

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

Dec 3, 2023 - 08:55 am GMT

PDB ID	:	2V68
Title	:	Crystal structure of Chlamydomonas reinhardtii Rubisco with large- subunit
		mutations V331A, T342I
Authors	:	Karkehabadi, S.; Satagopan, S.; Taylor, T.C.; Spreitzer, R.J.; Andersson, I.
Deposited on	:	2007-07-13
Resolution	:	2.30 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	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
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

# PERCENTILES INFOmissingINFO



# 1 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 40965 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.

• Molecule 1 is a protein called RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	Δ	466	Total	С	Ν	0	$\mathbf{S}$	0	3	0
1	Л	400	3644	2303	642	675	24	0	5	0
1	В	467	Total	С	Ν	0	S	0	4	0
1	D	407	3651	2306	643	678	24	0	4	0
1	C	467	Total	С	Ν	0	S	0	2	0
1		407	3649	2306	643	676	24	0	5	0
1	Л	465	Total	С	Ν	0	S	0	3	0
	D	405	3640	2301	641	674	24		5	0
1	F	466	Total	С	Ν	Ο	$\mathbf{S}$	0	2	0
1	Ľ	400	3643	2303	642	674	24	0	5	0
1	F	467	Total	С	Ν	0	$\mathbf{S}$	0	4	0
	Г	407	3653	2308	643	678	24	0	4	0
1	С	466	Total	С	Ν	0	$\mathbf{S}$	0	2	0
	G	400	3643	2302	642	675	24	0	5	0
1	ц	466	Total	С	Ν	0	S	0	2	0
1	11	400	3644	2303	642	675	24	U	່ <u>ບ</u>	U

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	46	PRO	LEU	conflict	UNP P00877
А	331	ALA	VAL	engineered mutation	UNP P00877
А	342	ILE	THR	engineered mutation	UNP P00877
В	46	PRO	LEU	conflict	UNP P00877
В	331	ALA	VAL	engineered mutation	UNP P00877
В	342	ILE	THR	engineered mutation	UNP P00877
С	46	PRO	LEU	conflict	UNP P00877
С	331	ALA	VAL	engineered mutation	UNP P00877
С	342	ILE	THR	engineered mutation	UNP P00877
D	46	PRO	LEU	conflict	UNP P00877
D	331	ALA	VAL	engineered mutation	UNP P00877
D	342	ILE	THR	engineered mutation	UNP P00877



Chain	Residue	Modelled	Actual	Comment	Reference
E	46	PRO	LEU	conflict	UNP P00877
E	331	ALA	VAL	engineered mutation	UNP P00877
E	342	ILE	THR	engineered mutation	UNP P00877
F	46	PRO	LEU	conflict	UNP P00877
F	331	ALA	VAL	engineered mutation	UNP P00877
F	342	ILE	THR	engineered mutation	UNP P00877
G	46	PRO	LEU	conflict	UNP P00877
G	331	ALA	VAL	engineered mutation	UNP P00877
G	342	ILE	THR	engineered mutation	UNP P00877
Н	46	PRO	LEU	conflict	UNP P00877
Н	331	ALA	VAL	engineered mutation	UNP P00877
Н	342	ILE	THR	engineered mutation	UNP P00877

• Molecule 2 is a protein called RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 1.

Mol	Chain	Residues		$\mathbf{A}$	toms			ZeroOcc	AltConf	Trace
0	т	140	Total	С	Ν	0	S	0	0	0
	1	140	1143	739	190	203	11	0	0	0
0	т	140	Total	С	Ν	0	S	0	0	0
	J	140	1143	739	190	203	11	0	0	0
0	V	140	Total	С	Ν	0	S	0	1	0
	Λ	140	1145	740	190	203	12	0	L	0
0	т	140	Total	С	Ν	0	S	0	0	0
		140	1143	739	190	203	11		0	0
0	м	140	Total	С	Ν	0	S	0	0	0
	111	140	1143	739	190	203	11	0	0	0
9	N	140	Total	С	Ν	0	S	0	1	0
	11	140	1145	740	190	203	12	0	L	0
9	0	140	Total	С	Ν	0	S	0	1	0
	0	140	1145	740	190	203	12	0	L	0
9	D	140	Total	С	Ν	0	S	0	0	0
	1	140	1143	739	190	203	11		0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	Total Mg 1 1	0	0
3	В	1	Total Mg 1 1	0	0
3	С	1	Total Mg 1 1	0	0



Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total Mg 1 1	0	0
3	Е	1	Total Mg 1 1	0	0
3	F	1	Total Mg 1 1	0	0
3	G	1	Total Mg 1 1	0	0
3	Н	1	Total Mg 1 1	0	0

• Molecule 4 is 2-CARBOXYARABINITOL-1,5-DIPHOSPHATE (three-letter code: CAP) (formula:  $C_6H_{14}O_{13}P_2$ ).



Mol	Chain	Residues	A	Ator	ns		ZeroOcc	AltConf
4	Λ	1	Total	С	Ο	Р	0	0
4	Л	1	21	6	13	2	0	0
4	В	1	Total	С	Ο	Р	0	0
4	D	1	21	6	13	2	0	0
4	С	1	Total	С	Ο	Р	0	0
4	U	1	21	6	13	2	0	0
4	Л	1	Total	С	Ο	Р	0	0
4	D	T	21	6	13	2	0	0
1	F	1	Total	С	Ο	Р	0	0
4	Ľ	T	21	6	13	2	0	0
1	F	1	Total	Ċ	Ō	Р	0	0
-	Ľ	1	21	6	13	2	0	0



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
4	С	1	Total	С	Ο	Р	0	0	
4	4 G	L	21	6	13	2	0		
4	ц	1	Total	С	Ο	Р	0	0	
4	4 H		21	6	13	2	0		

• Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
5	А	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 4  2  2 \end{array}$	0	0
5	А	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 4  2  2 \end{array}$	0	0
5	А	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 4  2  2 \end{array}$	0	0
5	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
5	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
5	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
5	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
5	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0



Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
5	С	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 4  2  2 \end{array}$	0	0
5	С	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 4  2  2 \end{array}$	0	0
5	С	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 4  2  2 \end{array}$	0	0
5	С	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 4  2  2 \end{array}$	0	0
5	D	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 4  2  2 \end{array}$	0	0
5	D	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 4  2  2 \end{array}$	0	0
5	D	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 4  2  2 \end{array}$	0	0
5	D	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 4  2  2 \end{array}$	0	0
5	Е	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 4  2  2 \end{array}$	0	0
5	Е	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 4  2  2 \end{array}$	0	0
5	Е	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 4  2  2 \end{array}$	0	0
5	F	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 4  2  2 \end{array}$	0	0
5	F	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 4  2  2 \end{array}$	0	0
5	F	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 4  2  2 \end{array}$	0	0
5	F	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 4  2  2 \end{array}$	0	0
5	F	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
5	F	1	$\begin{array}{c ccc} \hline \text{Total} & \text{C} & \text{O} \\ \hline 4 & 2 & 2 \end{array}$	0	0
5	G	1	$\begin{array}{c ccc} \hline Total & C & O \\ \hline 4 & 2 & 2 \end{array}$	0	0
5	G	1	$\begin{array}{c cc} Total & C & O \\ 4 & 2 & 2 \end{array}$	0	0
5	G	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0



Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	Н	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
5	Н	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
5	Н	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
5	Н	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
5	Н	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
5	Н	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
5	Ι	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
5	Ι	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
5	J	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
5	J	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
5	K	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
5	К	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
5	L	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 4  2  2 \end{array}$	0	0
5	М	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 4  2  2 \end{array}$	0	0
5	Ν	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
5	Ν	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
5	О	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
5	О	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
5	Р	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0

• Molecule 6 is water.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	237	Total O 237 237	0	0
6	В	216	Total   O     216   216	0	0
6	С	233	Total   O     233   233	0	0
6	D	211	Total   O     211   211	0	0
6	Е	225	Total   O     225   225	0	0
6	F	211	Total   O     211   211	0	0
6	G	221	Total   O     221   221	0	0
6	Н	234	Total   O     234   234	0	0
6	Ι	58	Total   O     58   58	0	0
6	J	57	$\begin{array}{cc} \text{Total} & \text{O} \\ 57 & 57 \end{array}$	0	0
6	К	62	Total   O     62   62	0	0
6	L	78	Total O 78 78	0	0
6	М	62	Total   O     62   62	0	0
6	Ν	58	Total   O     58   58	0	0
6	О	56	Total   O     56   56	0	0
6	Р	57	$\begin{array}{cc} \text{Total} & \text{O} \\ 57 & 57 \end{array}$	0	0

SEQUENCE-PLOTS INFOmissingINFO



# 2 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	120.42Å 178.24Å 122.76Å	Deperitor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $117.72^{\circ}$ $90.00^{\circ}$	Depositor
$\mathbf{P}_{\text{oscolution}}(\hat{\mathbf{A}})$	30.00 - 2.30	Depositor
Resolution (A)	29.71 - 2.22	EDS
% Data completeness	99.8 (30.00-2.30)	Depositor
(in resolution range)	98.5(29.71-2.22)	EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.71 (at 2.22 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
P. P.	0.172 , $0.203$	Depositor
$n, n_{free}$	0.173 , $0.176$	DCC
$R_{free}$ test set	10093 reflections $(4.55\%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	20.9	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.34 , $34.0$	EDS
L-test for $twinning^2$	$<  L  > = 0.50, < L^2 > = 0.33$	Xtriage
	0.000 for -h-l,k,h	
	0.000 for l,k,-h-l	
Estimated twinning fraction	0.010 for h,-k,-h-l	Xtriage
	0.009 for -h-l,-k,l	
	0.105 for l,-k,h	
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	40965	wwPDB-VP
Average B, all atoms $(Å^2)$	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.91% 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.

# 3 Model quality (i)

# 3.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MME, MG, HYP, SMC, KCX, EDO, CAP

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	Bo	nd lengths	Bond angles	
		RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	А	0.51	0/3698	0.57	0/4996
1	В	0.56	0/3712	0.59	0/5015
1	С	0.55	0/3703	0.61	0/5003
1	D	0.56	1/3694~(0.0%)	0.61	0/4991
1	Ε	0.55	0/3697	0.60	0/4996
1	F	0.55	0/3712	0.60	0/5015
1	G	0.55	0/3698	0.61	0/4996
1	Н	0.56	0/3698	0.62	0/4996
2	Ι	0.49	0/1166	0.57	0/1584
2	J	0.53	0/1166	0.60	0/1584
2	Κ	0.54	0/1174	0.61	0/1594
2	L	0.54	0/1166	0.63	0/1584
2	М	0.53	0/1166	0.60	0/1584
2	Ν	0.53	0/1174	0.59	0/1594
2	0	0.53	0/1174	0.59	0/1594
2	Р	0.55	0/1166	0.61	0/1584
All	All	0.54	1/38964~(0.0%)	0.60	0/52710

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	172	CYS	CB-SG	-5.89	1.72	1.81

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.



### 3.2 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	3644	0	3551	38	0
1	В	3651	0	3550	44	0
1	С	3649	0	3556	36	0
1	D	3640	0	3548	37	0
1	Е	3643	0	3551	39	0
1	F	3653	0	3558	40	0
1	G	3643	0	3547	32	0
1	Н	3644	0	3551	43	0
2	Ι	1143	0	1122	13	0
2	J	1143	0	1122	12	0
2	K	1145	0	1123	9	0
2	L	1143	0	1122	14	0
2	М	1143	0	1122	15	0
2	N	1145	0	1123	19	0
2	0	1145	0	1123	10	0
2	Р	1143	0	1122	12	0
3	А	1	0	0	0	0
3	В	1	0	0	0	0
3	С	1	0	0	0	0
3	D	1	0	0	0	0
3	Е	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	Н	1	0	0	0	0
4	А	21	0	7	0	0
4	В	21	0	7	0	0
4	С	21	0	7	0	0
4	D	21	0	8	0	0
4	Ε	21	0	7	0	0
4	F	21	0	7	0	0
4	G	21	0	7	0	0
4	Н	21	0	7	0	0
5	А	20	0	30	1	0
5	В	16	0	24	3	0
5	С	20	0	30	0	0
5	D	16	0	24	2	0
5	Е	12	0	18	0	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	24	0	36	1	0
5	G	12	0	18	2	0
5	Н	24	0	36	1	0
5	Ι	8	0	12	0	0
5	J	8	0	12	0	0
5	Κ	8	0	12	1	0
5	L	4	0	6	0	0
5	М	4	0	6	1	0
5	Ν	8	0	12	3	0
5	0	8	0	12	0	0
5	Р	4	0	6	0	0
6	А	237	0	0	1	0
6	В	216	0	0	4	0
6	С	233	0	0	2	0
6	D	211	0	0	2	0
6	Е	225	0	0	2	0
6	F	211	0	0	4	0
6	G	221	0	0	2	0
6	Н	234	0	0	1	0
6	Ι	58	0	0	0	0
6	J	57	0	0	0	0
6	Κ	62	0	0	1	0
6	L	78	0	0	2	0
6	М	62	0	0	0	0
6	Ν	58	0	0	1	0
6	0	56	0	0	0	0
6	Р	57	0	0	0	0
All	All	40965	0	37742	367	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 (367) 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:A:267:HIS:HD2	1:A:277:ASN:HD22	1.06	0.99
1:H:267:HIS:HD2	1:H:277:ASN:HD22	1.05	0.98
1:D:267:HIS:HD2	1:D:277:ASN:HD22	1.08	0.98
1:F:267:HIS:HD2	1:F:277:ASN:HD22	1.12	0.97
1:E:267:HIS:HD2	1:E:277:ASN:HD22	1.00	0.97
1:C:267:HIS:HD2	1:C:277:ASN:HD22	1.12	0.95



