP P11076
			-	expression tag	UNP P11076
	12	TYR	-	expression tag	UNP P11076

There are 48 discrepancies between the modelled and reference sequences:



Chain	Residue	Modelled	Actual	Comment	Reference
Ι	13	PHE	-	expression tag	UNP P11076
Ι	14	GLN	-	expression tag	UNP P11076
Ι	15	GLY	-	expression tag	UNP P11076
Ι	16	SER	-	expression tag	UNP P11076
Ι	17	GLY	-	expression tag	UNP P11076
Ι	71	LEU	GLN	engineered mutation	UNP P11076

• Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula:  $C_{10}H_{17}N_6O_{13}P_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf		
4	F	1	Total	С	Ν	Ο	Р	0	0	
4	4 Γ	L	32	10	6	13	3	0		
4	т	1	Total	С	Ν	Ο	Р	0	0	
4 L	1	32	10	6	13	3	0	0		
4	C	1	Total	С	Ν	Ο	Р	0	0	
4	4 C	1	32	10	6	13	3	0	0	
4	т	1	Total	С	Ν	Ο	Р	0	0	
4	1	1	32	10	6	13	3	0	0	

• Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	F	1	Total Mg 1 1	0	0



Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	L	1	Total Mg 1 1	0	0
5	С	1	Total Mg 1 1	0	0
5	Ι	1	Total Mg 1 1	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: Chs5p



















• Molecule 3: ADP-ribosylation factor 1





## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	114.66Å 208.17Å 155.08Å	Deperitor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $105.48^{\circ}$ $90.00^{\circ}$	Depositor
Posclution(Å)	43.17 - 3.35	Depositor
Resolution (A)	50.00 - 3.35	EDS
% Data completeness	97.0 (43.17-3.35)	Depositor
(in resolution range)	91.2(50.00-3.35)	EDS
R <sub>merge</sub>	(Not available)	Depositor
R <sub>sym</sub>	0.09	Depositor
$< I/\sigma(I) > 1$	1.55 (at 3.33Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
D D.	0.279 , $0.310$	Depositor
$\mathbf{n}, \mathbf{n}_{free}$	0.285 , $0.312$	DCC
$R_{free}$ test set	2557 reflections $(2.63%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	93.0	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.27, 57.0	EDS
L-test for twinning <sup>2</sup>	$<  L  > = 0.47, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	26303	wwPDB-VP
Average B, all atoms $(Å^2)$	107.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 9.45% 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: MG, GNP

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
	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	А	0.21	0/1818	0.42	0/2456
1	D	0.21	0/1379	0.39	0/1862
1	G	0.20	0/1679	0.40	0/2269
1	J	0.20	0/1258	0.39	0/1699
2	В	0.21	0/4175	0.36	0/5634
2	Ε	0.21	0/4571	0.37	0/6183
2	Н	0.20	0/2740	0.33	0/3682
2	Κ	0.21	0/4901	0.36	0/6630
3	С	0.20	0/1070	0.35	0/1442
3	F	0.20	0/1194	0.34	0/1609
3	Ι	0.20	0/667	0.34	0/887
3	L	0.20	0/1131	0.36	0/1521
All	All	0.21	0/26583	0.37	0/35874

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	1788	0	1872	20	0



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4	પ્ય	00	

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1357	0	1435	15	0
1	G	1655	0	1743	21	0
1	J	1240	0	1325	16	0
2	В	4108	0	4150	52	0
2	Е	4493	0	4560	40	0
2	Н	2711	0	2781	15	0
2	Κ	4809	0	4841	46	0
3	С	1056	0	1042	10	0
3	F	1173	0	1158	10	0
3	Ι	666	0	681	6	0
3	L	1115	0	1109	23	0
4	С	32	0	13	1	0
4	F	32	0	13	0	0
4	Ι	32	0	13	1	0
4	L	32	0	13	1	0
5	С	1	0	0	0	0
5	F	1	0	0	0	0
5	Ι	1	0	0	0	0
5	L	1	0	0	0	0
All	All	26303	0	26749	259	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 (259) 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 (Å)	overlap (Å)
2:B:26:VAL:O	2:B:28:GLN:N	1.72	1.19
3:L:100:ILE:O	3:L:103:ALA:N	1.85	1.09
2:B:22:ARG:O	2:B:23:ARG:NE	1.88	1.06
3:L:100:ILE:HG23	3:L:101:GLY:H	1.31	0.96
3:L:100:ILE:HG23	3:L:101:GLY:N	1.81	0.93
3:L:100:ILE:CG2	3:L:101:GLY:H	1.83	0.90
1:A:151:THR:HG22	1:A:153:SER:H	1.42	0.85
2:B:21:GLN:HE22	2:B:22:ARG:HD3	1.42	0.81
3:L:100:ILE:O	3:L:102:GLU:N	2.15	0.79
2:B:24:ALA:O	2:B:26:VAL:HG23	1.88	0.74
1:D:75:GLY:HA2	2:E:317:ILE:HG23	1.69	0.73
2:K:218:GLN:HE22	2:K:421:LEU:HD12	1.53	0.73
1:G:72:GLU:O	1:G:76:THR:OG1	2.06	0.73
2:B:24:ALA:O	2:B:26:VAL:N	2.21	0.73



