

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

#### Mar 11, 2025 – 06:11 PM EDT

PDB ID	:	8VC0
Title	:	HIV-1 CA crosslinked pentamer in complex with GS-CA1
Authors	:	Piacentini, J.; Ganser-Pornillos, B.K.; Pornillos, O.
Deposited on	:	2023-12-13
Resolution	:	3.46  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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

# 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 3.46 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
	$(\# {\rm Entries})$	$(\# { m Entries},  { m resolution}  { m range}({ m \AA}))$
$R_{free}$	164625	1597 (3.52-3.40)
Clashscore	180529	1041 (3.50-3.42)
Ramachandran outliers	177936	1026 (3.50-3.42)
Sidechain outliers	177891	1027 (3.50-3.42)
RSRZ outliers	164620	1596 (3.52-3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	231	4% 78%	9%	13%
1	В	231	3% 	9%	15%
1	С	231	<sup>2%</sup> 75%	8%	16%
1	D	231	3% 79%	7%	13%
1	Е	231	8%	12%	13%



Conti	nued from	<i>i</i> previous	page		
Mol	Chain	Length	Quality of chain		
1	F	231	2% <b>7</b> 9%	8%	13%
1	G	231	3% 78%	7%	15%
1	Н	231	3% 81%	9%	11%
1	Ι	231	4% 77%	8%	14%
1	J	231	7%	11%	12%



#### 8VC0

# 2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 28350 atoms, of which 13387 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	201	Total	С	Н	Ν	0	S	0	Ο	0
L	Π	201	2805	919	1344	254	276	12	0	0	0
1	В	196	Total	С	Η	Ν	Ο	$\mathbf{S}$	0	0	0
		150	2637	877	1249	244	255	12	0	0	0
1	C	103	Total	С	Η	Ν	Ο	$\mathbf{S}$	0	0	0
1	U	155	2416	822	1101	231	253	9	0	0	0
1	а	200	Total	С	Η	Ν	Ο	$\mathbf{S}$	0	0	0
	D	200	2653	885	1245	243	269	11	0	0	0
1	F	202	Total	С	Η	Ν	0	$\mathbf{S}$	0	0	0
L	Ľ	202	2934	948	1433	261	280	12	0	0	0
1	F	201	Total	С	Η	Ν	0	$\mathbf{S}$	0	0	0
1	Г	201	2822	924	1365	251	271	11	0	0	0
1	C	107	Total	С	Η	Ν	Ο	$\mathbf{S}$	0	0	0
1	G	197	2657	880	1265	239	260	13	0	0	0
1	Ц	206	Total	С	Η	Ν	0	$\mathbf{S}$	0	0	0
	11	200	2796	930	1321	257	277	11	0	0	0
1	т	108	Total	С	Η	Ν	0	$\mathbf{S}$	0	0	0
	1	190	2665	889	1256	249	261	10	U	U	0
1	т	203	Total	С	Н	Ν	0	S	0	0	0
	J	203	2965	956	1448	265	284	12	0	U	0

• Molecule 1 is a protein called Capsid protein p24.

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	21	CYS	ASN	engineered mutation	UNP P12497
А	22	CYS	ALA	engineered mutation	UNP P12497
А	184	ALA	TRP	engineered mutation	UNP P12497
А	185	ALA	MET	engineered mutation	UNP P12497
В	21	CYS	ASN	engineered mutation	UNP P12497
В	22	CYS	ALA	engineered mutation	UNP P12497
В	184	ALA	TRP	engineered mutation	UNP P12497
В	185	ALA	MET	engineered mutation	UNP P12497
С	21	CYS	ASN	engineered mutation	UNP P12497



Chain	Residue	Modelled	Actual	Comment	Reference
С	22	CYS	ALA	engineered mutation	UNP P12497
С	184	ALA	TRP	engineered mutation	UNP P12497
С	185	ALA	MET	engineered mutation	UNP P12497
D	21	CYS	ASN	engineered mutation	UNP P12497
D	22	CYS	ALA	engineered mutation	UNP P12497
D	184	ALA	TRP	engineered mutation	UNP P12497
D	185	ALA	MET	engineered mutation	UNP P12497
Е	21	CYS	ASN	engineered mutation	UNP P12497
Е	22	CYS	ALA	engineered mutation	UNP P12497
Е	184	ALA	TRP	engineered mutation	UNP P12497
Е	185	ALA	MET	engineered mutation	UNP P12497
F	21	CYS	ASN	engineered mutation	UNP P12497
F	22	CYS	ALA	engineered mutation	UNP P12497
F	184	ALA	TRP	engineered mutation	UNP P12497
F	185	ALA	MET	engineered mutation	UNP P12497
G	21	CYS	ASN	engineered mutation	UNP P12497
G	22	CYS	ALA	engineered mutation	UNP P12497
G	184	ALA	TRP	engineered mutation	UNP P12497
G	185	ALA	MET	engineered mutation	UNP P12497
Н	21	CYS	ASN	engineered mutation	UNP P12497
Н	22	CYS	ALA	engineered mutation	UNP P12497
Н	184	ALA	TRP	engineered mutation	UNP P12497
Н	185	ALA	MET	engineered mutation	UNP P12497
Ι	21	CYS	ASN	engineered mutation	UNP P12497
Ι	22	CYS	ALA	engineered mutation	UNP P12497
Ι	184	ALA	TRP	engineered mutation	UNP P12497
Ι	185	ALA	MET	engineered mutation	UNP P12497
J	21	CYS	ASN	engineered mutation	UNP P12497
J	22	CYS	ALA	engineered mutation	UNP P12497
J	184	ALA	TRP	engineered mutation	UNP P12497
J	185	ALA	MET	engineered mutation	UNP P12497