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
2:N:39:ILE:HG12	5:N:1141:EDO:H21	1.52	0.92
1:B:267:HIS:HD2	1:B:277:ASN:HD22	1.11	0.91
1:E:184:ASN:HD22	2:K:115:GLN:HE21	1.09	0.91
1:G:184:ASN:HD22	2:M:115:GLN:HE21	1.18	0.90
1:G:267:HIS:HD2	1:G:277:ASN:HD22	1.18	0.89
1:B:184:ASN:HD22	2:L:115:GLN:HE21	1.19	0.88
1:F:267:HIS:CD2	1:F:277:ASN:HD22	1.94	0.85
1:E:267:HIS:CD2	1:E:277:ASN:HD22	1.91	0.84
1:A:267:HIS:CD2	1:A:277:ASN:HD22	1.96	0.83
1:A:184:ASN:HD22	2:O:115:GLN:HE21	1.28	0.82
1:C:184:ASN:HD22	2:I:115:GLN:HE21	1.29	0.80
2:N:82:GLY:H	5:N:1141:EDO:H22	1.47	0.80
1:D:184:ASN:HD22	2:N:115:GLN:HE21	1.27	0.80
1:F:184:ASN:HD22	2:P:115:GLN:HE21	1.29	0.79
1:H:267:HIS:CD2	1:H:277:ASN:HD22	1.95	0.79
1:C:267:HIS:CD2	1:C:277:ASN:HD22	1.98	0.78
1:B:267:HIS:CD2	1:B:277:ASN:HD22	1.98	0.78
1:D:267:HIS:CD2	1:D:277:ASN:HD22	2.00	0.77
1:B:468:GLU:H	5:B:1479:EDO:H12	1.51	0.75
2:I:134:PRO:HG2	2:I:137:LYS:HB2	1.69	0.74
2:P:22:THR:H	2:P:25:GLN:HE21	1.36	0.73
1:C:431:ARG:HH21	1:C:432:ASN:HD21	1.38	0.72
2:O:22:THR:H	2:O:25:GLN:HE21	1.34	0.72
1:G:267:HIS:CD2	1:G:277:ASN:HD22	2.06	0.72
1:C:202:ASP:OD1	1:C:238:HIS:HE1	1.71	0.71
2:L:22:THR:H	2:L:25:GLN:HE21	1.39	0.71
2:M:22:THR:H	2:M:25:GLN:HE21	1.37	0.71
1:E:431:ARG:HH21	1:E:432:ASN:HD21	1.39	0.70
2:I:22:THR:H	2:I:25:GLN:HE21	1.40	0.70
1:F:431:ARG:HH21	1:F:432:ASN:HD21	1.41	0.69
1:B:14:LYS:HE3	6:B:2003:HOH:O	1.94	0.67
6:B:2105:HOH:O	1:D:161:LYS:HE2	1.94	0.67
1:G:431:ARG:HH21	1:G:432:ASN:HD21	1.41	0.67
1:H:184:ASN:HD22	2:J:115:GLN:HE21	1.43	0.66
1:G:468:GLU:H	5:G:1480:EDO:H12	1.60	0.65
1:A:431:ARG:HH21	1:A:432:ASN:HD21	1.44	0.65
6:E:2114:HOH:O	2:M:10:LYS:HE3	1.97	0.64
2:P:134:PRO:HG2	2:P:137:LYS:HB2	1.78	0.64
2:N:22:THR:H	2:N:25:GLN:HE21	1.43	0.64
1:C:180:LEU:HA	2:I:115:GLN:HE22	1.63	0.64
1:H:338[B]:GLU:HG3	1:H:471:THR:HG21	1.79	0.64



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:10:GLY:HA3	2:L:84:ARG:HH22	1.63	0.64
1:D:180:LEU:HA	2:N:115:GLN:HE22	1.63	0.63
1:B:180:LEU:HA	2:L:115:GLN:HE22	1.63	0.63
1:D:202:ASP:OD1	1:D:238:HIS:HE1	1.82	0.63
1:E:202:ASP:OD1	1:E:238:HIS:HE1	1.81	0.63
1:D:431:ARG:HH21	1:D:432:ASN:HD21	1.45	0.62
1:H:202:ASP:OD1	1:H:238:HIS:HE1	1.82	0.62
1:H:290:LEU:HG	2:P:66:LEU:HD11	1.79	0.62
1:H:431:ARG:HH21	1:H:432:ASN:HD21	1.47	0.62
1:E:338[B]:GLU:HG3	1:E:471:THR:HG21	1.81	0.62
1:G:200:THR:OG1	1:G:238:HIS:HD2	1.83	0.62
1:G:383:HIS:H	1:G:386:HIS:HD2	1.46	0.62
2:K:22:THR:H	2:K:25:GLN:HE21	1.48	0.62
1:D:290:LEU:HG	2:L:66:LEU:HD11	1.81	0.62
1:F:180:LEU:HA	2:P:115:GLN:HE22	1.65	0.62
1:E:239:TYR:HE2	1:E:401:GLN:HE22	1.48	0.62
1:G:239:TYR:HE2	1:G:401:GLN:HE22	1.47	0.61
1:F:200:THR:OG1	1:F:238:HIS:HD2	1.83	0.61
1:G:202:ASP:OD1	1:G:238:HIS:HE1	1.82	0.61
1:B:200:THR:OG1	1:B:238:HIS:HD2	1.84	0.61
1:B:338[B]:GLU:HG3	1:B:471:THR:HG21	1.82	0.61
1:C:338[B]:GLU:HG3	1:C:471:THR:HG21	1.82	0.61
1:G:180:LEU:HA	2:M:115:GLN:HE22	1.66	0.61
1:A:338[B]:GLU:HG3	1:A:471:THR:HG21	1.83	0.61
1:H:180:LEU:HA	2:J:115:GLN:HE22	1.65	0.61
1:A:267:HIS:HE1	6:B:2124:HOH:O	1.82	0.60
2:J:22:THR:H	2:J:25:GLN:HE21	1.49	0.60
1:A:202:ASP:OD1	1:A:238:HIS:HE1	1.84	0.60
6:F:2110:HOH:O	1:H:161:LYS:HE2	2.01	0.60
1:A:239:TYR:HE2	1:A:401:GLN:HE22	1.49	0.60
1:G:290:LEU:HG	2:O:66:LEU:HD11	1.82	0.60
1:D:239:TYR:HE2	1:D:401:GLN:HE22	1.49	0.60
1:C:290:LEU:HG	2:K:66:LEU:HD11	1.84	0.59
1:A:200:THR:OG1	1:A:238:HIS:HD2	1.84	0.59
1:G:338[B]:GLU:HG3	1:G:471:THR:HG21	1.84	0.59
1:B:239:TYR:HE2	1:B:401:GLN:HE22	1.49	0.59
1:E:161:LYS:HE2	6:G:2104:HOH:O	2.03	0.59
1:F:202:ASP:OD1	1:F:238:HIS:HE1	1.84	0.59
1:B:431:ARG:HH21	1:B:432:ASN:HD21	1.51	0.58
1:A:180:LEU:HA	2:O:115:GLN:HE22	1.67	0.58
1:F:383:HIS:H	1:F:386:HIS:HD2	1.52	0.58



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:E:200:THR:OG1	1:E:238:HIS:HD2	1.85	0.57
1:B:229:GLN:HE21	1:B:236:LYS:H	1.52	0.57
1:C:383:HIS:H	1:C:386:HIS:HD2	1.52	0.57
1:F:239:TYR:HE2	1:F:401:GLN:HE22	1.51	0.57
2:L:128:THR:HG23	6:L:2072:HOH:O	2.04	0.57
1:C:200:THR:OG1	1:C:238:HIS:HD2	1.87	0.57
1:B:290:LEU:HG	2:J:66:LEU:HD11	1.85	0.57
1:G:229:GLN:HE21	1:G:236:LYS:H	1.52	0.56
1:H:377:VAL:HG22	1:H:399:CYS:HB3	1.88	0.56
2:K:109:ALA:HB3	2:K:119:MET:HG3	1.86	0.56
6:E:2135:HOH:O	1:F:267:HIS:HE1	1.87	0.56
1:F:338[B]:GLU:HG3	1:F:471:THR:HG21	1.88	0.56
1:G:422:VAL:HG13	1:G:451:TRP:CH2	2.41	0.56
1:B:18:LYS:O	5:B:1481:EDO:H21	2.07	0.55
1:G:431:ARG:HE	1:G:432:ASN:ND2	2.05	0.55
2:I:109:ALA:HB3	2:I:119:MET:HG3	1.88	0.55
2:J:9:ASN:HD21	2:J:138:ARG:HG2	1.71	0.55
1:E:180:LEU:HA	2:K:115:GLN:HE22	1.72	0.55
1:H:200:THR:OG1	1:H:238:HIS:HD2	1.90	0.55
1:C:239:TYR:HE2	1:C:401:GLN:HE22	1.53	0.54
1:C:431:ARG:HE	1:C:432:ASN:ND2	2.06	0.54
1:G:383:HIS:H	1:G:386:HIS:CD2	2.25	0.54
1:F:267:HIS:HD2	1:F:277:ASN:ND2	1.94	0.54
1:E:192:CYS:HB3	1:E:197:LEU:HD12	1.89	0.54
1:A:431:ARG:HE	1:A:432:ASN:ND2	2.06	0.54
2:P:109:ALA:HB3	2:P:119:MET:HG3	1.89	0.54
1:E:383:HIS:H	1:E:386:HIS:HD2	1.55	0.54
1:G:431:ARG:HE	1:G:432:ASN:HD22	1.55	0.54
1:B:422:VAL:HG13	1:B:451:TRP:CH2	2.43	0.54
1:D:469:PHE:CZ	5:D:1478:EDO:H12	2.42	0.53
1:F:431:ARG:HE	1:F:432:ASN:ND2	2.06	0.53
1:C:267:HIS:HE1	6:D:2134:HOH:O	1.90	0.53
1:F:290:LEU:HG	2:N:66:LEU:HD11	1.90	0.53
1:G:267:HIS:HE1	6:H:2137:HOH:O	1.91	0.53
1:C:382:ILE:HA	1:C:386:HIS:HD2	1.73	0.53
1:B:382:ILE:HA	1:B:386:HIS:HD2	1.74	0.53
1:A:383:HIS:H	1:A:386:HIS:HD2	1.56	0.53
1:B:383:HIS:H	1:B:386:HIS:HD2	1.56	0.53
1:H:431:ARG:HE	1:H:432:ASN:ND2	2.07	0.53
1:A:290:LEU:HG	2:I:66:LEU:HD11	1.91	0.52
1:H:414:ALA:HB3	1:H:415:PRO:HD3	1.91	0.52



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
2:N:82:GLY:H	5:N:1141:EDO:C2	2.18	0.52
1:D:200:THR:OG1	1:D:238:HIS:HD2	1.92	0.52
1:C:382:ILE:HA	1:C:386:HIS:CD2	2.45	0.52
1:D:338[B]:GLU:HG3	1:D:471:THR:HG21	1.91	0.52
1:E:431:ARG:HE	1:E:432:ASN:HD22	1.56	0.51
1:F:181:SER:H	2:P:115:GLN:NE2	2.08	0.51
1:A:431:ARG:HE	1:A:432:ASN:HD22	1.57	0.51
1:E:290:LEU:HG	2:M:66:LEU:HD11	1.91	0.51
1:F:383:HIS:H	1:F:386:HIS:CD2	2.28	0.51
2:N:109:ALA:HB3	2:N:119:MET:HG3	1.90	0.51
1:B:202:ASP:OD1	1:B:238:HIS:HE1	1.93	0.51
1:C:229:GLN:HE21	1:C:236:LYS:H	1.59	0.51
1:H:422:VAL:HG13	1:H:451:TRP:CH2	2.45	0.51
2:M:9:ASN:HD21	2:M:138:ARG:HG2	1.75	0.51
1:B:200:THR:O	1:B:238:HIS:HA	2.11	0.51
1:A:161:LYS:HE2	6:C:2119:HOH:O	2.11	0.50
1:F:431:ARG:HE	1:F:432:ASN:HD22	1.57	0.50
1:C:383:HIS:H	1:C:386:HIS:CD2	2.29	0.50
1:C:181:SER:H	2:I:115:GLN:NE2	2.09	0.50
1:D:379:SER:HB2	1:D:401:GLN:HB2	1.93	0.50
1:B:431:ARG:HE	1:B:432:ASN:ND2	2.10	0.50
1:H:229:GLN:HE21	1:H:236:LYS:H	1.58	0.50
1:B:382:ILE:HA	1:B:386:HIS:CD2	2.47	0.50
1:B:431:ARG:HE	1:B:432:ASN:HD22	1.59	0.50
1:H:382:ILE:HA	1:H:386:HIS:HD2	1.75	0.50
1:D:201:KCX:HB2	1:D:239:TYR:CD2	2.47	0.50
2:M:109:ALA:HB3	2:M:119:MET:HG3	1.93	0.50
2:N:87:MET:HE3	6:N:2013:HOH:O	2.11	0.50
2:O:109:ALA:HB3	2:O:119:MET:HG3	1.93	0.50
1:E:181:SER:H	2:K:115:GLN:NE2	2.10	0.49
1:G:227:LYS:HA	5:M:1141:EDO:H12	1.93	0.49
1:H:383:HIS:H	1:H:386:HIS:HD2	1.58	0.49
2:L:9:ASN:HD21	2:L:138:ARG:HG2	1.78	0.49
1:A:422:VAL:HG13	1:A:451:TRP:CH2	2.47	0.49
1:E:201:KCX:HB2	1:E:239:TYR:CD2	2.47	0.49
1:F:185:TYR:O	1:F:189:VAL:HG23	2.12	0.49
1:E:190:TYR:CZ	1:E:227:LYS:HE3	2.47	0.49
1:H:431:ARG:HE	1:H:432:ASN:HD22	1.59	0.49
1:A:382:ILE:HA	1:A:386:HIS:HD2	1.77	0.48
1:H:181:SER:H	2:J:115:GLN:NE2	2.11	0.48
1:A:383:HIS:H	1:A:386:HIS:CD2	2.31	0.48