	A	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
2:E:362:VAL:HG13	2:E:363:LYS:HG2	1.73	0.70	
2:B:26:VAL:HG12	2:B:27:GLY:N	2.06	0.70	
3:L:96:ASP:OD2	3:L:96:ASP:N	2.25	0.69	
2:K:162:ILE:HB	2:K:170:SER:HB3	1.74	0.69	
1:G:241:ARG:H	1:G:241:ARG:HD3	1.60	0.67	
2:B:21:GLN:OE1	2:B:22:ARG:HB3	1.96	0.66	
2:B:21:GLN:HE22	2:B:22:ARG:CD	2.08	0.65	
1:G:71:LEU:O	1:G:76:THR:HG23	1.97	0.64	
2:E:685:MET:HB2	2:E:689:LYS:HD3	1.80	0.64	
3:L:99:ARG:O	3:L:99:ARG:HG3	1.97	0.64	
2:K:459:LYS:HE3	2:K:574:LEU:HD13	1.79	0.64	
1:G:33:VAL:HG13	1:G:34:LEU:HD12	1.81	0.63	
3:L:100:ILE:CG2	3:L:101:GLY:N	2.44	0.63	
3:L:100:ILE:O	3:L:101:GLY:C	2.37	0.63	
2:B:21:GLN:NE2	2:B:22:ARG:HG2	2.13	0.62	
3:L:73:ARG:HG3	3:L:74:ILE:HG12	1.80	0.62	
1:A:71:LEU:O	1:A:76:THR:OG1	2.17	0.62	
2:E:452:MET:SD	2:E:452:MET:N	2.72	0.61	
2:E:637:THR:OG1	2:E:640:GLN:OE1	2.18	0.61	
1:A:166:HIS:ND1	1:A:170:ASP:OD2	2.34	0.60	
1:A:34:LEU:HD22	1:D:6:VAL:HG11	1.82	0.60	
3:C:125:ALA:HB3	3:C:157:ALA:HA	1.82	0.60	
1:A:35:LEU:HB3	1:A:39:VAL:HG21	1.84	0.60	
2:E:144:ARG:NH1	2:E:195:GLU:OE2	2.34	0.60	
2:E:218:GLN:HE22	2:E:421:LEU:HD12	1.67	0.60	
2:E:550:ASP:OD2	2:E:587:ARG:NH1	2.35	0.59	
2:E:4:GLN:H	2:E:115:LEU:HD11	1.68	0.59	
2:B:459:LYS:HD3	2:B:574:LEU:HD13	1.85	0.59	
2:K:144:ARG:NH1	2:K:195:GLU:OE2	2.36	0.59	
3:F:37:LEU:HB3	3:F:56:VAL:HG11	1.85	0.59	
1:J:59:GLN:NE2	2:K:375:GLU:OE2	2.35	0.58	
1:D:33:VAL:HG13	1:D:34:LEU:HD12	1.84	0.58	
3:L:140:THR:HG22	3:L:145:LEU:HD12	1.86	0.58	
2:K:118:ASP:OD1	2:K:118:ASP:N	2.37	0.58	
2:E:500:ARG:NH2	2:E:541:ASP:OD1	2.36	0.58	
2:B:25:ARG:HG3	2:B:25:ARG:O	2.04	0.57	
2:K:3:SER:O	2:K:5:THR:N	2.35	0.57	
1:A:22:THR:OG1	1:A:24:ASP:OD1	2.19	0.57	
2:K:685:MET:HB2	2:K:689:LYS:HD3	1.86	0.57	
1:A:75:GLY:HA2	2:B:317:ILE:HG23	1.87	0.57	
2:K:140:TRP:O	2:K:203:ARG:NH1	2.36	0.57	



			Interatomic Clash		
Atom-1	Atom-2	distance (Å)	overlap (Å)		
2:H:307:ILE:HD13	2:H:323:ILE:HG12	1.87	0.57		
1:G:75:GLY:HA2	2:H:317:ILE:HG23	1.87	0.57		
2:B:500:ARG:NH2	2:B:541:ASP:OD1	2.38	0.57		
3:L:100:ILE:C	3:L:102:GLU:N	2.59	0.56		
1:A:109:LYS:HE3	1:A:152:THR:HB	1.88	0.56		
3:L:93:ASP:CG	3:L:96:ASP:OD2	2.43	0.56		
1:A:176:VAL:HG12	1:A:214:HIS:HB2	1.88	0.56		
3:F:104:ARG:NH1	3:F:142:LYS:O	2.39	0.56		
1:J:144:GLU:OE1	1:J:160:LYS:NZ	2.39	0.55		
2:H:255:LEU:HD12	2:H:271:LEU:HB2	1.88	0.55		
1:J:103:LEU:HD21	1:J:108:LEU:HB3	1.87	0.55		
2:B:685:MET:HB2	2:B:689:LYS:HD3	1.89	0.55		
2:B:550:ASP:OD2	2:B:587:ARG:NH1	2.40	0.54		
2:B:457:GLU:OE2	2:B:458:GLN:N	2.41	0.54		
2:K:148:VAL:HG21	2:K:196:THR:HG21	1.89	0.53		
3:C:37:LEU:HD21	3:C:166:LEU:HB3	1.89	0.53		
1:G:151:THR:OG1	1:G:154:GLY:O	2.24	0.53		
2:E:459:LYS:HD2	2:E:574:LEU:HD13	1.90	0.53		
2:B:144:ARG:NH1	2:B:195:GLU:OE2	2.42	0.53		
1:G:71:LEU:O	1:G:76:THR:CG2	2.57	0.53		
2:K:696:SER:HB3	3:L:79:ARG:HD2	1.90	0.53		
1:D:8:LEU:HD22	1:D:22:THR:HG22	1.90	0.53		
3:F:125:ALA:HB3	3:F:157:ALA:HA	1.91	0.53		
3:I:37:LEU:HD21	3:I:166:LEU:HB3	1.91	0.53		
2:E:18:ALA:HB1	2:E:37:LEU:HD21	1.91	0.52		
3:L:125:ALA:HB3	3:L:157:ALA:HA	1.90	0.52		
2:K:120:PRO:O	2:K:122:ILE:HG13	2.09	0.52		
2:B:218:GLN:HE22	2:B:421:LEU:HD12	1.75	0.52		
2:B:307:ILE:HD13	2:B:323:ILE:HG12	1.91	0.52		
2:B:21:GLN:CG	2:B:22:ARG:N	2.73	0.52		
3:F:26:ASP:O	3:F:99:ARG:NH2	2.42	0.52		
2:E:259:THR:HA	2:E:416:LYS:HD2	1.92	0.51		
2:B:21:GLN:NE2	2:B:22:ARG:CG	2.73	0.51		
2:B:696:SER:O	3:C:79:ARG:NE	2.44	0.51		
2:B:244:LEU:HD12	2:B:247:LEU:HD12	1.91	0.51		
2:B:537:GLU:O	2:B:539:TRP:N	2.43	0.51		
1:J:83:VAL:HG12	1:J:159:GLU:HG3	1.91	0.51		
1:G:12:LYS:HG3	2:K:381:PRO:HD2	1.93	0.51		
1:A:54:GLU:HA	1:A:57:LYS:HE2	1.91	0.50		
2:B:255:LEU:HD12	2:B:271:LEU:HB2	1.92	0.50		
2:K:195:GLU:OE2	2:K:251:LYS:NZ	2.44	0.50		