• Molecule 2 is N-[(1S)-1-{(3M)-3-{4-chloro-3-[(cyclopropanesulfonyl)amino]-1-(2,2-difluoroet hyl)-1H-indazol-7-yl}-6-[3-(methanesulfonyl)-3-methylbut-1-yn-1-yl]pyridin-2-yl}-2-(3,5-difluorophenyl)ethyl]-2-[(3bS,4aR)-3-(difluoromethyl)-5,5-difluoro-3b,4,4a,5-tetrahydro-1H-cy clopropa[3,4]cyclopenta[1,2-c]pyrazol-1-yl]acetamide (three-letter code: A1AAO) (formula:  $C_{41}H_{36}ClF_8N_7O_5S_2$ ) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms								ZeroOcc	AltConf
0	Λ	1	Total	С	Cl	F	Η	Ν	0	S	0	0
	A	1	100	41	1	8	36	7	5	2	0	0
9	В	1	Total	С	Cl	F	Η	Ν	0	$\mathbf{S}$	0	0
	D	1	100	41	1	8	36	7	5	2	0	0
9	С	1	Total	С	Cl	F	Η	Ν	0	$\mathbf{S}$	0	0
	U	1	100	41	1	8	36	7	5	2	0	0
9	Л	1	Total	С	Cl	F	Η	Ν	0	$\mathbf{S}$	0	0
	D	1	100	41	1	8	36	7	5	2	0	0
9	F	1	Total	С	Cl	F	Η	Ν	0	S	0	0
	Ľ	1	100	41	1	8	36	7	5	2	0	0
9	F	1	Total	С	Cl	F	Η	Ν	0	S	0	0
	Ľ	1	100	41	1	8	36	7	5	2	0	0
9	С	1	Total	С	Cl	F	Η	Ν	0	S	0	0
	G	1	100	41	1	8	36	7	5	2	0	0
9	Ц	1	Total	С	Cl	F	Η	Ν	Ο	$\mathbf{S}$	0	0
	11	1	100	41	1	8	36	7	5	2	0	0
9	Т	1	Total	С	Cl	F	Η	Ν	0	S	0	0
	1	T	100	41	1	8	36	7	5	2		0
9	т	1	Total	С	Cl	F	Η	Ν	0	S	0	0
	1	L	100	41	1	8	36	7	5	2		U



# 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: Capsid protein p24









## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants	137.40Å $149.46$ Å $157.11$ Å	Deperitor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
$\mathbf{P}_{\text{oscolution}}(\hat{\mathbf{A}})$	42.18 - 3.46	Depositor
Resolution (A)	42.18 - 3.46	EDS
% Data completeness	57.8 (42.18-3.46)	Depositor
(in resolution range)	58.0(42.18-3.46)	EDS
R <sub>merge</sub>	0.11	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.56 (at 3.48 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
D D.	0.257 , $0.315$	Depositor
$\Pi, \Pi_{free}$	0.257 , $0.314$	DCC
$R_{free}$ test set	2162 reflections $(5.14\%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	45.2	Xtriage
Anisotropy	1.000	Xtriage
Bulk solvent $k_{sol}(e/A^3)$ , $B_{sol}(A^2)$	0.33, 20.6	EDS
L-test for twinning <sup>2</sup>	$< L >=0.47, < L^2>=0.29$	Xtriage
Estimated twinning fraction	0.029 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	28350	wwPDB-VP
Average B, all atoms $(Å^2)$	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 38.61 % 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 3.5912e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

<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: A1AAO

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			
IVIOI	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5		
1	А	0.25	0/1491	0.45	0/2035		
1	В	0.24	0/1418	0.44	0/1937		
1	С	0.24	0/1340	0.42	0/1835		
1	D	0.24	0/1437	0.43	0/1969		
1	Ε	0.25	0/1533	0.45	0/2089		
1	F	0.24	0/1488	0.44	0/2036		
1	G	0.25	0/1421	0.44	0/1947		
1	Н	0.24	0/1507	0.44	0/2061		
1	Ι	0.25	0/1439	0.44	0/1966		
1	J	0.25	0/1549	0.46	0/2110		
All	All	0.25	0/14623	0.44	0/19985		

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	1461	1344	1344	13	0
1	В	1388	1249	1249	12	0
1	C	1315	1101	1101	11	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1408	1245	1245	8	0
1	Е	1501	1433	1433	14	0
1	F	1457	1365	1365	10	0
1	G	1392	1265	1265	7	0
1	Н	1475	1321	1321	10	0
1	Ι	1409	1256	1256	11	0
1	J	1517	1448	1448	12	0
2	А	64	36	0	0	0
2	В	64	36	0	0	0
2	С	64	36	0	0	0
2	D	64	36	0	0	0
2	Е	64	36	0	0	0
2	F	64	36	0	0	0
2	G	64	36	0	0	0
2	Н	64	36	0	0	0
2	Ι	64	36	0	0	0
2	J	64	36	0	1	0
All	All	14963	13387	13027	107	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 4.