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:431:ARG:HE	1:D:432:ASN:ND2	2.11	0.48
1:A:381:GLY:HA2	1:B:66:TRP:CD1	2.49	0.48
1:F:382:ILE:HA	1:F:386:HIS:HD2	1.78	0.48
1:D:382:ILE:HA	1:D:386:HIS:HD2	1.79	0.48
1:D:422:VAL:HG13	1:D:451:TRP:CH2	2.49	0.48
1:D:431:ARG:HE	1:D:432:ASN:HD22	1.61	0.48
1:E:422:VAL:HG13	1:E:451:TRP:CH2	2.49	0.48
2:O:42:LEU:HD21	2:O:93:ILE:HG12	1.95	0.48
1:A:273:GLY:HA3	1:B:273:GLY:HA3	1.96	0.48
1:B:345:PHE:O	1:B:349:MET:HG3	2.14	0.48
1:B:414:ALA:HB3	1:B:415:PRO:HD3	1.95	0.48
1:C:298:HIS:ND1	1:C:302:ASP:OD2	2.34	0.48
1:F:192:CYS:HB3	1:F:197:LEU:HD12	1.96	0.48
1:G:190:TYR:CZ	1:G:227:LYS:HE3	2.49	0.48
1:B:293:ILE:HG13	1:B:318:LEU:HD21	1.96	0.47
1:A:181:SER:H	2:O:115:GLN:NE2	2.12	0.47
1:C:93:GLU:HB3	1:C:96:GLN:HB2	1.96	0.47
2:N:22:THR:H	2:N:25:GLN:NE2	2.11	0.47
1:E:267:HIS:HE1	6:F:2133:HOH:O	1.97	0.47
1:E:431:ARG:HE	1:E:432:ASN:ND2	2.12	0.47
1:A:414:ALA:HB3	1:A:415:PRO:HD3	1.96	0.47
1:E:382:ILE:HA	1:E:386:HIS:HD2	1.78	0.47
1:E:383:HIS:H	1:E:386:HIS:CD2	2.31	0.47
1:C:431:ARG:HE	1:C:432:ASN:HD22	1.62	0.47
1:G:382:ILE:HA	1:G:386:HIS:HD2	1.79	0.47
1:F:229:GLN:HE21	1:F:236:LYS:H	1.62	0.47
1:F:382:ILE:HA	1:F:386:HIS:CD2	2.49	0.47
2:P:38:TRP:CD2	2:P:118:ILE:HG21	2.49	0.47
2:P:42:LEU:HD21	2:P:93:ILE:HG12	1.96	0.47
1:B:383:HIS:H	1:B:386:HIS:CD2	2.32	0.47
1:H:382:ILE:HA	1:H:386:HIS:CD2	2.49	0.47
1:A:201:KCX:HB2	1:A:239:TYR:CD2	2.50	0.47
1:G:158:GLU:CD	1:G:325:HIS:HE2	2.17	0.47
2:J:109:ALA:HB3	2:J:119:MET:HG3	1.97	0.47
1:C:392:GLU:CD	1:C:438:ALA:HB2	2.35	0.47
1:F:170:LEU:HD11	1:F:421:ARG:HA	1.96	0.47
2:N:9:ASN:HD21	2:N:138:ARG:HG2	1.80	0.47
1:G:382:ILE:HA	1:G:386:HIS:CD2	2.50	0.46
1:H:239:TYR:HE2	1:H:401:GLN:HE22	1.61	0.46
1:H:138:LEU:O	1:H:316:LYS:NZ	2.45	0.46
2:N:42:LEU:HD21	2:N:93:ILE:HG12	1.96	0.46



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:E:381:GLY:HA2	1:F:66:TRP:CD1	2.51	0.46
1:G:293:ILE:HG13	1:G:318:LEU:HD21	1.97	0.46
2:I:125:ARG:HD2	2:I:132:PHE:CE2	2.50	0.46
1:C:201:KCX:HB2	1:C:239:TYR:CD2	2.51	0.46
1:D:192:CYS:HB3	1:D:197:LEU:HD12	1.98	0.46
1:E:93:GLU:HB3	1:E:96:GLN:HB2	1.98	0.46
1:B:178:LEU:HD22	1:B:211:PHE:HZ	1.80	0.46
1:B:468:GLU:H	5:B:1479:EDO:C1	2.24	0.46
1:H:190:TYR:CZ	1:H:227:LYS:HE3	2.50	0.46
6:A:2146:HOH:O	1:B:267:HIS:HE1	1.99	0.46
1:E:382:ILE:HA	1:E:386:HIS:CD2	2.50	0.46
2:L:125:ARG:HD2	2:L:132:PHE:CE2	2.51	0.46
2:M:107:LEU:O	2:M:120:GLY:HA2	2.16	0.46
1:A:382:ILE:HA	1:A:386:HIS:CD2	2.50	0.45
1:A:229:GLN:HE21	1:A:236:LYS:H	1.63	0.45
1:D:383:HIS:H	1:D:386:HIS:HD2	1.64	0.45
1:B:125:PHE:HB2	6:B:2062:HOH:O	2.16	0.45
1:B:175:LYS:HA	1:B:176:PRO:C	2.37	0.45
1:G:190:TYR:CE1	1:G:227:LYS:HG2	2.51	0.45
1:G:468:GLU:H	5:G:1480:EDO:C1	2.28	0.45
1:H:383:HIS:H	1:H:386:HIS:CD2	2.34	0.45
2:J:38:TRP:CD2	2:J:118:ILE:HG21	2.52	0.45
1:D:295:ARG:HG2	1:D:327:HIS:HB2	1.98	0.45
1:B:251:MET:O	1:B:255:VAL:HG23	2.17	0.45
2:I:42:LEU:HD21	2:I:93:ILE:HG12	1.97	0.45
1:E:277:ASN:HD21	1:E:293:ILE:HD12	1.82	0.45
1:F:259[B]:GLU:OE1	2:P:61:GLY:HA3	2.16	0.45
1:C:239:TYR:HB3	1:C:266:MET:HB3	1.99	0.45
1:D:239:TYR:HB3	1:D:266:MET:HB3	1.99	0.45
1:E:331:ALA:HA	1:E:337:GLY:O	2.17	0.45
2:K:9:ASN:HD21	2:K:138:ARG:HG2	1.82	0.45
2:L:109:ALA:HB3	2:L:119:MET:HG3	1.99	0.45
1:F:173:THR:HB	1:F:175:LYS:HE2	1.99	0.45
1:F:298:HIS:ND1	1:F:302:ASP:OD2	2.38	0.45
1:H:192:CYS:HB3	1:H:197:LEU:HD12	1.99	0.45
1:B:170:LEU:HD11	1:B:421:ARG:HA	2.00	0.45
2:M:85:ASP:HA	2:M:86:PRO:HD2	1.90	0.45
2:M:134:PRO:HG2	2:M:137:LYS:HB2	1.99	0.45
1:F:258:LYS:HA	2:N:65:CYS:SG	2.57	0.44
2:M:125:ARG:HD2	2:M:132:PHE:CE2	2.52	0.44
2:P:107:LEU:O	2:P:120:GLY:HA2	2.16	0.44



			Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:F:201:KCX:HB2	1:F:239:TYR:CD2	2.52	0.44
1:D:414:ALA:HB3	1:D:415:PRO:HD3	1.98	0.44
1:E:197:LEU:HG	1:E:417:ALA:HB1	2.00	0.44
1:H:93:GLU:HB3	1:H:96:GLN:HB2	1.98	0.44
2:I:38:TRP:CD2	2:I:118:ILE:HG21	2.52	0.44
1:D:178:LEU:HD22	1:D:211:PHE:HZ	1.82	0.44
1:G:175:LYS:HA	1:G:176:PRO:C	2.38	0.44
1:H:170:LEU:HD11	1:H:421:ARG:HA	2.00	0.44
1:B:93:GLU:HB3	1:B:96:GLN:HB2	1.99	0.44
1:F:197:LEU:HG	1:F:417:ALA:HB1	2.00	0.44
1:G:185:TYR:O	1:G:189:VAL:HG23	2.17	0.44
2:J:42:LEU:HD21	2:J:93:ILE:HG12	2.00	0.44
2:L:42:LEU:HD21	2:L:93:ILE:HG12	2.00	0.44
1:E:178:LEU:HD22	1:E:211:PHE:HZ	1.83	0.44
1:E:414:ALA:HB3	1:E:415:PRO:HD3	1.99	0.44
1:H:201:KCX:HB2	1:H:239:TYR:CD2	2.53	0.44
1:A:93:GLU:HB3	1:A:96:GLN:HB2	1.99	0.44
1:D:383:HIS:H	1:D:386:HIS:CD2	2.36	0.44
1:G:181:SER:H	2:M:115:GLN:NE2	2.16	0.44
1:D:170:LEU:HD11	1:D:421:ARG:HA	1.99	0.43
1:A:336:GLU:O	5:A:1484:EDO:H11	2.19	0.43
1:D:293:ILE:HG13	1:D:318:LEU:HD21	2.00	0.43
1:D:469:PHE:CE2	5:D:1478:EDO:H12	2.53	0.43
1:F:72:ASP:OD2	5:F:1484:EDO:H21	2.19	0.43
2:I:3:VAL:O	2:I:139:SER:HA	2.18	0.43
1:B:190:TYR:CE1	1:B:227:LYS:HG2	2.53	0.43
1:C:379:SER:HB2	1:C:401:GLN:HB2	2.00	0.43
2:N:107:LEU:O	2:N:120:GLY:HA2	2.17	0.43
1:A:170:LEU:HD11	1:A:421:ARG:HA	2.01	0.43
5:K:1142:EDO:H12	6:K:2034:HOH:O	2.18	0.43
1:A:66:TRP:CD1	1:B:381:GLY:HA2	2.54	0.43
1:A:277:ASN:HD21	1:A:293:ILE:HD12	1.83	0.43
1:D:277:ASN:HD21	1:D:293:ILE:HD12	1.84	0.43
1:H:277:ASN:HD21	1:H:293:ILE:HD12	1.84	0.43
2:K:42:LEU:HD21	2:K:93:ILE:HG12	2.01	0.43
2:M:42:LEU:HD21	2:M:93:ILE:HG12	2.00	0.43
1:F:295:ARG:HG2	1:F:327:HIS:HB2	1.99	0.43
2:J:39:ILE:O	2:J:109:ALA:HA	2.18	0.43
1:A:190:TYR:CZ	1:A:227:LYS:HE3	2.54	0.43
1:H:18:LYS:O	5:H:1482:EDO:H21	2.19	0.43
1:B:201:KCX:HB2	1:B:239:TYR:CD2	2.53	0.42



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:E:62:SER:O	1:F:177:LYS:HB2	2.18	0.42
1:B:199:PHE:HA	1:B:237:GLY:O	2.19	0.42
6:F:2194:HOH:O	2:N:139:SER:HB3	2.19	0.42
1:H:197:LEU:HG	1:H:417:ALA:HB1	2.00	0.42
1:C:66:TRP:CD1	1:D:381:GLY:HA2	2.54	0.42
1:C:190:TYR:CZ	1:C:227:LYS:HE3	2.54	0.42
1:F:277:ASN:HD21	1:F:293:ILE:HD12	1.84	0.42
1:H:241:ASN:ND2	1:H:243:THR:OG1	2.52	0.42
2:I:107:LEU:O	2:I:120:GLY:HA2	2.19	0.42
2:J:5:THR:HG22	2:J:138:ARG:O	2.20	0.42
1:B:277:ASN:HD21	1:B:293:ILE:HD12	1.85	0.42
6:C:2143:HOH:O	1:D:267:HIS:HE1	2.01	0.42
1:F:190:TYR:CZ	1:F:227:LYS:HE3	2.54	0.42
1:H:36:ILE:N	1:H:36:ILE:HD12	2.35	0.42
2:N:38:TRP:CD2	2:N:118:ILE:HG21	2.55	0.42
2:J:22:THR:H	2:J:25:GLN:NE2	2.14	0.42
2:O:9:ASN:HD21	2:O:138:ARG:HG2	1.84	0.42
1:H:152:PRO:HB2	1:H:153:HIS:CD2	2.54	0.42
1:A:200:THR:OG1	1:A:238:HIS:CD2	2.71	0.42
1:B:185:TYR:O	1:B:189:VAL:HG23	2.19	0.42
6:F:2118:HOH:O	2:N:10:LYS:HE3	2.20	0.42
1:C:197:LEU:HG	1:C:417:ALA:HB1	2.02	0.41
1:C:258:LYS:HA	2:K:65:CYS:SG	2.60	0.41
1:H:175:LYS:HA	1:H:176:PRO:C	2.40	0.41
1:A:192:CYS:HB3	1:A:197:LEU:HD12	2.02	0.41
1:C:339:ARG:HH22	1:C:392:GLU:CD	2.24	0.41
1:F:339:ARG:HH22	1:F:392:GLU:CD	2.24	0.41
2:M:39:ILE:O	2:M:109:ALA:HA	2.20	0.41
1:C:277:ASN:HD21	1:C:293:ILE:HD12	1.84	0.41
1:E:293:ILE:HG13	1:E:318:LEU:HD21	2.03	0.41
1:H:293:ILE:HG13	1:H:318:LEU:HD21	2.02	0.41
2:N:125:ARG:HD2	2:N:132:PHE:CE2	2.56	0.41
1:C:185:TYR:O	1:C:189:VAL:HG23	2.19	0.41
1:D:153:HIS:HE1	6:D:2138:HOH:O	2.02	0.41
1:H:165:TYR:CD1	2:P:117:GLN:HB3	2.56	0.41
2:O:107:LEU:O	2:O:120:GLY:HA2	2.19	0.41
1:D:181:SER:H	2:N:115:GLN:NE2	2.19	0.41
1:E:66:TRP:CD1	1:F:381:GLY:HA2	2.54	0.41
1:E:214:TRP:CD2	1:E:253:ARG:HG2	2.56	0.41
2:L:38:TRP:CD2	2:L:118:ILE:HG21	2.56	0.41
1:E:161:LYS:CE	6:G:2104:HOH:O	2.65	0.41