		Interatomic	Clash	
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)	
2:B:21:GLN:HG3	2:B:22:ARG:H	1.77	0.50	
2:K:550:ASP:OD2	2:K:587:ARG:NH1	2.44	0.50	
2:H:692:ASN:HD22	3:I:73:ARG:HB3	1.76	0.50	
3:F:37:LEU:HD13	3:F:170:LEU:HD11	1.94	0.49	
1:J:54:GLU:HA	1:J:57:LYS:HZ3	1.77	0.49	
1:D:144:GLU:HB3	1:D:162:ILE:HG22	1.94	0.49	
2:H:370:LYS:HB2	2:H:393:ILE:HG21	1.94	0.49	
2:H:396:LYS:NZ	2:H:486:GLU:OE2	2.43	0.49	
1:D:101:LEU:HD11	1:D:111:LEU:HD22	1.94	0.49	
2:E:454:VAL:HG22	2:E:455:GLN:H	1.77	0.49	
3:C:30:LYS:NZ	4:C:201:GNP:O1B	2.36	0.49	
2:E:244:LEU:HD12	2:E:247:LEU:HD12	1.95	0.49	
3:C:37:LEU:HD13	3:C:170:LEU:HD11	1.95	0.49	
2:E:707:ASP:HA	2:E:711:LEU:HB3	1.94	0.49	
2:K:38:ILE:HG12	2:K:137:ILE:HG23	1.95	0.48	
2:K:322:LEU:O	2:K:326:GLN:HG2	2.14	0.48	
2:B:21:GLN:HE22	2:B:22:ARG:HG2	1.78	0.48	
2:K:307:ILE:HD13	2:K:323:ILE:HG12	1.96	0.48	
2:K:194:ALA:HA	2:K:244:LEU:HD21	1.95	0.48	
2:K:664:HIS:CG	2:K:705:LEU:HD11	2.49	0.48	
2:K:255:LEU:HD12	2:K:271:LEU:HB2	1.95	0.47	
2:E:4:GLN:HA	2:E:115:LEU:HD21	1.95	0.47	
2:E:457:GLU:HA	2:E:459:LYS:HE2	1.96	0.47	
2:B:3:SER:O	2:B:5:THR:N	2.45	0.47	
2:B:427:ILE:HG21	2:B:433:LEU:HD11	1.96	0.47	
2:K:26:VAL:HG12	2:K:165:SER:HA	1.97	0.47	
2:E:307:ILE:HD13	2:E:323:ILE:HG12	1.96	0.47	
2:E:370:LYS:HB2	2:E:393:ILE:HG21	1.95	0.47	
2:B:21:GLN:HE22	2:B:22:ARG:CG	2.26	0.47	
2:B:707:ASP:HA	2:B:711:LEU:HB3	1.97	0.47	
1:G:13:LEU:HD23	1:G:18:ALA:HB2	1.96	0.47	
2:K:389:LEU:O	2:K:393:ILE:HG12	2.14	0.47	
2:B:622:HIS:NE2	2:B:684:ASP:OD2	2.46	0.47	
2:B:304:ILE:HG12	2:B:351:LEU:HD21	1.95	0.47	
3:I:140:THR:HG23	3:I:145:LEU:HB2	1.96	0.47	
2:E:437:LEU:HD12	2:E:438:PRO:HD2	1.95	0.47	
3:L:115:GLU:OE1	3:L:115:GLU:N	2.46	0.47	
1:G:235:ASN:O	1:G:236:ASN:HB2	2.15	0.47	
2:K:173:PRO:HG2	2:K:189:VAL:HG22	1.97	0.47	
2:E:255:LEU:HD12	2:E:271:LEU:HB2	1.97	0.47	
2:B:389:LEU:O	2:B:393:ILE:HG12	2.15	0.46	