All (107) 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)
1:D:27:VAL:HG11	1:D:59:VAL:HG13	1.55	0.88
1:I:27:VAL:HG11	1:I:59:VAL:HG13	1.59	0.83
1:B:150:ILE:HG21	1:B:172:LEU:HD23	1.62	0.81
1:D:81:ASP:OD1	1:D:101:GLY:N	2.15	0.79
1:F:12:HIS:NE2	1:F:111:LEU:HD21	1.98	0.78
1:A:104:ILE:HG23	1:A:126:VAL:HG13	1.69	0.74
1:H:27:VAL:HG11	1:H:59:VAL:HG13	1.71	0.72
1:E:27:VAL:HG11	1:E:59:VAL:HG13	1.75	0.69
1:D:143:ARG:NH1	1:D:175:GLU:O	2.28	0.67
1:J:27:VAL:HG11	1:J:59:VAL:HG13	1.77	0.65
1:J:81:ASP:OD1	1:J:101:GLY:N	2.30	0.65
1:B:168:PHE:CE2	1:B:172:LEU:HD11	2.32	0.65
1:F:27:VAL:HG11	1:F:59:VAL:HG13	1.80	0.64
1:E:150:ILE:N	1:E:175:GLU:OE2	2.29	0.64
1:C:159:GLU:OE2	1:C:167:ARG:NH2	2.31	0.64
1:B:81:ASP:OD1	1:B:101:GLY:N	2.31	0.64



		Interatomic	Clash		
Atom-1	Atom-2	distance (Å)	overlap (Å)		
1:G:103:ASP:OD1	1:G:108:THR:OG1	2.17	0.63		
1:G:27:VAL:HG11	1:G:59:VAL:HG13	1.81	0.63		
1:A:27:VAL:HG11	1:A:59:VAL:HG13	1.80	0.62		
1:I:49:PRO:O	1:I:53:ASN:ND2	2.34	0.61		
1:F:168:PHE:CE2	1:F:172:LEU:HD11	2.36	0.60		
1:D:49:PRO:O	1:D:53:ASN:ND2	2.34	0.60		
1:E:49:PRO:O	1:E:53:ASN:ND2	2.35	0.60		
1:B:27:VAL:HG11	1:B:59:VAL:HG13	1.83	0.59		
1:B:135:ILE:O	1:B:139:ASN:ND2	2.35	0.59		
1:G:135:ILE:O	1:G:139:ASN:ND2	2.34	0.58		
1:J:135:ILE:O	1:J:139:ASN:ND2	2.37	0.58		
1:B:150:ILE:CG2	1:B:172:LEU:HD23	2.32	0.58		
1:A:135:ILE:O	1:A:139:ASN:ND2	2.35	0.57		
1:B:97:ARG:NH1	1:B:103:ASP:OD2	2.35	0.57		
1:A:151:LEU:HD23	1:A:189:LEU:HD21	1.87	0.57		
1:B:49:PRO:O	1:B:53:ASN:ND2	2.37	0.57		
1:A:49:PRO:O	1:A:53:ASN:ND2	2.39	0.56		
1:B:69:LEU:HD11	1:B:134:ILE:HA	1.88	0.56		
1:J:104:ILE:HG23	1:J:126:VAL:HG13	1.88	0.56		
1:I:159:GLU:OE2	1:I:167:ARG:NH2	2.34	0.55		
1:F:49:PRO:O	1:F:53:ASN:ND2	2.39	0.55		
1:G:49:PRO:O	1:G:53:ASN:ND2	2.40	0.54		
1:G:15:ILE:HD13	1:G:20:LEU:HD21	1.89	0.54		
1:H:135:ILE:O	1:H:139:ASN:ND2	2.40	0.54		
1:A:97:ARG:NH1	1:A:103:ASP:OD2	2.41	0.54		
1:C:49:PRO:O	1:C:53:ASN:ND2	2.39	0.53		
1:A:151:LEU:HD23	1:A:189:LEU:CD2	2.39	0.53		
1:C:104:ILE:HG23	1:C:126:VAL:HG13	1.91	0.52		
1:F:195:ASN:O	1:F:199:LYS:N	2.37	0.52		
1:F:135:ILE:O	1:F:139:ASN:ND2	2.41	0.52		
1:H:15:ILE:HD13	1:H:20:LEU:HD21	1.91	0.52		
1:J:49:PRO:O	1:J:53:ASN:ND2	2.41	0.52		
1:J:15:ILE:HD13	1:J:20:LEU:HD21	1.92	0.51		
1:J:150:ILE:N	1:J:175:GLU:OE2	2.39	0.51		
1:C:195:ASN:O	1:C:199:LYS:N	2.31	0.51		
1:E:15:ILE:HD13	1:E:20:LEU:HD21	1.93	0.51		
1:D:135:ILE:O	1:D:139:ASN:ND2	2.43	0.51		
1:E:135:ILE:O	1:E:139:ASN:ND2	2.41	0.51		
1:D:104:ILE:HG23	1:D:126:VAL:HG13	1.92	0.51		
1:D:37:ILE:HB	1:D:38:PRO:HD3	1.93	0.50		
1:H:104:ILE:CD1	1:H:126:VAL:HG13	2.41	0.50		