	A 4	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
2:L:87:MET:HE3	6:L:2054:HOH:O	2.20	0.41
1:D:229:GLN:HE21	1:D:236:LYS:H	1.68	0.41
1:G:197:LEU:HG	1:G:417:ALA:HB1	2.02	0.41
1:A:175:LYS:HA	1:A:176:PRO:C	2.41	0.41
1:A:239:TYR:HE2	1:A:401:GLN:NE2	2.16	0.41
1:C:170:LEU:HD11	1:C:421:ARG:HA	2.03	0.41
1:E:229:GLN:HE21	1:E:236:LYS:H	1.68	0.41
1:F:331:ALA:HA	1:F:337:GLY:O	2.21	0.41
2:I:39:ILE:O	2:I:109:ALA:HA	2.20	0.41
1:A:214:TRP:CD2	1:A:253:ARG:HG2	2.56	0.41
1:B:110:GLU:HB3	1:B:147:THR:HB	2.02	0.41
1:B:181:SER:H	2:L:115:GLN:NE2	2.19	0.41
1:C:331:ALA:HA	1:C:337:GLY:O	2.21	0.41
1:C:368:TRP:O	1:C:369:SMC:C	2.68	0.41
1:D:382:ILE:HA	1:D:386:HIS:CD2	2.56	0.41
1:E:273:GLY:HA3	1:F:273:GLY:HA3	2.02	0.41
1:G:192:CYS:HB3	1:G:197:LEU:HD12	2.02	0.41
1:G:414:ALA:HB3	1:G:415:PRO:HD3	2.02	0.41
1:H:214:TRP:CE3	1:H:253:ARG:HG2	2.56	0.41
1:B:295:ARG:HG2	1:B:327:HIS:HB2	2.02	0.41
1:D:165:TYR:CD1	2:L:117:GLN:HB3	2.56	0.41
1:H:178:LEU:HD22	1:H:211:PHE:HZ	1.86	0.41
1:H:267:HIS:HB2	1:H:280:LEU:HD23	2.03	0.41
2:O:39:ILE:O	2:O:109:ALA:HA	2.20	0.41
1:H:368:TRP:O	1:H:369:SMC:C	2.68	0.40
2:M:39:ILE:HA	2:M:40:PRO:HD3	1.96	0.40
1:A:345:PHE:O	1:A:349:MET:HG3	2.22	0.40
1:D:199:PHE:HA	1:D:237:GLY:O	2.20	0.40
1:C:143:ALA:HA	1:F:143:ALA:HA	2.03	0.40
1:E:200:THR:OG1	1:E:238:HIS:CD2	2.70	0.40
1:H:19:ASP:HB3	1:H:21:ARG:HG2	2.03	0.40
1:E:377:VAL:HG22	1:E:399:CYS:HB3	2.04	0.40
1:H:298:HIS:ND1	1:H:302:ASP:OD2	2.36	0.40

There are no symmetry-related clashes.



### 3.3 Torsion angles (i)

#### 3.3.1 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	ntiles
1	А	462/475~(97%)	448 (97%)	13 (3%)	1 (0%)	47	58
1	В	464/475~(98%)	452 (97%)	12 (3%)	0	100	100
1	С	463/475~(98%)	449 (97%)	14 (3%)	0	100	100
1	D	461/475~(97%)	447 (97%)	14(3%)	0	100	100
1	Ε	462/475~(97%)	449 (97%)	12 (3%)	1 (0%)	47	58
1	F	464/475~(98%)	449 (97%)	15 (3%)	0	100	100
1	G	462/475~(97%)	450 (97%)	12 (3%)	0	100	100
1	Н	462/475~(97%)	450 (97%)	12 (3%)	0	100	100
2	Ι	138/140~(99%)	132 (96%)	6 (4%)	0	100	100
2	J	138/140~(99%)	133~(96%)	5(4%)	0	100	100
2	Κ	139/140~(99%)	132~(95%)	7 (5%)	0	100	100
2	L	138/140~(99%)	133~(96%)	5(4%)	0	100	100
2	М	138/140~(99%)	134 (97%)	4 (3%)	0	100	100
2	Ν	139/140~(99%)	133~(96%)	6 (4%)	0	100	100
2	Ο	$13\overline{9/140}~(99\%)$	132 (95%)	7(5%)	0	100	100
2	Р	138/140~(99%)	132 (96%)	6 (4%)	0	100	100
All	All	4807/4920 (98%)	4655 (97%)	150 (3%)	2(0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Ε	11	ALA
1	А	11	ALA



#### 2V68

#### 3.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
1	А	370/375~(99%)	363~(98%)	7~(2%)	57	73
1	В	371/375~(99%)	364~(98%)	7 (2%)	57	73
1	С	370/375~(99%)	362~(98%)	8 (2%)	52	69
1	D	370/375~(99%)	363~(98%)	7 (2%)	57	73
1	Ε	370/375~(99%)	363~(98%)	7(2%)	57	73
1	F	371/375~(99%)	363~(98%)	8 (2%)	52	69
1	G	370/375~(99%)	362~(98%)	8 (2%)	52	69
1	Н	370/375~(99%)	361 (98%)	9(2%)	49	66
2	Ι	122/122~(100%)	118 (97%)	4 (3%)	38	53
2	J	122/122~(100%)	119 (98%)	3 (2%)	47	65
2	Κ	123/122 (101%)	120 (98%)	3 (2%)	49	66
2	L	122/122~(100%)	119 (98%)	3 (2%)	47	65
2	М	122/122 (100%)	118 (97%)	4 (3%)	38	53
2	Ν	123/122~(101%)	120 (98%)	3 (2%)	49	66
2	Ο	123/122~(101%)	118 (96%)	5 (4%)	30	43
2	Р	122/122 (100%)	119 (98%)	3 (2%)	47	65
All	All	3941/3976~(99%)	3852 (98%)	89 (2%)	50	67

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	14	LYS
1	А	94	ASP
1	А	185	TYR
1	А	203	ASP
1	А	239	TYR
1	А	241	ASN
1	А	460	GLU
1	В	14	LYS



Mol	Chain	Res	Type
1	В	94	ASP
1	В	185	TYR
1	В	203	ASP
1	В	239	TYR
1	В	241	ASN
1	В	460	GLU
1	С	14	LYS
1	С	94	ASP
1	С	185	TYR
1	С	203	ASP
1	С	241	ASN
1	С	392	GLU
1	С	431	ARG
1	С	460	GLU
1	D	14	LYS
1	D	94	ASP
1	D	185	TYR
1	D	203	ASP
1	D	241	ASN
1	D	439	ARG
1	D	460	GLU
1	Е	14	LYS
1	Е	94	ASP
1	Е	185	TYR
1	Е	203	ASP
1	Ε	241	ASN
1	Е	439	ARG
1	Ε	460	GLU
1	F	14	LYS
1	F	94	ASP
1	F	185	TYR
1	F	203	ASP
1	F	239	TYR
1	F	241	ASN
1	F	392	GLU
1	F	460	GLU
1	G	14	LYS
1	G	94	ASP
1	G	185	TYR
1	G	203	ASP
1	G	239	TYR
1	G	241	ASN



Mol	Chain	Res	Type
1	G	439	ARG
1	G	460	GLU
1	Н	14	LYS
1	Н	94	ASP
1	Н	185	TYR
1	Н	203	ASP
1	Н	239	TYR
1	Н	241	ASN
1	Н	392	GLU
1	Н	431	ARG
1	Н	460	GLU
2	Ι	9	ASN
2	Ι	12	PHE
2	Ι	52	VAL
2	Ι	137	LYS
2	J	9	ASN
2	J	12	PHE
2	J	52	VAL
2	K	9	ASN
2	К	12	PHE
2	K	52	VAL
2	L	9	ASN
2	L	12	PHE
2	L	52	VAL
2	М	9	ASN
2	М	12	PHE
2	М	52	VAL
2	М	137	LYS
2	Ν	9	ASN
2	N	12	PHE
2	N	52	VAL
2	0	9	ASN
2	0	12	PHE
2	Ō	52	VAL
2	0	130	ARG
2	O	137	LYS
2	Р	9	ASN
2	Р	12	PHE
2	Р	52	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (128) such sidechains are listed below:



$\mathbf{Mol}$	Chain	Res	Type
1	А	153	HIS
1	А	163	ASN
1	А	229	GLN
1	А	238	HIS
1	А	241	ASN
1	А	267	HIS
1	А	277	ASN
1	А	304	GLN
1	А	386	HIS
1	А	401	GLN
1	А	432	ASN
1	В	153	HIS
1	В	229	GLN
1	В	238	HIS
1	В	241	ASN
1	В	267	HIS
1	В	277	ASN
1	В	304	GLN
1	В	386	HIS
1	В	401	GLN
1	В	432	ASN
1	С	153	HIS
1	С	229	GLN
1	С	238	HIS
1	С	241	ASN
1	С	267	HIS
1	С	277	ASN
1	С	304	GLN
1	С	386	HIS
1	С	401	GLN
1	С	432	ASN
1	D	153	HIS
1	D	229	GLN
1	D	238	HIS
1	D	241	ASN
1	D	267	HIS
1	D	277	ASN
1	D	304	GLN
1	D	386	HIS
1	D	401	GLN
1	D	432	ASN
1	Е	153	HIS
1	Е	163	ASN



Mol	Chain	Res	Type
1	Е	207	ASN
1	Е	229	GLN
1	Е	238	HIS
1	Е	241	ASN
1	Е	267	HIS
1	Е	277	ASN
1	Е	304	GLN
1	Е	386	HIS
1	Е	401	GLN
1	Е	432	ASN
1	F	153	HIS
1	F	229	GLN
1	F	238	HIS
1	F	241	ASN
1	F	267	HIS
1	F	277	ASN
1	F	304	GLN
1	F	386	HIS
1	F	401	GLN
1	F	432	ASN
1	G	153	HIS
1	G	229	GLN
1	G	238	HIS
1	G	241	ASN
1	G	267	HIS
1	G	277	ASN
1	G	304	GLN
1	G	386	HIS
1	G	401	GLN
1	G	432	ASN
1	Н	153	HIS
1	Н	163	ASN
1	Н	229	GLN
1	H	238	HIS
1	Н	241	ASN
1	Н	267	HIS
1	Н	277	ASN
1	Н	304	GLN
1	Н	386	HIS
1	Н	401	GLN
1	H	432	ASN
2	Ι	9	ASN



Mol	Chain	Res	Type
2	Ι	25	GLN
2	Ι	29	GLN
2	Ι	115	GLN
2	Ι	133	GLN
2	J	8	ASN
2	J	9	ASN
2	J	25	GLN
2	J	29	GLN
2	J	113	GLN
2	J	115	GLN
2	J	133	GLN
2	K	9	ASN
2	K	25	GLN
2	K	29	GLN
2	K	115	GLN
2	K	133	GLN
2	L	8	ASN
2	L	9	ASN
2	L	25	GLN
2	L	29	GLN
2	L	115	GLN
2	L	133	GLN
2	М	8	ASN
2	М	9	ASN
2	М	25	GLN
2	М	29	GLN
2	М	115	GLN
2	М	133	GLN
2	Ν	9	ASN
2	N	25	GLN
2	N	29	GLN
2	N	113	GLN
2	N	115	GLN
2	0	8	ASN
2	0	9	ASN
2	O	25	GLN
2	0	29	GLN
2	0	115	GLN
2	Р	9	ASN
2	Р	25	GLN
2	Р	29	GLN
2	Р	115	GLN



Continued from previous page...

Mol	Chain	Res	Type
2	Р	133	GLN

#### 3.3.3 RNA (i)

There are no RNA molecules in this entry.