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:44:ILE:HD11	1:D:59:GLN:HG3	1.97	0.46
1:D:106:ALA:HB3	2:E:363:LYS:HZ3	1.81	0.46
2:K:292:LEU:O	2:K:296:ILE:HG13	2.15	0.46
2:K:718:THR:O	2:K:721:THR:OG1	2.28	0.46
1:J:106:ALA:HB1	1:J:107:LYS:HB2	1.96	0.46
2:H:229:PHE:HE1	2:H:278:ILE:HG23	1.80	0.46
1:J:14:ASP:OD1	1:J:15:ALA:N	2.40	0.46
1:G:106:ALA:N	1:G:107:LYS:HA	2.31	0.46
1:J:44:ILE:HD11	1:G:59:GLN:HG3	1.98	0.46
2:B:21:GLN:HG3	2:B:22:ARG:N	2.31	0.46
1:A:77:HIS:O	1:A:79:PRO:HD3	2.16	0.46
1:D:106:ALA:HA	1:D:107:LYS:HA	1.77	0.46
2:K:622:HIS:NE2	2:K:684:ASP:OD2	2.46	0.46
2:B:21:GLN:OE1	2:B:22:ARG:HD2	2.16	0.45
2:K:131:HIS:HA	2:K:134:LYS:HD2	1.97	0.45
2:H:389:LEU:O	2:H:393:ILE:HG12	2.17	0.45
2:K:537:GLU:O	2:K:539:TRP:N	2.44	0.45
3:F:134:MET:HE1	3:F:142:LYS:HG3	1.99	0.45
1:A:106:ALA:HB1	1:A:151:THR:CG2	2.47	0.45
1:A:233:LYS:HB3	1:A:234:HIS:H	1.56	0.45
1:D:106:ALA:HB1	1:D:107:LYS:HB2	1.99	0.45
2:K:707:ASP:HA	2:K:711:LEU:HB3	1.99	0.45
2:H:207:ILE:HG23	2:H:208:MET:HG2	1.98	0.45
2:K:170:SER:OG	2:K:171:GLN:N	2.44	0.45
2:E:718:THR:O	2:E:721:THR:OG1	2.31	0.45
3:F:140:THR:HG23	3:F:145:LEU:HD12	1.99	0.45
3:L:30:LYS:NZ	4:L:201:GNP:O1B	2.46	0.45
1:J:113:LEU:O	1:J:120:SER:HB2	2.17	0.44
1:D:31:PRO:HG2	1:D:34:LEU:HD13	1.99	0.44
2:B:23:ARG:HA	2:B:23:ARG:HD3	1.72	0.44
3:L:116:LEU:O	3:L:151:ARG:NH1	2.49	0.44
2:E:537:GLU:O	2:E:539:TRP:N	2.45	0.44
1:G:82:PRO:HG3	1:G:149:LEU:HB2	1.98	0.44
2:E:389:LEU:O	2:E:393:ILE:HG12	2.16	0.44
3:L:37:LEU:HB3	3:L:56:VAL:HG11	1.99	0.44
2:K:465:LEU:HG	2:K:580:LEU:HD23	2.00	0.44
2:E:148:VAL:HG21	2:E:196:THR:HG21	1.98	0.44
2:K:334:LEU:HD11	2:K:351:LEU:HD12	1.99	0.44
2:E:296:ILE:HG23	2:E:300:PRO:HA	2.00	0.44
2:B:558:GLN:HE21	2:B:581:PHE:HZ	1.65	0.44
2:B:21:GLN:NE2	2:B:22:ARG:CD	2.77	0.44



	to do pagom	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:G:31:PRO:HG2	1:G:34:LEU:HD13	2.00	0.44	
3:C:115:GLU:OE1	3:C:115:GLU:N	2.46	0.44	
2:B:194:ALA:HA	2:B:244:LEU:HD21	2.00	0.43	
1:J:6:VAL:HG21	1:G:34:LEU:HG	1.99	0.43	
1:G:97:ALA:HB2	1:G:131:THR:HG22	2.00	0.43	
2:H:537:GLU:O	2:H:539:TRP:N	2.47	0.43	
3:I:30:LYS:NZ	4:I:201:GNP:O3G	2.39	0.43	
1:A:231:ARG:HB2	1:A:233:LYS:HG2	2.00	0.43	
3:F:79:ARG:HA	3:F:82:TYR:CD2	2.53	0.43	
1:A:106:ALA:HB1	1:A:151:THR:HG21	2.00	0.43	
2:K:134:LYS:HB3	2:K:135:ILE:HA	1.99	0.43	
2:E:119:THR:HA	2:E:120:PRO:HD2	1.94	0.43	
2:E:292:LEU:O	2:E:296:ILE:HG13	2.18	0.43	
2:K:11:LYS:HB2	2:K:432:ASN:HD21	1.83	0.43	
2:K:212:ARG:HH22	2:K:672:ILE:HG21	1.83	0.43	
2:H:675:ILE:HG12	2:H:710:ILE:HG23	2.01	0.43	
1:D:146:GLN:HB3	1:D:160:LYS:HA	2.01	0.43	
2:B:21:GLN:NE2	2:B:22:ARG:HD3	2.21	0.43	
2:K:11:LYS:HE2	2:K:123:TRP:HE1	1.84	0.42	
3:C:168:GLU:OE1	3:C:168:GLU:N	2.49	0.42	
1:D:150:ILE:HG23	1:D:155:THR:HG22	2.00	0.42	
2:B:23:ARG:HG3	2:B:424:ILE:HG22	2.00	0.42	
2:B:6:SER:HA	2:B:667:TYR:HD1	1.83	0.42	
2:B:21:GLN:CD	2:B:22:ARG:N	2.73	0.42	
2:K:329:SER:HA	2:K:330:PRO:HD3	1.84	0.42	
2:E:470:ALA:HA	2:E:546:LEU:HD23	2.00	0.42	
1:J:106:ALA:HA	1:J:107:LYS:HA	1.77	0.42	
2:E:140:TRP:O	2:E:203:ARG:NH1	2.50	0.42	
2:E:360:LEU:HD13	2:E:393:ILE:HD13	2.02	0.42	
1:J:135:SER:CB	3:L:99:ARG:HD2	2.49	0.42	
1:G:123:ILE:HD12	1:G:132:THR:HG21	2.01	0.42	
1:D:258:ARG:HD3	3:F:135:SER:HB3	2.02	0.42	
2:K:143:PHE:CZ	2:K:255:LEU:HD11	2.54	0.42	
2:H:360:LEU:HD13	2:H:393:ILE:HD13	2.00	0.42	
3:F:115:GLU:OE1	3:F:115:GLU:N	2.46	0.42	
2:K:6:SER:HB3	2:K:438:PRO:HB3	2.01	0.42	
2:E:285:LEU:HD21	2:E:315:LEU:HD11	2.01	0.42	
1:A:113:LEU:O	1:A:120:SER:OG	2.36	0.41	
2:K:29:PHE:CZ	2:K:34:PRO:HG3	2.54	0.41	
2:K:141:ASN:HB3	2:K:196:THR:HA	2.01	0.41	
2:E:141:ASN:HB3	2:E:196:THR:HA	2.00	0.41	