	te de pagem	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:I:112:GLN:OE1	1:I:112:GLN:N	2.45	0.50	
1:C:104:ILE:HD12	1:C:126:VAL:HG13	1.94	0.49	
1:A:24:VAL:HG21	1:E:39:MET:CE	2.42	0.49	
1:I:37:ILE:HB	1:I:38:PRO:HD3	1.94	0.49	
1:H:104:ILE:HD12	1:H:126:VAL:HG13	1.94	0.49	
1:I:104:ILE:CD1	1:I:126:VAL:HG13	2.43	0.49	
1:E:81:ASP:OD1	1:E:101:GLY:N	2.45	0.49	
1:C:69:LEU:HD11	1:C:134:ILE:HA	1.94	0.49	
1:A:104:ILE:HD12	1:A:126:VAL:HG13	1.95	0.48	
1:F:12:HIS:CE1	1:F:111:LEU:HD11	2.48	0.48	
1:A:12:HIS:ND1	1:A:12:HIS:O	2.46	0.48	
1:C:37:ILE:HB	1:C:38:PRO:HD3	1.96	0.47	
1:H:143:ARG:NH1	1:H:175:GLU:O	2.48	0.47	
1:G:69:LEU:HD11	1:G:134:ILE:HA	1.98	0.46	
1:J:12:HIS:O	1:J:12:HIS:ND1	2.48	0.46	
1:H:69:LEU:HD11	1:H:134:ILE:HA	1.98	0.46	
1:H:49:PRO:O	1:H:53:ASN:ND2	2.49	0.46	
1:I:12:HIS:NE2	1:I:111:LEU:HD11	2.31	0.46	
1:F:15:ILE:HD13	1:F:20:LEU:HD21	1.99	0.45	
1:H:37:ILE:HB	1:H:38:PRO:HD3	1.99	0.45	
1:J:107:THR:HG22	2:J:301:A1AAO:C69	2.46	0.45	
1:C:135:ILE:O	1:C:139:ASN:ND2	2.45	0.45	
1:J:37:ILE:HB	1:J:38:PRO:HD3	1.99	0.45	
1:E:37:ILE:HB	1:E:38:PRO:HD3	1.97	0.45	
1:E:104:ILE:HG23	1:E:126:VAL:HG13	1.99	0.45	
1:G:37:ILE:HB	1:G:38:PRO:HD3	2.00	0.44	
1:A:15:ILE:HD13	1:A:20:LEU:HD21	2.00	0.44	
1:E:186:THR:O	1:E:190:LEU:HB2	2.18	0.44	
1:B:37:ILE:HB	1:B:38:PRO:HD3	2.00	0.44	
1:E:161:PHE:O	1:E:165:VAL:HG23	2.18	0.44	
1:E:12:HIS:NE2	1:E:111:LEU:HD21	2.32	0.44	
1:F:50:GLN:OE1	1:F:111:LEU:HD13	2.18	0.43	
1:C:104:ILE:CD1	1:C:126:VAL:HG13	2.48	0.43	
1:B:32:PHE:HE1	1:B:138:LEU:HD22	1.84	0.43	
1:I:104:ILE:HD12	1:I:126:VAL:HG13	1.99	0.43	
1:I:104:ILE:HG23	1:I:126:VAL:HG13	1.99	0.43	
1:E:143:ARG:NH1	1:E:175:GLU:O	2.51	0.43	
1:F:37:ILE:HB	1:F:38:PRO:HD3	2.00	0.43	
1:I:103:ASP:OD1	1:I:108:THR:OG1	2.34	0.42	
1:E:205:LEU:HD23	1:E:209:ALA:HB1	2.01	0.42	
1:H:97:ARG:NH2	1:H:113:GLU:OE1	2.50	0.42	



2.00

2.51

2.36

2.51

2.22

2.54

2.55

2.35

Interatomic	Clash
distance (Å)	overlap (Å)
2.19	0.42

0.42

0.42

0.41

0.41

0.40

0.40

0.40

0.40

Continued from previous page...