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

48 non-standard protein/DNA/RNA residues 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	Turne	Chain	Dec	Tiple	B	ond leng	gths	E	Bond angles		
	Type	Unam	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z  > 2	
1	HYP	D	104	1	6,8,9	0.63	0	5,10,12	0.97	0	
1	SMC	С	256	1	5,6,7	0.93	0	$2,\!6,\!8$	1.11	0	
2	MME	Ι	1	2	7,8,9	2.80	1 (14%)	$5,\!8,\!10$	1.23	1 (20%)	
1	HYP	Е	104	1	6,8,9	0.68	0	5,10,12	1.10	0	
1	KCX	G	201	3,1	9,11,12	1.16	1 (11%)	5,12,14	1.24	1 (20%)	
1	SMC	А	256	1	5,6,7	0.78	0	2,6,8	0.98	0	
2	MME	Р	1	2	7,8,9	2.81	1 (14%)	5,8,10	1.30	1 (20%)	
1	KCX	А	201	3,1	9,11,12	1.10	1 (11%)	5,12,14	0.65	0	
1	SMC	F	369	1	5,6,7	0.93	0	2,6,8	0.50	0	
1	HYP	В	151	1	6,8,9	0.55	0	5,10,12	1.60	1 (20%)	
1	SMC	Н	256	1	5,6,7	0.71	0	2,6,8	0.41	0	
1	SMC	Е	369	1	5,6,7	0.77	0	$2,\!6,\!8$	1.07	0	
1	KCX	С	201	3,1	9,11,12	1.06	1 (11%)	$5,\!12,\!14$	0.89	0	
1	SMC	D	256	1	5,6,7	1.05	1 (20%)	2,6,8	1.64	1 (50%)	
1	KCX	D	201	3,1	9,11,12	1.08	1 (11%)	5,12,14	0.73	0	
1	SMC	Н	369	1	5,6,7	0.90	0	2,6,8	0.39	0	
1	HYP	А	151	1	6,8,9	0.66	0	5,10,12	1.47	0	
2	MME	K	1	2	7,8,9	2.79	1 (14%)	$5,\!8,\!10$	1.36	1 (20%)	
1	HYP	D	151	1	6,8,9	0.59	0	5,10,12	1.38	1 (20%)	
1	HYP	Е	151	1	6,8,9	0.71	0	5,10,12	1.19	0	



Mal	Turne	Chain	Dec	Tink	B	ond leng	$\mathbf{gths}$	Bond angles		
	Type	Ullalli	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
1	SMC	F	256	1	5,6,7	0.74	0	$2,\!6,\!8$	0.30	0
1	HYP	Н	104	1	6,8,9	0.56	0	5,10,12	1.10	0
1	HYP	С	104	1	$6,\!8,\!9$	0.47	0	5,10,12	1.01	0
1	KCX	F	201	$^{3,1}$	9,11,12	0.85	0	$5,\!12,\!14$	1.37	1 (20%)
2	MME	N	1	2	7,8,9	2.87	1 (14%)	$5,\!8,\!10$	1.19	0
1	KCX	Н	201	3,1	9,11,12	1.01	1 (11%)	5,12,14	0.47	0
1	SMC	В	256	1	5,6,7	0.53	0	2,6,8	0.62	0
1	SMC	В	369	1	5,6,7	0.69	0	2,6,8	0.90	0
1	SMC	Е	256	1	5,6,7	0.93	0	2,6,8	1.18	0
1	SMC	G	256	1	$5,\!6,\!7$	0.56	0	$2,\!6,\!8$	0.45	0
1	KCX	Е	201	3,1	9,11,12	1.05	1 (11%)	5,12,14	1.44	1 (20%)
1	HYP	F	104	1	6,8,9	0.59	0	5,10,12	1.08	0
1	SMC	G	369	1	5,6,7	1.08	0	2,6,8	0.53	0
1	HYP	F	151	1	6,8,9	0.74	0	5,10,12	1.51	1 (20%)
2	MME	М	1	2	7,8,9	2.74	1 (14%)	5,8,10	1.33	1 (20%)
1	SMC	С	369	1	$5,\!6,\!7$	0.81	0	2,6,8	0.51	0
2	MME	J	1	2	7,8,9	2.84	1 (14%)	5,8,10	1.24	1 (20%)
1	SMC	D	369	1	$5,\!6,\!7$	0.81	0	2,6,8	1.00	0
1	SMC	А	369	1	$5,\!6,\!7$	0.94	0	2,6,8	0.50	0
1	HYP	С	151	1	6,8,9	0.71	0	5,10,12	1.58	1 (20%)
1	HYP	В	104	1	6,8,9	0.65	0	5,10,12	1.00	0
1	HYP	G	104	1	6,8,9	0.63	0	5,10,12	1.23	0
1	HYP	G	151	1	6,8,9	0.42	0	5,10,12	1.40	0
2	MME	0	1	2	7,8,9	2.90	1 (14%)	5,8,10	1.21	1 (20%)
2	MME	L	1	2	7,8,9	2.70	1 (14%)	5,8,10	1.09	0
1	HYP	A	104	1	6,8,9	0.60	0	5,10,12	1.09	0
1	KCX	В	201	3,1	9,11,12	1.07	1 (11%)	$5,\!12,\!14$	0.69	0
1	HYP	Н	151	1	6,8,9	0.70	0	5,10,12	1.46	1 (20%)

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
1	HYP	D	104	1	-	0/0/11/13	0/1/1/1
1	SMC	С	256	1	-	0/3/5/7	-
2	MME	Ι	1	2	-	3/5/8/10	-
1	HYP	Е	104	1	-	0/0/11/13	0/1/1/1
1	KCX	G	201	3,1	-	0/9/10/12	-



Mol	Type	Chain	$\mathbf{Res}$	Link	Chirals	Torsions	Rings
1	SMC	А	256	1	-	0/3/5/7	-
2	MME	Р	1	2	-	2/5/8/10	-
1	KCX	А	201	3,1	-	0/9/10/12	-
1	SMC	F	369	1	-	1/3/5/7	-
1	HYP	В	151	1	-	0/0/11/13	0/1/1/1
1	SMC	Н	256	1	_	0/3/5/7	_
1	SMC	Е	369	1	-	1/3/5/7	-
1	KCX	С	201	3,1	-	0/9/10/12	-
1	SMC	D	256	1	-	0/3/5/7	-
1	KCX	D	201	3,1	-	0/9/10/12	_
1	SMC	Н	369	1	-	1/3/5/7	-
1	HYP	A	151	1	-	0/0/11/13	0/1/1/1
2	MME	Κ	1	2	-	2/5/8/10	-
1	HYP	D	151	1	-	0/0/11/13	0/1/1/1
1	HYP	Е	151	1	-	0/0/11/13	0/1/1/1
1	SMC	F	256	1	-	0/3/5/7	-
1	HYP	Н	104	1	-	0/0/11/13	0/1/1/1
1	HYP	С	104	1	-	0/0/11/13	0/1/1/1
1	KCX	F	201	3,1	-	0/9/10/12	-
2	MME	N	1	2	-	3/5/8/10	-
1	KCX	Н	201	3,1	_	0/9/10/12	_
1	SMC	В	256	1	-	0/3/5/7	-
1	SMC	В	369	1	-	1/3/5/7	-
1	SMC	Е	256	1	-	0/3/5/7	-
1	SMC	G	256	1	-	0/3/5/7	-
1	KCX	Е	201	3,1	-	1/9/10/12	-
1	HYP	F	104	1	-	0/0/11/13	0/1/1/1
1	SMC	G	369	1	-	1/3/5/7	-
1	HYP	F	151	1	-	0/0/11/13	0/1/1/1
2	MME	М	1	2	-	3/5/8/10	-
1	SMC	С	369	1	-	1/3/5/7	-
2	MME	J	1	2	-	3/5/8/10	-
1	SMC	D	369	1	_	1/3/5/7	_
1	SMC	A	369	1	_	1/3/5/7	_
1	HYP	С	151	1	-	0/0/11/13	0/1/1/1
1	HYP	В	104	1	-	0/0/11/13	0/1/1/1
1	HYP	G	104	1	-	0/0/11/13	0/1/1/1
1	HYP	G	151	1	-	0/0/11/13	0/1/1/1
2	MME	0	1	2	-	2/5/8/10	-
2	MME	L	1	2	_	3/5/8/10	_
1	HYP	A	104	1	-	0/0/11/13	0/1/1/1



Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	KCX	В	201	3,1	-	0/9/10/12	-
1	HYP	Н	151	1	-	0/0/11/13	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	0	1	MME	CM-N	-7.34	1.27	1.46
2	Р	1	MME	CM-N	-7.27	1.27	1.46
2	Ι	1	MME	CM-N	-7.26	1.27	1.46
2	J	1	MME	CM-N	-7.25	1.27	1.46
2	Ν	1	MME	CM-N	-7.21	1.27	1.46
2	Κ	1	MME	CM-N	-7.08	1.28	1.46
2	М	1	MME	CM-N	-6.99	1.28	1.46
2	L	1	MME	CM-N	-6.90	1.28	1.46
1	D	201	KCX	CE-NZ	2.52	1.51	1.46
1	С	201	KCX	OQ1-CX	2.23	1.25	1.21
1	Н	201	KCX	OQ1-CX	2.23	1.25	1.21
1	А	201	KCX	CE-NZ	2.16	1.51	1.46
1	Е	201	KCX	CE-NZ	2.12	1.51	1.46
1	G	201	KCX	CE-NZ	2.08	1.50	1.46
1	В	201	KCX	OQ1-CX	2.06	1.25	1.21
1	D	256	SMC	CB-SG	2.06	1.83	1.80

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
1	F	201	KCX	OQ1-CX-NZ	-3.02	120.27	124.96
1	Е	201	KCX	OQ1-CX-NZ	-2.87	120.51	124.96
1	G	201	KCX	OQ1-CX-NZ	-2.40	121.24	124.96
2	Р	1	MME	CM-N-CA	2.35	120.96	113.64
1	В	151	HYP	O-C-CA	-2.33	118.67	124.78
1	С	151	HYP	CG-CB-CA	-2.32	101.03	103.96
2	K	1	MME	CM-N-CA	2.31	120.83	113.64
1	D	256	SMC	CS-SG-CB	2.26	105.45	101.30
2	М	1	MME	CM-N-CA	2.20	120.47	113.64
1	F	151	HYP	CG-CB-CA	-2.13	101.28	103.96
2	0	1	MME	CM-N-CA	2.08	120.10	113.64
2	Ι	1	MME	CM-N-CA	2.07	120.07	113.64
1	D	151	HYP	O-C-CA	-2.06	119.38	124.78
2	J	1	MME	CM-N-CA	2.04	119.99	113.64
1	Н	151	HYP	O-C-CA	-2.04	119.44	124.78



There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	J	1	MME	C-CA-CB-CG
2	J	1	MME	CB-CG-SD-CE
2	L	1	MME	CB-CG-SD-CE
2	0	1	MME	CB-CG-SD-CE
2	Ι	1	MME	CB-CG-SD-CE
2	Κ	1	MME	CB-CG-SD-CE
2	М	1	MME	CB-CG-SD-CE
2	Ν	1	MME	CB-CG-SD-CE
2	Р	1	MME	CB-CG-SD-CE
2	Ι	1	MME	C-CA-CB-CG
2	Κ	1	MME	C-CA-CB-CG
2	L	1	MME	C-CA-CB-CG
2	М	1	MME	C-CA-CB-CG
2	Ν	1	MME	C-CA-CB-CG
2	0	1	MME	C-CA-CB-CG
2	Р	1	MME	C-CA-CB-CG
2	J	1	MME	N-CA-CB-CG
1	А	369	SMC	N-CA-CB-SG
1	В	369	SMC	N-CA-CB-SG
1	С	369	SMC	N-CA-CB-SG
1	D	369	SMC	N-CA-CB-SG
1	Е	369	SMC	N-CA-CB-SG
1	F	369	SMC	N-CA-CB-SG
1	G	369	SMC	N-CA-CB-SG
1	Н	369	SMC	N-CA-CB-SG
2	Ι	1	MME	N-CA-CB-CG
2	L	1	MME	N-CA-CB-CG
2	Ν	1	MME	N-CA-CB-CG
1	Е	201	KCX	CG-CD-CE-NZ
2	М	1	MME	N-CA-CB-CG

There are no ring outliers.

9 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	А	201	KCX	1	0
1	С	201	KCX	1	0
1	D	201	KCX	1	0
1	Н	369	SMC	1	0
1	F	201	KCX	1	0



	v	±	1 0		
Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	Н	201	KCX	1	0
1	Е	201	KCX	1	0
1	С	369	SMC	1	0
1	В	201	KCX	1	0

Continued from previous page...

### 3.5 Carbohydrates (i)

There are no monosaccharides in this entry.