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:B:29:PHE:HD1	2:B:29:PHE:HA	1.77	0.41
2:E:103:THR:O	2:E:107:ILE:HG13	2.20	0.41
1:G:46:LYS:HE2	1:G:48:GLN:HE21	1.84	0.41
3:L:37:LEU:HD13	3:L:170:LEU:HD11	2.01	0.41
1:A:101:LEU:HD11	1:A:111:LEU:HD22	2.02	0.41
1:J:109:LYS:HB2	1:J:150:ILE:HG22	2.01	0.41
3:L:100:ILE:HG22	3:L:101:GLY:H	1.80	0.41
1:D:12:LYS:HE2	1:D:12:LYS:HB3	1.91	0.41
2:B:32:LEU:HB2	2:B:419:TYR:CE1	2.56	0.41
2:B:140:TRP:O	2:B:203:ARG:NH1	2.42	0.41
2:B:259:THR:HA	2:B:416:LYS:HD2	2.01	0.41
2:H:304:ILE:HG12	2:H:351:LEU:HD21	2.01	0.41
1:A:215:PHE:CZ	1:A:233:LYS:HE2	2.56	0.41
2:K:285:LEU:HD21	2:K:315:LEU:HD11	2.03	0.41
2:B:26:VAL:C	2:B:28:GLN:H	2.03	0.41
2:H:551:LEU:HD23	2:H:588:LEU:HD13	2.03	0.41
3:C:130:LEU:HA	3:C:131:PRO:HD3	1.92	0.41
3:L:79:ARG:HA	3:L:82:TYR:CD2	2.54	0.41
2:E:222:GLU:OE1	2:E:222:GLU:N	2.50	0.41
2:B:21:GLN:O	2:B:22:ARG:HB3	2.21	0.41
2:B:101:ASP:OD1	2:B:103:THR:OG1	2.30	0.41
2:E:322:LEU:O	2:E:326:GLN:HG2	2.21	0.41
2:E:457:GLU:HB3	2:E:458:GLN:H	1.62	0.41
2:B:718:THR:O	2:B:721:THR:OG1	2.28	0.41
3:I:168:GLU:OE1	3:I:168:GLU:N	2.49	0.41
1:A:106:ALA:O	1:A:153:SER:OG	2.27	0.40
1:J:13:LEU:HD22	1:J:40:LYS:O	2.22	0.40
2:K:10:VAL:HG22	2:K:433:LEU:HB3	2.02	0.40
2:K:370:LYS:HB2	2:K:393:ILE:HG21	2.01	0.40
1:G:125:ASN:HB3	1:G:128:LYS:HB2	2.04	0.40
2:H:292:LEU:O	2:H:296:ILE:HG13	2.20	0.40
3:C:22:MET:HE1	3:C:34:LEU:HB2	2.04	0.40
3:C:158:THR:HG22	3:C:165:GLY:O	2.22	0.40
3:I:33:VAL:HG22	3:I:160:ALA:HB2	2.03	0.40
1:J:109:LYS:N	1:J:150:ILE:O	2.46	0.40
1:G:107:LYS:HE3	1:G:107:LYS:HB2	1.90	0.40
2:K:4:GLN:H	2:K:115:LEU:HD13	1.86	0.40
1:J:150:ILE:HG23	1:J:155:THR:HG22	2.02	0.40
1:G:81:SER:HA	1:G:82:PRO:HD3	1.91	0.40
2:E:10:VAL:HB	2:E:91:PHE:CD1	2.56	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	212/368~(58%)	190 (90%)	22 (10%)	0	100	100
1	D	162/368~(44%)	152 (94%)	10 (6%)	0	100	100
1	G	197/368~(54%)	183 (93%)	13 (7%)	1 (0%)	29	63
1	J	150/368 (41%)	139 (93%)	11 (7%)	0	100	100
2	В	469/739~(64%)	446 (95%)	19 (4%)	4 (1%)	17	51
2	Е	527/739~(71%)	503 (95%)	21 (4%)	3 (1%)	25	59
2	Н	300/739~(41%)	290 (97%)	10 (3%)	0	100	100
2	Κ	567/739~(77%)	536 (94%)	25~(4%)	6 (1%)	14	46
3	С	122/175~(70%)	120 (98%)	2(2%)	0	100	100
3	F	138/175~(79%)	136 (99%)	2(1%)	0	100	100
3	Ι	68/175~(39%)	66 (97%)	2(3%)	0	100	100
3	L	125/175~(71%)	119 (95%)	5 (4%)	1 (1%)	19	53
All	All	3037/5128~(59%)	2880 (95%)	142 (5%)	15 (0%)	29	63

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	Е	454	VAL
2	В	22	ARG
2	В	25	ARG
2	В	27	GLY
2	Е	451	PRO
3	L	101	GLY
1	G	80	GLU
2	Κ	31	ASP
2	Е	607	SER
2	Κ	119	THR
2	Κ	120	PRO
2	Κ	121	GLN



 $Continued \ from \ previous \ page...$ 

Mol	Chain	Res	Type
2	Κ	136	SER
2	Κ	364	ARG
2	В	26	VAL

#### 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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
1	А	207/333~(62%)	203~(98%)	4 (2%)	57	79
1	D	157/333~(47%)	156~(99%)	1 (1%)	86	93
1	G	193/333~(58%)	190~(98%)	3~(2%)	62	81
1	J	145/333~(44%)	143~(99%)	2(1%)	67	83
2	В	467/672~(70%)	464 (99%)	3~(1%)	86	93
2	Ε	512/672~(76%)	507~(99%)	5(1%)	76	87
2	Η	307/672~(46%)	306 (100%)	1 (0%)	92	97
2	Κ	545/672~(81%)	535~(98%)	10 (2%)	59	80
3	С	113/150~(75%)	113 (100%)	0	100	100
3	F	124/150~(83%)	124 (100%)	0	100	100
3	Ι	71/150~(47%)	71~(100%)	0	100	100
3	L	$11\overline{8}/150~(79\overline{\%})$	114 (97%)	4 (3%)	37	66
All	All	$2959/4620~(6\overline{4\%})$	2926 (99%)	33 (1%)	73	86