Atom-2

1:J:58:THR:HG23

1:A:38:PRO:HD3

1:I:139:ASN:ND2

1:B:108:THR:OG1

1:J:214:MET:CE

1:A:176:GLN:HG2

1:C:113:GLU:OE1

1:C:101:GLY:N

1:D:108:THR:OG1

Atom-1

1:J:54:THR:O

1:A:37:ILE:HB

1:I:135:ILE:O

1:B:103:ASP:OD1

1:J:202:LEU:HD13

1:A:176:GLN:O

1:C:97:ARG:NH2

1:C:81:ASP:OD1

1:D:103:ASP:OD1

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	193/231~(84%)	186 (96%)	7 (4%)	0	100	100
1	В	188/231 (81%)	181 (96%)	7 (4%)	0	100	100
1	С	183/231~(79%)	175~(96%)	8 (4%)	0	100	100
1	D	194/231~(84%)	186 (96%)	8 (4%)	0	100	100
1	Ε	196/231~(85%)	187 (95%)	9~(5%)	0	100	100
1	F	195/231~(84%)	186 (95%)	9~(5%)	0	100	100
1	G	193/231~(84%)	181 (94%)	12 (6%)	0	100	100
1	Н	198/231~(86%)	187 (94%)	11 (6%)	0	100	100
1	Ι	188/231~(81%)	181 (96%)	7 (4%)	0	100	100
1	J	197/231~(85%)	187 (95%)	10 (5%)	0	100	100
All	All	1925/2310 (83%)	1837 (95%)	88 (5%)	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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
1	А	141/193~(73%)	140~(99%)	1 (1%)	81	89
1	В	125/193~(65%)	124~(99%)	1 (1%)	79	87
1	С	108/193~(56%)	107~(99%)	1 (1%)	75	86
1	D	127/193~(66%)	126 (99%)	1 (1%)	79	87
1	Ε	152/193~(79%)	150 (99%)	2(1%)	65	81
1	F	142/193~(74%)	141 (99%)	1 (1%)	81	89
1	G	128/193~(66%)	125~(98%)	3(2%)	45	71
1	Н	136/193~(70%)	134 (98%)	2(2%)	60	78
1	Ι	127/193~(66%)	125~(98%)	2 (2%)	58	76
1	J	154/193~(80%)	150 (97%)	4 (3%)	41	68
All	All	1340/1930~(69%)	1322 (99%)	18 (1%)	65	81

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	166	ASP
1	В	166	ASP
1	С	166	ASP
1	D	166	ASP
1	Е	166	ASP
1	Е	176	GLN
1	F	166	ASP
1	G	32	PHE
1	G	79	GLU
1	G	166	ASP
1	Н	166	ASP
1	Н	176	GLN
1	Ι	145	TYR
1	Ι	166	ASP
1	J	32	PHE
1	J	166	ASP



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Mol	Chain	Res	Type
1	J	183	ASN
1	J	187	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

#### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

#### 5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry (i)

10 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).

Mal	Mol Type Chain		hain Bos Link		Bo	Bond lengths			Bond angles		
WIOI	туре	Ullalli	nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2	
2	A1AAO	Ι	301	-	56,71,71	0.96	1 (1%)	61,113,113	1.25	7 (11%)	
2	A1AAO	С	301	-	56,71,71	0.99	2 (3%)	61,113,113	1.21	7 (11%)	
2	A1AAO	Н	301	-	56,71,71	1.00	2 (3%)	61,113,113	1.21	7 (11%)	
2	A1AAO	Е	301	-	56,71,71	0.98	2 (3%)	61,113,113	1.26	6 (9%)	
2	A1AAO	J	301	-	56,71,71	0.97	1 (1%)	61,113,113	1.24	7 (11%)	
2	A1AAO	G	301	-	56,71,71	0.98	2 (3%)	61,113,113	1.20	6 (9%)	
2	A1AAO	D	301	-	56,71,71	0.97	1 (1%)	61,113,113	1.25	8 (13%)	



Mol Turno		Chain	Dec	Tink	Bo	ond leng	ths	Bo	nd angl	es
	Type	Ullaili	nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	A1AAO	А	301	-	56,71,71	0.97	2 (3%)	61,113,113	1.22	7 (11%)
2	A1AAO	В	301	-	56,71,71	0.97	2 (3%)	61,113,113	1.23	7 (11%)
2	A1AAO	F	301	-	56,71,71	0.97	2 (3%)	61,113,113	1.23	6 (9%)

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
2	A1AAO	Ι	301	-	-	3/38/77/77	0/8/8/8
2	A1AAO	С	301	-	-	4/38/77/77	0/8/8/8
2	A1AAO	Н	301	-	-	4/38/77/77	0/8/8/8
2	A1AAO	Е	301	-	-	3/38/77/77	0/8/8/8
2	A1AAO	J	301	-	-	6/38/77/77	0/8/8/8
2	A1AAO	G	301	-	-	4/38/77/77	0/8/8/8
2	A1AAO	D	301	-	-	4/38/77/77	0/8/8/8
2	A1AAO	А	301	-	-	4/38/77/77	0/8/8/8
2	A1AAO	В	301	-	-	4/38/77/77	0/8/8/8
2	A1AAO	F	301	_	_	5/38/77/77	0/8/8/8

$\Delta 11$ (	(17)	hond	longth	outliers	aro	listed	helow
AII (	( <b>1</b> )	bond	length	outners	are	nsteu	below.

Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	Ideal(Å)
2	Е	301	A1AAO	C72-C71	-2.29	1.39	1.43
2	А	301	A1AAO	C72-C71	-2.24	1.39	1.43
2	F	301	A1AAO	C72-C71	-2.20	1.40	1.43
2	G	301	A1AAO	C72-C71	-2.17	1.40	1.43
2	Е	301	A1AAO	C79-N77	-2.15	1.43	1.47
2	Н	301	A1AAO	C79-N77	-2.14	1.43	1.47
2	Н	301	A1AAO	C72-C71	-2.11	1.40	1.43
2	J	301	A1AAO	C79-N77	-2.11	1.43	1.47
2	В	301	A1AAO	C79-N77	-2.09	1.43	1.47
2	С	301	A1AAO	C79-N77	-2.08	1.43	1.47
2	В	301	A1AAO	C72-C71	-2.07	1.40	1.43
2	D	301	A1AAO	C79-N77	-2.07	1.43	1.47
2	Ι	301	A1AAO	C79-N77	-2.07	1.43	1.47
2	G	301	A1AAO	C79-N77	-2.04	1.43	1.47
2	F	301	A1AAO	C79-N77	-2.02	1.43	1.47



001000	naca jion	" proor	ouo puge				
Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
2	А	301	A1AAO	C79-N77	-2.02	1.43	1.47
2	С	301	A1AAO	C72-C71	-2.00	1.40	1.43

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
2	F	301	A1AAO	C5-N7-N6	4.43	108.30	104.48
2	Ι	301	A1AAO	C5-N7-N6	4.35	108.23	104.48
2	Е	301	A1AAO	C5-N7-N6	4.35	108.23	104.48
2	J	301	A1AAO	C5-N7-N6	4.32	108.21	104.48
2	В	301	A1AAO	C5-N7-N6	4.23	108.13	104.48
2	Н	301	A1AAO	C5-N7-N6	4.16	108.06	104.48
2	D	301	A1AAO	C5-N7-N6	4.14	108.05	104.48
2	С	301	A1AAO	C5-N7-N6	4.09	108.01	104.48
2	G	301	A1AAO	C5-N7-N6	4.04	107.97	104.48
2	А	301	A1AAO	C5-N7-N6	3.99	107.92	104.48
2	Е	301	A1AAO	C9-C4-C3	-3.51	105.75	108.40
2	D	301	A1AAO	C2-C1-N6	-3.41	105.17	106.61
2	J	301	A1AAO	C2-C1-N6	-3.40	105.18	106.61
2	F	301	A1AAO	C9-C4-C3	-3.38	105.86	108.40
2	Ι	301	A1AAO	C9-C4-C3	-3.29	105.92	108.40
2	Ι	301	A1AAO	C2-C1-N6	-3.27	105.23	106.61
2	J	301	A1AAO	C9-C4-C3	-3.26	105.94	108.40
2	В	301	A1AAO	C9-C4-C3	-3.25	105.95	108.40
2	D	301	A1AAO	C9-C4-C3	-3.24	105.96	108.40
2	А	301	A1AAO	C9-C4-C3	-3.20	105.99	108.40
2	G	301	A1AAO	C2-C1-N6	-3.14	105.29	106.61
2	G	301	A1AAO	C9-C4-C3	-3.11	106.05	108.40
2	Е	301	A1AAO	C2-C1-N6	-3.11	105.30	106.61
2	В	301	A1AAO	C2-C1-N6	-3.08	105.31	106.61
2	С	301	A1AAO	C9-C4-C3	-2.97	106.16	108.40
2	А	301	A1AAO	F10-C9-C1	-2.92	108.85	112.87
2	F	301	A1AAO	F10-C9-C1	-2.91	108.87	112.87
2	С	301	A1AAO	C2-C1-N6	-2.81	105.42	106.61
2	Н	301	A1AAO	C9-C4-C3	-2.78	106.30	108.40
2	Н	301	A1AAO	C2-C1-N6	-2.71	105.47	106.61
2	G	301	A1AAO	F10-C9-C1	-2.69	109.17	112.87
2	А	301	A1AAO	C2-C1-N6	-2.68	105.48	106.61
2	F	301	A1AAO	C2-C1-N6	-2.63	105.50	106.61
2	J	301	A1AAO	C44-N48-C43	2.62	119.38	117.29
2	Ι	301	A1AAO	C74-C69-C70	2.58	120.83	117.57
2	Е	301	A1AAO	F10-C9-C1	-2.57	109.33	112.87