### 3.6 Ligand geometry (i)

Of 65 ligands modelled in this entry, 8 are monoatomic - leaving 57 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	Tune	Chain	Dec	Tink	Bo	ond leng	ths	В	ond ang	gles
WIOI	Type	Ullalli	nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	EDO	D	1481	-	3,3,3	0.58	0	2,2,2	0.18	0
5	EDO	G	1480	-	3,3,3	0.47	0	2,2,2	0.25	0
5	EDO	Н	1482	-	3,3,3	0.53	0	2,2,2	0.17	0
5	EDO	J	1142	-	3,3,3	0.45	0	2,2,2	0.23	0
5	EDO	С	1477	-	3,3,3	0.52	0	2,2,2	0.22	0
4	CAP	С	477	3	17,20,20	0.81	0	22,31,31	0.85	0
4	CAP	Н	477	3	17,20,20	0.86	0	22,31,31	0.75	0
5	EDO	Р	1141	-	3,3,3	0.50	0	2,2,2	0.28	0
4	CAP	D	477	3	17,20,20	0.81	0	22,31,31	0.75	0
5	EDO	В	1480	-	3,3,3	0.73	0	2,2,2	0.12	0
5	EDO	Н	1476	-	3,3,3	0.80	0	2,2,2	0.14	0
5	EDO	0	1142	-	3,3,3	0.50	0	2,2,2	0.40	0
5	EDO	Е	1478	-	3,3,3	0.53	0	2,2,2	0.24	0
5	EDO	D	1478	-	3,3,3	0.55	0	2,2,2	0.08	0
5	EDO	А	1481	-	3,3,3	0.75	0	2,2,2	0.06	0
5	EDO	В	1479	-	3,3,3	0.50	0	2,2,2	0.25	0
5	EDO	Е	1476	-	3,3,3	0.63	0	2,2,2	0.05	0
5	EDO	K	1141	-	3,3,3	0.53	0	2,2,2	0.32	0
5	EDO	С	1481	-	3,3,3	0.61	0	2,2,2	0.17	0



Mal	Turne	Chain	Dec	Tink	Bo	ond leng	$_{\rm ths}$	В	ond ang	les
NIOI	туре	Chain	nes	LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	EDO	А	1483	-	3,3,3	0.48	0	2,2,2	0.41	0
5	EDO	L	1141	-	3,3,3	0.53	0	2,2,2	0.17	0
5	EDO	F	1481	-	3,3,3	0.52	0	2,2,2	0.28	0
5	EDO	Ι	1141	-	3,3,3	0.54	0	2,2,2	0.18	0
5	EDO	С	1480	-	3,3,3	0.64	0	2,2,2	0.09	0
5	EDO	F	1484	-	3,3,3	0.63	0	2,2,2	0.06	0
5	EDO	В	1481	-	3,3,3	0.47	0	2,2,2	0.05	0
5	EDO	D	1480	-	3,3,3	0.45	0	2,2,2	0.37	0
5	EDO	А	1484	-	3,3,3	0.48	0	2,2,2	0.30	0
5	EDO	F	1483	-	3,3,3	0.56	0	2,2,2	0.35	0
5	EDO	М	1141	-	3,3,3	0.49	0	2,2,2	0.11	0
4	CAP	А	477	3	17,20,20	0.96	0	22,31,31	0.74	0
5	EDO	С	1478	-	3,3,3	0.54	0	2,2,2	0.10	0
4	CAP	Е	477	3	17,20,20	0.74	0	22,31,31	0.96	0
5	EDO	Н	1478	-	3,3,3	0.42	0	2,2,2	0.26	0
4	CAP	G	477	3	17,20,20	0.91	0	22,31,31	0.98	1 (4%)
5	EDO	А	1482	-	3,3,3	0.66	0	2,2,2	0.22	0
5	EDO	D	1477	-	3,3,3	0.66	0	2,2,2	0.07	0
5	EDO	G	1478	-	3,3,3	0.43	0	2,2,2	0.19	0
5	EDO	Ν	1142	-	3,3,3	0.52	0	$2,\!2,\!2$	0.07	0
5	EDO	С	1482	-	3,3,3	0.65	0	2,2,2	0.23	0
5	EDO	Ι	1142	-	3, 3, 3	0.64	0	$2,\!2,\!2$	0.21	0
5	EDO	J	1141	-	3, 3, 3	0.49	0	$2,\!2,\!2$	0.25	0
5	EDO	0	1141	-	3, 3, 3	0.42	0	$2,\!2,\!2$	0.32	0
5	EDO	Н	1481	-	3, 3, 3	0.52	0	$2,\!2,\!2$	0.24	0
5	EDO	Κ	1142	-	3, 3, 3	0.47	0	$2,\!2,\!2$	0.33	0
5	EDO	G	1476	-	3, 3, 3	0.65	0	$2,\!2,\!2$	0.17	0
5	EDO	N	1141	-	3,3,3	0.61	0	2,2,2	0.13	0
4	CAP	F	477	3	$17,\!20,\!20$	0.74	0	22,31,31	0.95	1 (4%)
5	EDO	F	1479	-	3, 3, 3	0.48	0	$2,\!2,\!2$	0.16	0
5	EDO	Н	1483	-	3,3,3	0.66	0	2,2,2	0.12	0
5	EDO	Е	1480	-	3, 3, 3	0.58	0	$2,\!2,\!2$	0.15	0
5	EDO	F	1480	-	3, 3, 3	0.51	0	2,2,2	0.28	0
5	EDO	F	1482	-	3,3,3	0.60	0	$2,\!2,\!2$	0.11	0
5	EDO	В	1477	-	3,3,3	0.78	0	2,2,2	0.14	0
5	EDO	Н	1480	-	3,3,3	0.60	0	$2,\!2,\!2$	0.07	0
5	EDO	А	1477	-	3, 3, 3	0.48	0	$2,\!2,\!2$	0.29	0
4	CAP	В	477	3	17,20,20	0.99	1 (5%)	22,31,31	0.93	1 (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.



2	V	6	8

5   EDO   D   1481   -   - $1/1/1/1$ -     5   EDO   G   1480   -   - $0/1/1/1$ -     5   EDO   J   1142   -   - $0/1/1/1$ -     5   EDO   C   1477   -   - $0/1/1/1$ -     4   CAP   C   477   3   - $7/29/29/29$ -     4   CAP   D   477   3   - $1/1/1/1$ -     4   CAP   D   477   3   - $0/1/1/1$ -     5   EDO   B   1480   -   - $0/1/1/1$ -     5   EDO   D   1478   -   - $1/1/1/1$ -     5   EDO   E   1476   -   - $0/1/1/1$ -     5   EDO   E   1476   -   - $0/1/1/1$ - <t< th=""><th>Mol</th><th>Type</th><th>Chain</th><th>Res</th><th>Link</th><th>Chirals</th><th>Torsions</th><th>Rings</th></t<>	Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5   EDO   G   1480   -   - $1/1/1/1$ -     5   EDO   J   1142   -   - $0/1/1/1$ -     5   EDO   C   1477   -   - $0/1/1/1$ -     4   CAP   C   1477   3   - $7/29/29/29$ -     4   CAP   H   477   3   - $7/29/29/29$ -     5   EDO   P   1141   -   - $1/1/1/1$ -     4   CAP   D   477   3   - $7/29/29/29$ -     5   EDO   B   1480   -   - $0/1/1/1$ -     5   EDO   H   1476   - $0/1/1/1$ -   -     5   EDO   B   1479   - $1/1/1/1$ -   -     5   EDO   K   1141   -   - $0/1/1/1$ -	5	EDO	D	1481	_	_	1/1/1/1	-
5   EDO   H   1482   -   - $0/1/1/1$ -     5   EDO   C   1477   -   - $0/1/1/1$ -     4   CAP   C   477   3   - $7/29/29/29$ -     4   CAP   H   477   3   - $7/29/29/29$ -     5   EDO   P   1141   -   - $1/1/1/1$ -     4   CAP   D   477   3   - $7/29/29/29$ -     5   EDO   B   1480   -   - $0/1/1/1$ -     5   EDO   H   1476   -   0/1/1/1   -   -     5   EDO   D   1478   -   1/1/1/1   -   -     5   EDO   A   1481   -   0/1/1/1   -   -     5   EDO   K   1141   -   -   1/1/1/1   -	5	EDO	G	1480	_	_	1/1/1/1	-
5   EDO   J   1142   -   - $0/1/1/1$ -     5   EDO   C   1477   -   - $0/1/1/1$ -     4   CAP   C   477   3   - $7/29/29/29$ -     5   EDO   P   1141   -   - $1/1/1/1$ -     4   CAP   D   477   3   - $7/29/29/29$ -     5   EDO   B   1480   -   - $0/1/1/1$ -     4   CAP   D   477   3   - $7/29/29/29$ -     5   EDO   H   1476   -   - $0/1/1/1$ -     5   EDO   D   1478   -   - $1/1/1/1$ -     5   EDO   B   1479   -   - $1/1/1/1$ -     5   EDO   K   1141   -   - $1/1/1/1$ -	5	EDO	Н	1482	-	-	0/1/1/1	-
5   EDO   C   1477   -   - $0/1/1/1$ -     4   CAP   C   477   3   - $7/29/29/29$ -     4   CAP   H   477   3   - $7/29/29/29$ -     5   EDO   P   1141   -   - $1/1/1/1$ -     4   CAP   D   477   3   - $7/29/29/29$ -     5   EDO   B   1480   -   - $0/1/1/1$ -     5   EDO   H   1476   -   - $0/1/1/1$ -     5   EDO   D   1478   -   - $1/1/1/1$ -     5   EDO   A   1481   -   - $0/1/1/1$ -     5   EDO   K   1141   -   - $0/1/1/1$ -     5   EDO   K   1141   -   - $0/1/1/1$ -	5	EDO	J	1142	-	-	0/1/1/1	-
4   CAP   C   477   3   - $7/29/29/29$ -     4   CAP   H   477   3   - $7/29/29/29$ -     5   EDO   P   1141   -   - $1/1/1/1$ -     4   CAP   D   477   3   - $7/29/29/29$ -     5   EDO   B   1480   -   - $0/1/1/1$ -     5   EDO   H   1476   -   - $0/1/1/1$ -     5   EDO   D   1478   -   - $1/1/1/1$ -     5   EDO   A   1481   -   - $0/1/1/1$ -     5   EDO   K   1141   -   - $0/1/1/1$ -     5   EDO   K   1141   -   - $0/1/1/1$ -     5   EDO   K   1483   -   - $0/1/1/1$ -	5	EDO	С	1477	-	-	0/1/1/1	-
4   CAP   H   477   3   - $7/29/29/29$ -     5   EDO   P   1141   -   - $1/1/1/1$ -     4   CAP   D   477   3   - $7/29/29/29$ -     5   EDO   B   1480   -   - $0/1/1/1$ -     5   EDO   H   1476   - $0/1/1/1$ -     5   EDO   D   1478   - $1/1/1/1$ -     5   EDO   B   1479   - $1/1/1/1$ -     5   EDO   B   1479   - $0/1/1/1$ -     5   EDO   K   1141   - $0/1/1/1$ -     5   EDO   K   1141   - $0/1/1/1$ -     5   EDO   K   1141   - $0/1/1/1$ -     5   EDO   I   1481   - $0/1/1/1$	4	CAP	С	477	3	-	7/29/29/29	-
5 EDO P 1141 - - $1/1/1/1$ -   4 CAP D 477 3 - $7/29/29/29$ -   5 EDO B 1480 - - $0/1/1/1$ -   5 EDO H 1476 - - $0/1/1/1$ -   5 EDO D 1442 - - $1/1/1/1$ -   5 EDO D 1478 - - $1/1/1/1$ -   5 EDO D 1478 - - $1/1/1/1$ -   5 EDO A 1481 - - $1/1/1/1$ -   5 EDO K 1141 - - $0/1/1/1$ -   5 EDO K 1141 - - $0/1/1/1$ -   5 EDO K 1141 - - $1/1/1/1$ -   5 EDO K 1481 - - $0/1/1/1$ -	4	CAP	Н	477	3	-	7/29/29/29	-
4   CAP   D   477   3   - $7/29/29/29$ -     5   EDO   B   1480   -   - $0/1/1/1$ -     5   EDO   H   1476   -   - $0/1/1/1$ -     5   EDO   O   1142   -   - $1/1/1/1$ -     5   EDO   D   1478   -   - $1/1/1/1$ -     5   EDO   D   1478   -   - $1/1/1/1$ -     5   EDO   A   1481   -   - $0/1/1/1$ -     5   EDO   E   1479   -   - $0/1/1/1$ -     5   EDO   C   1481   -   - $0/1/1/1$ -     5   EDO   L   1141   -   - $1/1/1/1$ -     5   EDO   L   1141   -   - $1/1/1/1$ -	5	EDO	Р	1141	-	-	1/1/1/1	-
5   EDO   B   1480   -   - $0/1/1/1$ -     5   EDO   H   1476   -   - $0/1/1/1$ -     5   EDO   O   1142   -   - $1/1/1/1$ -     5   EDO   E   1478   -   - $1/1/1/1$ -     5   EDO   D   1478   -   - $1/1/1/1$ -     5   EDO   A   1481   -   - $1/1/1/1$ -     5   EDO   B   1479   -   - $1/1/1/1$ -     5   EDO   E   1476   -   - $0/1/1/1$ -     5   EDO   K   1141   -   - $0/1/1/1$ -     5   EDO   I   1141   -   - $1/1/1/1$ -     5   EDO   F   1480   -   - $0/1/1/1$ - <t< td=""><td>4</td><td>CAP</td><td>D</td><td>477</td><td>3</td><td>-</td><td>7/29/29/29</td><td>-</td></t<>	4	CAP	D	477	3	-	7/29/29/29	-
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	5	EDO	В	1480	-	-	0/1/1/1	-
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	5	EDO	Н	1476	-	-	0/1/1/1	-
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	5	EDO	0	1142	-	_	1/1/1/1	-
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	5	EDO	Е	1478	-	_	1/1/1/1	-
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	5	EDO	D	1478	-	-	1/1/1/1	-
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	5	EDO	А	1481	-	-	1/1/1/1	-
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	5	EDO	В	1479	-	-	1/1/1/1	-
5EDOK1141 $0/1/1/1$ -5EDOC1481 $0/1/1/1$ -5EDOA1483 $1/1/1/1$ -5EDOL1141 $0/1/1/1$ -5EDOF1481 $0/1/1/1$ -5EDOI1141 $0/1/1/1$ -5EDOC1480 $0/1/1/1$ -5EDOF1484 $0/1/1/1$ -5EDOB1481 $0/1/1/1$ -5EDOB1481 $0/1/1/1$ -5EDOD1480 $1/1/1/1$ -5EDOA1484 $1/1/1/1$ -5EDOA1483 $1/1/1/1$ -5EDOM1141 $1/1/1/1$ -4CAPA4773- $7/29/29/29$ -5EDOH1478 $0/1/1/1$ -4CAPG4773- $7/29/29/29$ -5EDOA1482 $0/1/1/1$ -5EDOD1477 $0/1/1/1$ -5EDOG1478 $1/1/1/1$ - <td>5</td> <td>EDO</td> <td>Е</td> <td>1476</td> <td>-</td> <td>-</td> <td>0/1/1/1</td> <td>-</td>	5	EDO	Е	1476	-	-	0/1/1/1	-
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	5	EDO	K	1141	-	-	0/1/1/1	-
5EDOA1483 $1/1/1/1$ -5EDOL1141 $1/1/1/1$ -5EDOF1481 $0/1/1/1$ -5EDOI1141 $1/1/1/1$ -5EDOC1480 $1/1/1/1$ -5EDOF1484 $0/1/1/1$ -5EDOB1481 $0/1/1/1$ -5EDOD1480 $1/1/1/1$ -5EDOA1484 $1/1/1/1$ -5EDOA1483 $1/1/1/1$ -5EDOA1483 $1/1/1/1$ -5EDOM1141 $1/1/1/1$ -4CAPA4773- $7/29/29/29$ -5EDOH1478 $0/1/1/1$ -4CAPG4773- $7/29/29/29$ -5EDOA1482 $0/1/1/1$ -5EDOG1478 $0/1/1/1$ -5EDOG1478 $0/1/1/1$ -5EDON1142 $0/1/1/1$ -5EDOC1482 $1/1/1/1$ - <td>5</td> <td>EDO</td> <td>С</td> <td>1481</td> <td>-</td> <td>-</td> <td>0/1/1/1</td> <td>-</td>	5	EDO	С	1481	-	-	0/1/1/1	-
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	5	EDO	А	1483	-	-	1/1/1/1	-
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	5	EDO	L	1141	-	-	1/1/1/1	-
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	5	EDO	F	1481	-	-	0/1/1/1	-
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	5	EDO	Ι	1141	-	-	1/1/1/1	-
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	5	EDO	С	1480	-	-	1/1/1/1	-
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	5	EDO	F	1484	-	-	0/1/1/1	-
5 EDO D 1480 - - 1/1/1/1 -   5 EDO A 1484 - - 1/1/1/1 -   5 EDO F 1483 - - 1/1/1/1 -   5 EDO M 1141 - - 1/1/1/1 -   4 CAP A 477 3 - 7/29/29/29 -   5 EDO C 1478 - - 1/1/1/1 -   4 CAP E 477 3 - 9/29/29/29 -   5 EDO C 1478 - - 0/1/1/1 -   4 CAP E 477 3 - 0/1/1/1 -   4 CAP G 477 3 - 0/1/1/1 -   5 EDO H 1478 - - 0/1/1/1 -   5 EDO D 1477 - - 0/1/1/1 -   5 EDO<	5	EDO	В	1481	-	-	0/1/1/1	-
5 EDO A 1484 - - 1/1/1/1 -   5 EDO F 1483 - - 1/1/1/1 -   5 EDO M 1141 - - 1/1/1/1 -   4 CAP A 477 3 - 7/29/29/29 -   5 EDO C 1478 - - 1/1/1/1 -   4 CAP E 477 3 - 9/29/29/29 -   5 EDO C 1478 - - 0/1/1/1 -   4 CAP E 477 3 - 9/29/29/29 -   5 EDO H 1478 - - 0/1/1/1 -   4 CAP G 477 3 - 7/29/29/29 -   5 EDO A 1482 - - 0/1/1/1 -   5 EDO G 1477 - - 0/1/1/1 -   5 <t< td=""><td>5</td><td>EDO</td><td>D</td><td>1480</td><td>-</td><td>-</td><td>1/1/1/1</td><td>-</td></t<>	5	EDO	D	1480	-	-	1/1/1/1	-
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	5	EDO	А	1484	-	-	1/1/1/1	-
5 EDO M 1141 - - 1/1/1/1 -   4 CAP A 477 3 - 7/29/29/29 -   5 EDO C 1478 - - 1/1/1/1 -   4 CAP E 477 3 - 9/29/29/29 -   5 EDO H 1478 - - 0/1/1/1 -   4 CAP E 477 3 - 9/29/29/29 -   5 EDO H 1478 - - 0/1/1/1 -   4 CAP G 477 3 - 7/29/29/29 -   5 EDO A 1482 - - 0/1/1/1 -   5 EDO D 1477 - - 0/1/1/1 -   5 EDO G 1478 - - 0/1/1/1 -   5 EDO N 1142 - - 0/1/1/1 -   5 <t< td=""><td>5</td><td>EDO</td><td>F</td><td>1483</td><td>-</td><td>-</td><td>1/1/1/1</td><td>-</td></t<>	5	EDO	F	1483	-	-	1/1/1/1	-
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	5	EDO	М	1141	-	-	1/1/1/1	-
5 EDO C 1478 - - 1/1/1/1 -   4 CAP E 477 3 - 9/29/29/29 -   5 EDO H 1478 - - 0/1/1/1 -   4 CAP G 477 3 - 0/1/1/1 -   4 CAP G 477 3 - 7/29/29/29 -   5 EDO A 1482 - - 0/1/1/1 -   5 EDO D 1477 - - 0/1/1/1 -   5 EDO G 1478 - - 0/1/1/1 -   5 EDO G 1478 - - 0/1/1/1 -   5 EDO G 1478 - - 0/1/1/1 -   5 EDO N 1142 - - 0/1/1/1 -   5 EDO C 1482 - - 1/1/1/1 -	4	CAP	А	477	3	-	7/29/29/29	-
4 CAP E 477 3 - 9/29/29/29 -   5 EDO H 1478 - - 0/1/1/1 -   4 CAP G 477 3 - 7/29/29/29 -   5 EDO A 1482 - - 0/1/1/1 -   5 EDO D 1477 - - 0/1/1/1 -   5 EDO G 1478 - - 0/1/1/1 -   5 EDO D 1477 - - 0/1/1/1 -   5 EDO G 1478 - - 0/1/1/1 -   5 EDO N 1142 - - 0/1/1/1 -   5 EDO C 1482 - - 1/1/1/1 -	5	EDO	С	1478	-	-	1/1/1/1	-
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	4	CAP	Е	477	3	-	9/29/29/29	-
4   CAP   G   477   3   -   7/29/29/29   -     5   EDO   A   1482   -   -   0/1/1/1   -     5   EDO   D   1477   -   -   0/1/1/1   -     5   EDO   G   1478   -   -   0/1/1/1   -     5   EDO   G   1478   -   -   0/1/1/1   -     5   EDO   N   1142   -   -   0/1/1/1   -     5   EDO   N   1142   -   -   0/1/1/1   -     5   EDO   C   1482   -   -   1/1/1/1   -	5	EDO	Н	1478	-	-	0/1/1/1	-
5   EDO   A   1482   -   -   0/1/1/1   -     5   EDO   D   1477   -   -   0/1/1/1   -     5   EDO   G   1477   -   -   0/1/1/1   -     5   EDO   G   1478   -   -   1/1/1/1   -     5   EDO   N   1142   -   -   0/1/1/1   -     5   EDO   C   1482   -   -   1/1/1/1   -	4	CAP	G	477	3	-	7/29/29/29	-
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	5	EDO	А	1482	-	-	0/1/1/1	-
5   EDO   G   1478   -   -   1/1/1/1   -     5   EDO   N   1142   -   -   0/1/1/1   -     5   EDO   C   1482   -   -   1/1/1/1   -	5	EDO	D	1477	-	-	0/1/1/1	-
5   EDO   N   1142   -   -   0/1/1/1   -     5   EDO   C   1482   -   -   1/1/1/1   -	5	EDO	G	1478	-	-	1/1/1/1	-
5 EDO C 1482 1/1/1/1 -	5	EDO	N	1142	-	-	0/1/1/1	-
	5	EDO	С	1482	-	-	1/1/1/1	-