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	76	THR
1	А	230	ILE
1	А	233	LYS
1	А	262	LEU
1	J	76	THR
1	J	160	LYS
1	G	152	THR



Mol	Chain	Res	Type
1	G	157	TRP
1	G	241	ARG
1	D	92	THR
2	Κ	118	ASP
2	Κ	121	GLN
2	Κ	122	ILE
2	Κ	123	TRP
2	Κ	130	PHE
2	Κ	158	VAL
2	Κ	450	ASN
2	Κ	454	VAL
2	Κ	457	GLU
2	Κ	459	LYS
2	Е	158	VAL
2	Е	452	MET
2	Е	454	VAL
2	Е	455	GLN
2	Е	456	LEU
2	В	21	GLN
2	В	22	ARG
2	В	23	ARG
2	Н	691	HIS
3	L	96	ASP
3	L	97	ARG
3	L	98	SER
3	L	168	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	205	GLN
1	J	146	GLN
1	G	48	GLN
1	D	166	HIS
2	Κ	21	GLN
2	Κ	28	GLN
2	Κ	218	GLN
2	Κ	342	HIS
2	Κ	432	ASN
2	Κ	495	GLN
2	Κ	664	HIS
2	Е	218	GLN



Mol	Chain	Res	Type
2	Е	342	HIS
2	Е	495	GLN
2	В	218	GLN
2	В	342	HIS
2	В	640	GLN
2	В	664	HIS
2	Н	478	GLN
2	Н	495	GLN
2	Н	616	GLN
2	Н	692	ASN
2	Н	704	GLN

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#### 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 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	Mal Tuna Chain Da		Dec	Tink	Bond lengths			Bond angles		
IVIOI	туре	Unam	nes	LINK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z  > 2
4	GNP	F	201	5	29,34,34	1.78	5 (17%)	33,54,54	2.38	9 (27%)
4	GNP	Ι	201	5	29,34,34	1.77	5 (17%)	33,54,54	2.37	9 (27%)



Mal Truna Chain		Dec	Tink	Bo	Bond lengths			Bond angles		
INIOI	туре	Unam	nes	LINK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	GNP	С	201	5	29,34,34	1.77	5 (17%)	33,54,54	2.38	9 (27%)
4	GNP	L	201	5	29,34,34	1.77	6 (20%)	33,54,54	2.36	9 (27%)

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	GNP	F	201	5	-	2/14/38/38	0/3/3/3
4	GNP	Ι	201	5	-	8/14/38/38	0/3/3/3
4	GNP	С	201	5	-	2/14/38/38	0/3/3/3
4	GNP	L	201	5	-	3/14/38/38	0/3/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	С	201	GNP	PB-O3A	-5.22	1.52	1.59
4	F	201	GNP	PB-O3A	-5.21	1.52	1.59
4	L	201	GNP	PB-O3A	-5.16	1.52	1.59
4	Ι	201	GNP	PB-O3A	-5.08	1.52	1.59
4	Ι	201	GNP	C6-N1	3.89	1.39	1.33
4	F	201	GNP	C6-N1	3.85	1.39	1.33
4	L	201	GNP	C6-N1	3.83	1.39	1.33
4	С	201	GNP	C6-N1	3.83	1.39	1.33
4	F	201	GNP	PG-O1G	3.34	1.51	1.46
4	Ι	201	GNP	PG-O1G	3.31	1.51	1.46
4	L	201	GNP	PG-O1G	3.29	1.51	1.46
4	С	201	GNP	PG-O1G	3.27	1.51	1.46
4	Ι	201	GNP	PB-O2B	-3.08	1.48	1.56
4	С	201	GNP	PB-O2B	-3.07	1.48	1.56
4	F	201	GNP	PB-O2B	-3.07	1.48	1.56
4	L	201	GNP	PB-O2B	-3.04	1.48	1.56
4	C	201	GNP	C8-N7	-2.17	1.30	1.34
4	Ι	201	GNP	C8-N7	-2.16	1.30	1.34
4	L	201	GNP	C8-N7	-2.16	1.30	1.34
4	F	201	GNP	C8-N7	-2.14	1.30	1.34
4	L	201	GNP	PG-O3G	-2.01	1.51	1.56