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	С	301	A1AAO	F10-C9-C1	-2.57	109.34	112.87
2	Е	301	A1AAO	C44-N48-C43	2.55	119.32	117.29
2	D	301	A1AAO	C74-C69-C70	2.52	120.76	117.57
2	В	301	A1AAO	F10-C9-C1	-2.50	109.43	112.87
2	Н	301	A1AAO	C44-N48-C43	2.49	119.28	117.29
2	С	301	A1AAO	C44-N48-C43	2.48	119.27	117.29
2	Н	301	A1AAO	F11-C9-C1	-2.48	109.46	112.87
2	А	301	A1AAO	C74-C69-C70	2.47	120.68	117.57
2	В	301	A1AAO	C74-C69-C70	2.45	120.67	117.57
2	J	301	A1AAO	C74-C69-C70	2.42	120.63	117.57
2	Н	301	A1AAO	F10-C9-C1	-2.42	109.54	112.87
2	Ι	301	A1AAO	F10-C9-C1	-2.41	109.55	112.87
2	D	301	A1AAO	F10-C9-C1	-2.35	109.64	112.87
2	F	301	A1AAO	C74-C69-C70	2.33	120.51	117.57
2	F	301	A1AAO	C44-N48-C43	2.32	119.13	117.29
2	Н	301	A1AAO	C74-C69-C70	2.30	120.47	117.57
2	С	301	A1AAO	C74-C69-C70	2.29	120.47	117.57
2	D	301	A1AAO	C44-N48-C43	2.29	119.11	117.29
2	А	301	A1AAO	C44-N48-C43	2.25	119.08	117.29
2	В	301	A1AAO	C44-N48-C43	2.24	119.07	117.29
2	G	301	A1AAO	C74-C69-C70	2.20	120.34	117.57
2	С	301	A1AAO	F11-C9-C1	-2.18	109.87	112.87
2	В	301	A1AAO	F11-C9-C1	-2.18	109.87	112.87
2	G	301	A1AAO	C44-N48-C43	2.17	119.02	117.29
2	А	301	A1AAO	F11-C9-C1	-2.15	109.92	112.87
2	J	301	A1AAO	F11-C9-C1	-2.15	109.92	112.87
2	Ι	301	A1AAO	C46-C47-C43	2.13	120.10	117.94
2	Е	301	A1AAO	C74-C69-C70	2.11	120.23	117.57
2	Ι	301	A1AAO	C44-N48-C43	2.10	118.96	117.29
2	J	301	A1AAO	F10-C9-C1	-2.09	109.99	112.87
2	D	301	A1AAO	F11-C9-C1	-2.06	110.04	112.87
2	D	301	A1AAO	C46-C47-C43	2.02	119.99	117.94

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There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	А	301	A1AAO	C50-C53-S56-O58
2	А	301	A1AAO	C76-N83-S89-O93
2	В	301	A1AAO	C50-C53-S56-O58
2	В	301	A1AAO	C76-N83-S89-O93
2	С	301	A1AAO	C50-C53-S56-O58



Mol	Chain	Res	Type	Atoms
2	D	301	A1AAO	C50-C53-S56-O58
2	D	301	A1AAO	C76-N83-S89-O93
2	D	301	A1AAO	C76-N83-S89-O94
2	F	301	A1AAO	C50-C53-S56-O58
2	G	301	A1AAO	C50-C53-S56-O58
2	Н	301	A1AAO	C50-C53-S56-O58
2	Ι	301	A1AAO	C76-N83-S89-O93
2	J	301	A1AAO	C45-C44-C49-C50
2	J	301	A1AAO	C50-C53-S56-O58
2	А	301	A1AAO	C76-N83-S89-C90
2	В	301	A1AAO	C76-N83-S89-C90
2	D	301	A1AAO	C76-N83-S89-C90
2	Ι	301	A1AAO	C76-N83-S89-C90
2	F	301	A1AAO	C44-C49-C50-C53
2	А	301	A1AAO	C76-N83-S89-O94
2	В	301	A1AAO	C76-N83-S89-O94
2	С	301	A1AAO	C76-N83-S89-O93
2	F	301	A1AAO	C76-N83-S89-O93
2	G	301	A1AAO	C76-N83-S89-O93
2	С	301	A1AAO	C76-N83-S89-C90
2	Е	301	A1AAO	C76-N83-S89-C90
2	F	301	A1AAO	C76-N83-S89-C90
2	G	301	A1AAO	C76-N83-S89-C90
2	Н	301	A1AAO	C76-N83-S89-C90
2	J	301	A1AAO	C76-N83-S89-C90
2	J	301	A1AAO	N48-C44-C49-C50
2	С	301	A1AAO	C76-N83-S89-O94
2	Е	301	A1AAO	C76-N83-S89-O93
2	Е	301	A1AAO	C76-N83-S89-O94
2	F	301	A1AAO	C76-N83-S89-O94
2	G	301	A1AAO	C76-N83-S89-O94
2	Н	301	A1AAO	C76-N83-S89-O93
2	Н	301	A1AAO	C76-N83-S89-O94
2	Ι	301	A1AAO	C76-N83-S89-O94
2	J	301	A1AAO	C76-N83-S89-O93
2	J	301	A1AAO	C76-N83-S89-O94