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



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	Ι	1142	-	-	1/1/1/1	-
5	EDO	J	1141	-	-	1/1/1/1	-
5	EDO	0	1141	-	-	0/1/1/1	-
5	EDO	Н	1481	-	-	1/1/1/1	-
5	EDO	K	1142	-	-	0/1/1/1	-
5	EDO	G	1476	-	-	0/1/1/1	-
5	EDO	Ν	1141	-	-	1/1/1/1	-
4	CAP	F	477	3	-	7/29/29/29	-
5	EDO	F	1479	-	-	0/1/1/1	-
5	EDO	Н	1483	-	-	0/1/1/1	-
5	EDO	Е	1480	-	-	0/1/1/1	-
5	EDO	F	1480	-	-	0/1/1/1	-
5	EDO	F	1482	-	-	0/1/1/1	-
5	EDO	В	1477	-	-	0/1/1/1	-
5	EDO	Н	1480	-	-	0/1/1/1	-
5	EDO	А	1477	-	-	0/1/1/1	-
4	CAP	В	477	3	-	8/29/29/29	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	В	477	CAP	C4-C3	-2.39	1.51	1.54

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	G	477	CAP	O2-C2-C	-3.22	103.09	108.97
4	F	477	CAP	O2-C2-C	-2.41	104.56	108.97
4	В	477	CAP	02-C2-C	-2.01	105.30	108.97

All (3) bond angle outliers are listed below:

There are no chirality outliers.

All (82) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	А	477	CAP	O6-C-C2-C1
4	А	477	CAP	O7-C-C2-C1
4	А	477	CAP	O6-C-C2-O2
4	А	477	CAP	O7-C-C2-O2
4	А	477	CAP	C2-C3-C4-O4
4	А	477	CAP	O3-C3-C4-O4
4	В	477	CAP	O6-C-C2-C1



Mol	Chain	Res	Type	Atoms
4	В	477	CAP	O6-C-C2-O2
4	В	477	CAP	O7-C-C2-O2
4	В	477	CAP	C2-C3-C4-O4
4	В	477	CAP	O3-C3-C4-O4
4	С	477	CAP	O6-C-C2-C1
4	С	477	CAP	O7-C-C2-C1
4	С	477	CAP	O6-C-C2-O2
4	С	477	CAP	O7-C-C2-O2
4	С	477	CAP	C2-C3-C4-O4
4	С	477	CAP	O3-C3-C4-O4
4	D	477	CAP	O6-C-C2-C1
4	D	477	CAP	O7-C-C2-C1
4	D	477	CAP	O6-C-C2-O2
4	D	477	CAP	O7-C-C2-O2
4	D	477	CAP	C2-C3-C4-O4
4	D	477	CAP	O3-C3-C4-O4
4	Е	477	CAP	O6-C-C2-C1
4	Е	477	CAP	O7-C-C2-C1
4	Е	477	CAP	O6-C-C2-O2
4	Е	477	CAP	O7-C-C2-O2
4	Е	477	CAP	C2-C3-C4-O4
4	Е	477	CAP	O3-C3-C4-O4
4	F	477	CAP	O6-C-C2-C1
4	F	477	CAP	O7-C-C2-C1
4	F	477	CAP	O6-C-C2-O2
4	F	477	CAP	O7-C-C2-O2
4	F	477	CAP	C2-C3-C4-O4
4	F	477	CAP	O3-C3-C4-O4
4	G	477	CAP	O6-C-C2-C1
4	G	477	CAP	O7-C-C2-C1
4	G	477	CAP	O6-C-C2-O2
4	G	477	CAP	O7-C-C2-O2
4	G	477	CAP	C2-C3-C4-O4
4	G	477	CAP	O3-C3-C4-O4
4	H	477	CAP	O6-C-C2-C1
4	Н	477	CAP	07-C-C2-C1
4	Н	477	CAP	O6-C-C2-O2
4	Н	477	CAP	07-C-C2-O2
4	Н	477	CAP	C2-C3-C4-O4
4	Н	477	CAP	O3-C3-C4-O4
5	В	1479	EDO	01-C1-C2-O2
5	A	1483	EDO	01-C1-C2-O2

Continued from previous page...



Mol	Chain	Res	Type	Atoms
5	Р	1141	EDO	O1-C1-C2-O2
4	В	477	CAP	O7-C-C2-C1
5	А	1484	EDO	O1-C1-C2-O2
5	F	1483	EDO	O1-C1-C2-O2
5	Н	1481	EDO	O1-C1-C2-O2
5	Ι	1141	EDO	O1-C1-C2-O2
5	Ι	1142	EDO	O1-C1-C2-O2
5	N	1141	EDO	O1-C1-C2-O2
4	А	477	CAP	O2-C2-C3-C4
4	В	477	CAP	O2-C2-C3-C4
4	С	477	CAP	O2-C2-C3-C4
4	D	477	CAP	O2-C2-C3-C4
4	Е	477	CAP	O2-C2-C3-C4
4	F	477	CAP	O2-C2-C3-C4
4	G	477	CAP	O2-C2-C3-C4
4	Н	477	CAP	O2-C2-C3-C4
5	С	1482	EDO	O1-C1-C2-O2
5	G	1480	EDO	O1-C1-C2-O2
5	D	1480	EDO	O1-C1-C2-O2
5	Е	1478	EDO	O1-C1-C2-O2
4	Е	477	CAP	C2-C3-C4-C5
5	М	1141	EDO	O1-C1-C2-O2
5	L	1141	EDO	O1-C1-C2-O2
5	D	1478	EDO	O1-C1-C2-O2
5	G	1478	EDO	O1-C1-C2-O2
5	J	1141	EDO	O1-C1-C2-O2
5	0	1142	EDO	O1-C1-C2-O2
5	А	1481	EDO	O1-C1-C2-O2
5	С	1478	EDO	O1-C1-C2-O2
5	С	1480	EDO	O1-C1-C2-O2
5	D	1481	EDO	O1-C1-C2-O2
4	Е	477	CAP	O3-C3-C4-C5
4	В	477	CAP	C2-C3-C4-C5

Continued from previous page...