All (36) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	F	201	GNP	C5-C6-N1	-8.59	111.68	123.43
4	L	201	GNP	C5-C6-N1	-8.58	111.70	123.43
4	С	201	GNP	C5-C6-N1	-8.55	111.74	123.43
4	Ι	201	GNP	C5-C6-N1	-8.54	111.75	123.43
4	С	201	GNP	C2-N1-C6	5.65	124.90	115.93
4	F	201	GNP	C2-N1-C6	5.64	124.90	115.93
4	L	201	GNP	C2-N1-C6	5.64	124.90	115.93
4	Ι	201	GNP	C2-N1-C6	5.61	124.85	115.93
4	F	201	GNP	O2B-PB-O1B	3.92	118.14	109.92
4	С	201	GNP	O2B-PB-O1B	3.86	118.01	109.92
4	L	201	GNP	O2B-PB-O1B	3.86	118.00	109.92
4	Ι	201	GNP	O2B-PB-O1B	3.81	117.92	109.92
4	С	201	GNP	PB-O3A-PA	-3.53	120.18	132.62
4	F	201	GNP	PB-O3A-PA	-3.43	120.54	132.62
4	L	201	GNP	PB-O3A-PA	-3.34	120.86	132.62
4	Ι	201	GNP	O3G-PG-O1G	-3.33	105.08	113.45
4	С	201	GNP	O3G-PG-O1G	-3.33	105.08	113.45
4	Ι	201	GNP	PB-O3A-PA	-3.33	120.90	132.62
4	F	201	GNP	O3G-PG-O1G	-3.31	105.14	113.45
4	L	201	GNP	O3G-PG-O1G	-3.28	105.21	113.45
4	С	201	GNP	C2-N3-C4	-3.12	111.79	115.36
4	L	201	GNP	C2-N3-C4	-3.10	111.81	115.36
4	С	201	GNP	O2G-PG-O3G	3.08	115.84	107.64
4	L	201	GNP	O2G-PG-O3G	3.07	115.81	107.64
4	F	201	GNP	C2-N3-C4	-3.07	111.85	115.36
4	F	201	GNP	O2G-PG-O3G	3.07	115.80	107.64
4	Ι	201	GNP	C2-N3-C4	-3.06	111.86	115.36
4	Ι	201	GNP	O2G-PG-O3G	3.06	115.79	107.64
4	F	201	GNP	N3-C2-N1	-2.44	123.97	127.22
4	Ι	201	GNP	N3-C2-N1	-2.41	124.00	127.22
4	С	201	GNP	N3-C2-N1	-2.41	124.01	127.22
4	L	201	GNP	N3-C2-N1	-2.40	124.02	127.22
4	F	201	GNP	O1G-PG-N3B	-2.27	108.42	111.77
4	Ι	201	GNP	O1G-PG-N3B	-2.22	108.50	111.77
4	L	201	GNP	O1G-PG-N3B	-2.14	108.62	111.77
4	С	201	GNP	O1G-PG-N3B	-2.07	108.73	111.77

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	201	GNP	PB-N3B-PG-O1G
4	F	201	GNP	PG-N3B-PB-O1B



Mol	Chain	Res	Type	Atoms
4	L	201	GNP	PB-N3B-PG-O1G
4	L	201	GNP	PG-N3B-PB-O1B
4	С	201	GNP	PB-N3B-PG-O1G
4	С	201	GNP	PG-N3B-PB-O1B
4	Ι	201	GNP	PB-N3B-PG-O1G
4	Ι	201	GNP	PG-N3B-PB-O1B
4	Ι	201	GNP	PG-N3B-PB-O3A
4	Ι	201	GNP	PA-O3A-PB-O1B
4	Ι	201	GNP	PA-O3A-PB-O2B
4	Ι	201	GNP	C5'-O5'-PA-O3A
4	Ι	201	GNP	C5'-O5'-PA-O2A
4	L	201	GNP	O4'-C4'-C5'-O5'
4	Ι	201	GNP	C5'-O5'-PA-O1A

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There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	Ι	201	GNP	1	0
4	С	201	GNP	1	0
4	L	201	GNP	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	$OWAB(Å^2)$	Q<0.9
1	А	226/368~(61%)	0.27	7 (3%) 49 52	63, 102, 153, 199	0
1	D	171/368~(46%)	0.61	16 (9%) 8 10	58, 103, 174, 290	0
1	G	211/368~(57%)	0.57	19 (9%) 9 11	61, 108, 176, 203	0
1	J	158/368~(42%)	0.41	13 (8%) 11 13	62, 93, 159, 233	0
2	В	507/739~(68%)	0.23	14 (2%) 53 55	24, 102, 149, 204	0
2	Ε	557/739~(75%)	0.14	10 (1%) 68 71	53, 90, 147, 273	0
2	Н	338/739~(45%)	0.51	33 (9%) 7 9	86, 133, 179, 213	0
2	Κ	593/739~(80%)	0.17	13 (2%) 62 65	53, 79, 143, 231	0
3	С	134/175~(76%)	0.33	9 (6%) 17 20	79, 123, 176, 197	0
3	F	146/175~(83%)	0.50	11 (7%) 14 16	76, 118, 157, 185	0
3	Ι	86/175~(49%)	0.75	14 (16%) 1 2	92, 127, 179, 204	0
3	L	139/175~(79%)	0.65	16 (11%) 4 5	24, 115, 147, 174	0
All	All	$326\overline{6}/5128~(63\%)$	0.33	175 (5%) 25 28	24, 103, 163, 290	0

All (175) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	Κ	187	LEU	7.2
3	F	121	TRP	6.3
1	D	106	ALA	5.9
1	G	243	GLU	5.9
2	Е	628	ASP	5.4
3	Ι	88	VAL	5.2
3	С	87	GLY	5.2
1	J	38	ASN	4.7
1	D	92	THR	4.6
2	В	250	GLU	4.5
3	F	63	PHE	4.5



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Mol	Chain	Res	Type	RSRZ
2	Е	118	ASP	4.5
3	L	124	PHE	4.5
2	Н	196	THR	4.4
2	В	433	LEU	4.3
1	J	145	PHE	4.3
1	J	96	LEU	4.1
3	L	122	LEU	4.1
1	D	263	ASP	4.1
1	G	215	PHE	4.1
1	J	92	THR	4.0
2	Н	202	VAL	4.0
1	G	199	ILE	4.0
2	Κ	458	GLN	3.9
1	G	242	PRO	3.8
1	G	72	GLU	3.7
3	С	153	TRP	3.7
3	Ι	69	GLY	3.7
3	L	121	TRP	3.6
2	Н	610	CYS	3.6
3	L	140	THR	3.6
1	G	103	LEU	3.5
2	Н	189	VAL	3.5
1	А	104	GLY	3.5
3	Ι	21	LEU	3.4
3	С	63	PHE	3.4
3	F	65	VAL	3.4
2	Κ	219	ASN	3.3
3	F	141	GLU	3.3
3	С	21	LEU	3.3
1	G	49	VAL	3.3
1	J	106	ALA	3.3
2	Н	192	ILE	3.2
2	Н	659	ILE	3.2
1	D	143	TYR	3.2
2	Н	256	ASP	3.2
1	G	238	PRO	3.1
2	Н	502	LYS	3.1
2	Н	556	ASP	3.1
3	F	166	LEU	3.1
1	D	139	VAL	3.1
2	K	564	PHE	3.0
3	С	155	ILE	3.0