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There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	301	A1AAO	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 sufficient 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	<RSRZ $>$	#RS	SRZ>	>2	$OWAB(Å^2)$	Q<0.9
1	А	201/231~(87%)	0.29	9 (4%)	39	29	24, 44, 63, 79	0
1	В	196/231~(84%)	0.27	8 (4%)	42	31	28, 48, 68, 74	0
1	С	193/231~(83%)	0.24	5 (2%)	57	42	27, 49, 67, 75	0
1	D	200/231~(86%)	0.34	8 (4%)	43	32	27, 49, 62, 71	0
1	Ε	202/231~(87%)	0.46	18 (8%)	17	14	24, 40, 56, 67	0
1	F	201/231~(87%)	0.22	4 (1%)	64	48	25, 45, 65, 74	0
1	G	197/231~(85%)	0.28	7(3%)	46	34	28, 48, 66, 78	0
1	Н	206/231~(89%)	0.15	8 (3%)	44	33	26, 42, 65, 75	0
1	Ι	198/231~(85%)	0.27	9 (4%)	39	29	26, 44, 65, 73	0
1	J	203/231~(87%)	0.45	16 (7%)	20	17	25, 37, 55, 65	0
All	All	1997/2310~(86%)	0.30	92 (4%)	38	29	24, 44, 65, 79	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	179	GLN	5.5
1	G	183	ASN	4.4
1	D	186	THR	4.1
1	Ι	186	THR	4.0
1	А	143	ARG	3.8
1	G	104	ILE	3.8
1	В	21	CYS	3.7
1	J	150	ILE	3.6
1	J	70	LYS	3.5
1	J	65	ALA	3.4
1	J	219	GLN	3.4
1	Е	65	ALA	3.3
1	G	178	SER	3.3



8V	C0
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Mol	Chain	Res	Type	RSRZ
1	D	198	CYS	3.3
1	Е	185	ALA	3.2
1	В	12	HIS	3.2
1	Н	183	ASN	3.2
1	А	20	LEU	3.2
1	J	145	TYR	3.1
1	Е	186	THR	3.1
1	Е	204	ALA	3.1
1	Ι	198	CYS	3.0
1	В	2	ILE	3.0
1	D	106	GLY	2.8
1	Е	62	HIS	2.8
1	В	104	ILE	2.8
1	G	181	VAL	2.8
1	Е	180	GLU	2.7
1	J	176	GLN	2.6
1	Ι	175	GLU	2.6
1	А	28	GLU	2.6
1	Е	45	GLU	2.6
1	F	35	GLU	2.6
1	Е	31	ALA	2.6
1	Н	198	CYS	2.6
1	Е	70	LYS	2.6
1	Е	127	GLY	2.6
1	J	127	GLY	2.6
1	В	20	LEU	2.5
1	Ι	191	VAL	2.5
1	Ι	197	ASP	2.5
1	J	134	ILE	2.5
1	Ι	81	ASP	2.5
1	D	31	ALA	2.5
1	Н	186	THR	2.5
1	J	147	PRO	2.4
1	А	150	ILE	2.4
1	Е	184	ALA	2.4
1	Н	184	ALA	2.4
1	В	114	GLN	2.4
1	F	81	ASP	2.4
1	Ι	150	ILE	2.4
1	Е	183	ASN	2.4
1	J	98	GLU	2.4
1	J	143	ARG	2.4



Mol	Chain	Res	Type	RSRZ
1	J	131	LYS	2.3
1	А	186	THR	2.3
1	Н	121	ASN	2.3
1	G	180	GLU	2.3
1	J	151	LEU	2.3
1	D	153	ILE	2.3
1	Е	177	ALA	2.3
1	J	44	SER	2.3
1	С	182	LYS	2.2
1	F	31	ALA	2.2
1	А	1	PRO	2.2
1	С	161	PHE	2.2
1	С	183	ASN	2.2
1	С	209	ALA	2.2
1	Н	28	GLU	2.2
1	G	206	GLY	2.1
1	Н	140	LYS	2.1
1	А	11	VAL	2.1
1	Е	67	GLN	2.1
1	Е	150	ILE	2.1
1	С	207	PRO	2.1
1	D	178	SER	2.1
1	А	195	ASN	2.1
1	J	129	ILE	2.1
1	А	182	LYS	2.1
1	D	33	SER	2.1
1	Е	149	SER	2.1
1	Е	30	LYS	2.1
1	В	1	PRO	2.1
1	D	104	ILE	2.1
1	F	166	ASP	2.1
1	Н	195	ASN	2.0
1	Е	145	TYR	2.0
1	Ι	190	LEU	2.0
1	Ι	183	ASN	2.0
1	В	182	LYS	2.0
1	J	185	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,  $95^{th}$  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(Å <sup>2</sup> )	Q < 0.9
2	A1AAO	Е	301	64/64	0.86	0.15	$25,\!44,\!96,\!103$	0
2	A1AAO	J	301	64/64	0.87	0.15	20,42,92,118	0
2	A1AAO	В	301	64/64	0.88	0.13	22,46,76,102	0
2	A1AAO	G	301	64/64	0.89	0.12	24,43,71,87	0
2	A1AAO	С	301	64/64	0.89	0.12	23,48,81,99	0
2	A1AAO	Ι	301	64/64	0.90	0.13	21,41,72,81	0
2	A1AAO	D	301	64/64	0.90	0.12	$25,\!49,\!76,\!87$	0
2	A1AAO	F	301	64/64	0.91	0.14	22,30,72,79	0
2	A1AAO	Н	301	64/64	0.91	0.12	20,42,85,103	0
2	A1AAO	А	301	64/64	0.93	0.13	21,32,64,75	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.