Mol

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1

1

3

1

1

3

3

2

2

2 1

2

3

2

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458	GLN	2.9
139	SER	2.9
493	TRP	2.9
98	TRP	2.8
10	VAL	2.8
93	ASP	2.8
456	LEU	2.8
142	LYS	2.8
440	ASP	2.8
140	ASP	2.8
666	TRP	2.8
239	ILE	2.7
710	ILE	2.7
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164

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166

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84

88

91

LYS

ARG

VAL

LEU

ALA

LEU

VAL

VAL

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В

Ι

Κ

3	$\mathbf{L}$	142	LYS	2.8		
2	Κ	440	ASP	2.8		
1	J	140	ASP	2.8		
2	В	666	TRP	2.8		
1	G	239	ILE	2.7		
2	Н	710	ILE	2.7		
3	Ι	90	PHE	2.7		
2	Н	553	THR	2.7		
3	Ι	145	LEU	2.7		
1	J	112	ILE	2.7		
3	L	145	LEU	2.7		
2	Н	552	LYS	2.7		
2	Н	607	SER	2.7		
2	Κ	557 TRP		2.7		
1	D	262	LEU	2.7		
2	Н	232	GLY	2.6		
2	В	344	GLN	2.6		
3	С	22	MET	2.6		
2	В	654	ASP	2.6		
3	L	148	ILE	2.6		
2	Н	549	GLU	2.6		
2	Κ	91	PHE	2.5		
2	Κ	20	HIS	2.5		
3	L	63	PHE	2.5		
1	A	176	176 VAL			
3	Ι	123	VAL	2.5		
1	А	49	VAL	2.5		
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Mol	Chain	Res	Type	RSRZ		
2	В	421	LEU	2.5		
2	Н	678	LEU	2.5		
2	Н	347	PHE	2.5		
1	D	81	SER	2.5		
1	G	106	ALA	2.5		
2	Н	344	GLN	2.5		
2	Κ	151	ILE	2.5		
1	G	159	GLU	2.5		
2	Н	500	ARG	2.5		
2	Н	501	SER	2.5		
1	D	93	SER	2.5		
2	Н	199	SER	2.5		
3	F	153	TRP	2.4		
2	Н	488	VAL	2.4		
2	Е	624	ARG	2.4		
2	Е	20	HIS	2.4		
3	F	142	LYS	2.4		
1	G	190	LEU	2.4		
2	K	150	ILE	2.4		
2	Н	254	TYR	2.4		
2	Е	4	GLN	2.4		
1	D	159	GLU	2.4		
2	Е	91	PHE	2.4		
1	J	139	VAL	2.4		
3	L	90	PHE	2.4		
2	Н	345	LEU	2.3		
1	А	63	PHE	2.3		
2	Н	255	LEU	2.3		
1	G	82	PRO	2.3		
1	G	216	VAL	2.3		
3	L	67	ASP	2.3		
3	L	137	ALA	2.3		
1	G	230	ILE	2.3		
1	G	240	VAL	2.3		
3	Ι	35	TYR	2.3		
2	Н	198	MET	2.2		
1	А	103	LEU	2.2		
1	А	158	SER	2.2		
2	В	140	TRP	2.2		
2	Н	654	ASP	2.2		
2	K	560	GLU	2.2		
	D	100	AGD			

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 ASP
 2.2

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Mol	Chain	Res	Type	RSRZ
2	K	234	LEU	2.2
2	В	189	VAL	2.2
3	С	81	TYR	2.2
2	В	263	ASN	2.2
2	Е	138	SER	2.2
2	Н	416	LYS	2.2
1	G	245	VAL	2.2
3	С	172	TRP	2.2
3	L	155	ILE	2.2
1	J	84	LEU	2.1
3	Ι	157	ALA	2.1
3	L	141	GLU	2.1
3	Ι	33	VAL	2.1
3	Ι	74	ILE	2.1
1	D	94	CYS	2.1
3	F	56	VAL	2.1
1	G	45	ILE	2.1
1	J	153	SER	2.1
2	В	6	SER	2.1
3	F	90	PHE	2.1
2	Н	554	TYR	2.1
1	D	257	VAL	2.1
3	L	95	ASN	2.1
3	F	68	VAL	2.1
1	D	259	GLY	2.0
2	В	334	LEU	2.0
2	Е	644	SER	2.0
2	Н	475	SER	2.0
2	В	662	TRP	2.0
3	F	136	ALA	2.0
2	Н	663	ASN	2.0
2	Н	609	VAL	2.0
3	L	116	LEU	2.0
1	А	177	CYS	2.0
1	D	38	ASN	2.0
3	Ι	81	TYR	2.0
1	D	168	MET	2.0
3	Ι	48	THR	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,  $95^{th}$  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	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q < 0.9
5	MG	С	202	1/1	0.91	0.16	60,60,60,60	0
4	GNP	L	201	32/32	0.93	0.18	86,112,138,201	0
4	GNP	F	201	32/32	0.94	0.15	98,129,153,381	0
4	GNP	С	201	32/32	0.95	0.15	53,82,103,108	0
4	GNP	Ι	201	32/32	0.96	0.15	50,94,122,244	0
5	MG	L	202	1/1	0.97	0.18	$51,\!51,\!51,\!51$	0
5	MG	F	202	1/1	0.97	0.19	59, 59, 59, 59, 59	0
5	MG	Ι	202	1/1	0.98	0.11	83,83,83,83	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.