There are no ring outliers.

10 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	1480	EDO	2	0
5	Н	1482	EDO	1	0
5	D	1478	EDO	2	0
5	В	1479	EDO	2	0



Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	1484	EDO	1	0
5	В	1481	EDO	1	0
5	А	1484	EDO	1	0
5	М	1141	EDO	1	0
5	K	1142	EDO	1	0
5	Ν	1141	EDO	3	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 similar 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.























# 3.7 Other polymers (i)

There are no such residues in this entry.

## 3.8 Polymer linkage issues (i)

There are no chain breaks in this entry.





# 4 Fit of model and data (i)

## 4.1 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 $>$	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	А	461/475~(97%)	-0.40	2 (0%) 92 95	11, 16, 31, 40	0
1	В	462/475~(97%)	-0.38	5 (1%) 80 85	11, 16, 31, 42	0
1	С	462/475~(97%)	-0.43	5 (1%) 80 85	11, 16, 31, 41	0
1	D	460/475~(96%)	-0.38	4 (0%) 84 88	11, 16, 31, 42	0
1	Е	461/475~(97%)	-0.40	6 (1%) 77 81	11, 16, 31, 40	0
1	F	462/475~(97%)	-0.41	8 (1%) 70 76	11, 16, 31, 44	1 (0%)
1	G	461/475~(97%)	-0.42	3 (0%) 87 91	11, 16, 31, 40	0
1	Н	461/475~(97%)	-0.45	2 (0%) 92 95	11, 16, 31, 40	0
2	Ι	139/140~(99%)	-0.15	2 (1%) 75 80	12, 22, 34, 37	1 (0%)
2	J	139/140~(99%)	0.00	6 (4%) 35 42	13, 22, 36, 40	1 (0%)
2	K	139/140~(99%)	-0.20	3 (2%) 62 69	12, 22, 35, 37	1 (0%)
2	L	139/140~(99%)	-0.40	0 100 100	13, 22, 34, 36	0
2	М	139/140~(99%)	-0.40	0 100 100	13, 22, 34, 36	0
2	Ν	139/140~(99%)	-0.24	1 (0%) 87 91	12, 22, 36, 40	0
2	Ο	139/140~(99%)	-0.17	2 (1%) 75 80	12, 22, 34, 37	1 (0%)
2	Р	139/140~(99%)	-0.18	1 (0%) 87 91	13, 22, 34, 37	0
All	All	4802/4920 (97%)	-0.36	50 (1%) 82 86	11, 17, 32, 44	5 (0%)

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	J	127	LYS	4.1
1	В	10	GLY	4.0
1	F	11	ALA	3.9
1	С	10	GLY	3.8
1	Е	92	GLY	3.6



2V6	58
-----	----

Mol	Chain	Res	Type	RSRZ
1	F	10	GLY	3.5
1	С	9	ALA	3.3
1	С	94	ASP	3.3
1	В	439	ARG	3.2
1	А	464	GLU	3.2
1	F	9	ALA	3.2
2	Ι	128	THR	3.1
2	J	84	ARG	3.1
2	J	128	THR	3.0
2	J	130	ARG	3.0
1	G	439	ARG	2.9
1	D	92	GLY	2.9
1	D	439	ARG	2.8
1	F	47	GLY	2.8
2	N	84	ARG	2.8
1	В	9	ALA	2.8
2	0	84	ARG	2.7
1	В	28	ASP	2.7
1	Е	10	GLY	2.6
1	С	464	GLU	2.6
1	F	94	ASP	2.5
1	Е	11	ALA	2.5
1	F	464	GLU	2.5
1	Е	94	ASP	2.4
1	Н	94	ASP	2.4
2	К	128	THR	2.3
2	J	136	ASN	2.3
2	К	127	LYS	2.3
1	D	436	ASP	2.3
1	G	464	GLU	2.2
1	Е	89	PRO	2.2
1	Е	28	ASP	2.2
1	A	28	ASP	2.2
1	G	10	GLY	2.2
2	Р	128	THR	2.2
2	K	136	ASN	2.1
1	C	11	ALA	2.1
1	Н	464	GLU	2.1
1	F	451	TRP	2.1
1	В	94	ASP	2.1
2	0	136	ASN	2.1
1	F	450	LYS	2.1



Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	464	GLU	2.0
2	Ι	22	THR	2.0
2	J	129	ALA	2.0

#### 4.2 Non-standard residues in protein, DNA, RNA chains (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
2	MME	K	1	9/10	0.90	0.15	26,27,31,33	0
1	HYP	Н	151	8/9	0.91	0.12	12,13,13,13	0
2	MME	J	1	9/10	0.92	0.14	26,26,31,33	0
2	MME	М	1	9/10	0.92	0.15	26,27,30,33	0
1	HYP	А	104	8/9	0.93	0.09	13,14,14,14	0
2	MME	Р	1	9/10	0.93	0.14	25,26,32,33	0
1	HYP	F	104	8/9	0.94	0.08	13,14,14,14	0
2	MME	L	1	9/10	0.94	0.12	26,27,31,33	0
1	HYP	А	151	8/9	0.94	0.11	12,13,13,13	0
2	MME	N	1	9/10	0.94	0.15	26,27,31,33	0
1	SMC	А	256	7/8	0.94	0.09	10,12,13,13	0
1	HYP	Е	104	8/9	0.95	0.09	13,14,14,14	0
1	HYP	Е	151	8/9	0.95	0.09	12,13,13,13	0
1	HYP	С	104	8/9	0.95	0.08	13,14,14,15	0
1	KCX	С	201	12/13	0.95	0.10	12,13,14,14	0
2	MME	0	1	9/10	0.95	0.09	26,27,31,33	0
1	SMC	С	369	7/8	0.95	0.09	16,16,17,19	0
1	HYP	D	151	8/9	0.96	0.09	12,13,13,13	0
1	KCX	D	201	12/13	0.96	0.11	12,13,13,14	0
1	KCX	А	201	12/13	0.96	0.10	12,13,13,14	0
1	SMC	А	369	7/8	0.96	0.09	16,16,17,19	0
1	SMC	Е	256	7/8	0.96	0.09	10,12,13,13	0
1	KCX	В	201	12/13	0.96	0.11	12,13,14,14	0
1	SMC	G	369	7/8	0.96	0.08	16,16,17,19	0
1	HYP	Н	104	8/9	0.96	0.08	13,14,14,15	0
1	SMC	F	256	7/8	0.97	0.08	11,12,13,14	0
1	SMC	F	369	7/8	0.97	0.10	16,17,18,19	0
1	HYP	G	104	8/9	0.97	0.08	13,13,14,14	0
1	HYP	G	151	8/9	0.97	0.08	13,13,13,14	0
1	KCX	G	201	12/13	0.97	0.13	12,13,13,14	0



Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(Å^2)$	Q<0.9
1	SMC	D	256	7/8	0.97	0.07	9,12,12,13	0
1	SMC	D	369	7/8	0.97	0.08	16,16,18,19	0
1	HYP	В	151	8/9	0.97	0.06	13,13,13,14	0
1	KCX	Н	201	12/13	0.97	0.12	12,13,13,14	0
1	SMC	Н	256	7/8	0.97	0.08	11,12,12,13	0
2	MME	Ι	1	9/10	0.97	0.09	26,26,31,33	0
1	HYP	D	104	8/9	0.97	0.07	13,13,14,14	0
1	KCX	Е	201	12/13	0.97	0.10	12,13,13,14	0
1	HYP	В	104	8/9	0.97	0.07	13,13,14,14	0
1	SMC	Е	369	7/8	0.97	0.07	16,16,18,19	0
1	SMC	С	256	7/8	0.97	0.08	10,12,12,13	0
1	HYP	F	151	8/9	0.97	0.09	13,13,13,14	0
1	KCX	F	201	12/13	0.97	0.09	12,13,14,15	0
1	SMC	В	369	7/8	0.98	0.09	16,16,17,19	0
1	SMC	Н	369	7/8	0.98	0.06	16,16,17,19	0
1	SMC	В	256	7/8	0.98	0.08	10,12,12,13	0
1	HYP	С	151	8/9	0.98	0.07	13,13,14,14	0
1	SMC	G	256	7/8	0.98	0.08	10,12,13,13	0

### 4.3 Carbohydrates (i)

There are no monosaccharides in this entry.

### 4.4 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	$B-factors(Å^2)$	Q<0.9
5	EDO	Ι	1142	4/4	0.62	0.29	41,42,42,43	0
5	EDO	Ν	1141	4/4	0.69	0.21	30,32,34,35	0
5	EDO	С	1482	4/4	0.70	0.27	33,38,38,38	0
5	EDO	F	1481	4/4	0.71	0.29	41,41,41,42	0
5	EDO	Н	1483	4/4	0.76	0.25	39,42,42,43	0
5	EDO	F	1484	4/4	0.79	0.19	24,26,28,29	0
5	EDO	Е	1480	4/4	0.79	0.20	42,43,43,44	0
5	EDO	А	1482	4/4	0.80	0.16	31,32,32,33	0
5	EDO	L	1141	4/4	0.82	0.19	47,47,48,48	0
5	EDO	B	1480	4/4	0.82	0.18	29,30,31,32	0



Continued from previous page										
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(A^2)$	Q < 0.9		
5	EDO	С	1477	4/4	0.83	0.22	38,38,39,40	0		
5	EDO	Н	1480	4/4	0.85	0.15	$35,\!38,\!39,\!39$	0		
5	EDO	М	1141	4/4	0.86	0.22	33,34,34,36	0		
5	EDO	F	1479	4/4	0.86	0.18	36, 36, 37, 37	0		
5	EDO	Р	1141	4/4	0.86	0.20	$48,\!50,\!51,\!52$	0		
5	EDO	Ι	1141	4/4	0.88	0.19	$35,\!35,\!35,\!35$	0		
5	EDO	0	1142	4/4	0.88	0.20	31,32,34,36	0		
5	EDO	D	1478	4/4	0.88	0.20	35, 36, 38, 38	0		
5	EDO	J	1142	4/4	0.89	0.23	$26,\!28,\!32,\!33$	0		
5	EDO	С	1481	4/4	0.89	0.18	27,30,30,30	0		
5	EDO	K	1141	4/4	0.90	0.20	30,32,34,35	0		
5	EDO	Н	1476	4/4	0.90	0.13	17,20,21,21	0		
5	EDO	В	1477	4/4	0.90	0.14	16,16,18,18	0		
5	EDO	D	1481	4/4	0.91	0.12	32,33,34,34	0		
5	EDO	Е	1476	4/4	0.91	0.16	22,22,24,25	0		
5	EDO	А	1481	4/4	0.91	0.12	21,21,22,23	0		
5	EDO	G	1480	4/4	0.91	0.14	38,38,38,39	0		
5	EDO	А	1484	4/4	0.92	0.18	41,43,43,45	0		
5	EDO	Н	1481	4/4	0.92	0.21	39,40,41,41	0		
5	EDO	С	1480	4/4	0.92	0.16	20,24,24,25	0		
5	EDO	D	1477	4/4	0.92	0.15	20,21,21,22	0		
5	EDO	Н	1482	4/4	0.93	0.10	21,21,22,22	0		
5	EDO	K	1142	4/4	0.93	0.11	40,40,40,41	0		
5	EDO	F	1482	4/4	0.93	0.21	28,30,32,34	0		
5	EDO	Н	1478	4/4	0.93	0.16	29,30,31,31	0		
5	EDO	F	1480	4/4	0.93	0.20	35,37,37,37	0		
5	EDO	N	1142	4/4	0.93	0.09	$25,\!26,\!26,\!28$	0		
5	EDO	J	1141	4/4	0.93	0.14	28,29,30,31	0		
5	EDO	С	1478	4/4	0.93	0.12	27,27,28,28	0		
5	EDO	В	1479	4/4	0.94	0.15	33,33,34,35	0		
5	EDO	0	1141	4/4	0.94	0.15	32,33,34,37	0		
5	EDO	G	1476	4/4	0.94	0.11	20,20,23,23	0		
5	EDO	А	1477	4/4	0.94	0.20	21,22,23,24	0		
5	EDO	G	1478	4/4	0.95	0.11	$25,\!25,\!25,\!25$	0		
5	EDO	D	1480	4/4	0.95	0.09	24,28,28,29	0		
5	EDO	F	1483	4/4	0.95	0.10	21,23,26,27	0		
5	EDO	Е	1478	4/4	0.96	0.09	23,25,26,26	0		
4	CAP	Е	477	21/21	0.96	0.10	14,16,17,19	0		
5	EDO	А	1483	4/4	0.96	0.08	19,20,20,23	0		
4	CAP	D	477	21/21	0.97	0.11	14,16,17,18	0		
4	CAP	С	477	21/21	0.98	0.08	13,16,18,19	0		
3	MG	А	476	1/1	0.98	0.10	14,14,14,14	0		

 $\alpha$ 1 L.



2V68
------

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	MG	С	476	1/1	0.98	0.06	14,14,14,14	0
5	EDO	В	1481	4/4	0.98	0.09	20,21,21,24	0
4	CAP	F	477	21/21	0.98	0.08	14,16,17,19	0
4	CAP	G	477	21/21	0.98	0.09	14,16,17,18	0
3	MG	D	476	1/1	0.98	0.04	14,14,14,14	0
3	MG	Е	476	1/1	0.98	0.06	14,14,14,14	0
3	MG	Н	476	1/1	0.98	0.08	14,14,14,14	0
4	CAP	А	477	21/21	0.98	0.12	14,16,17,18	0
4	CAP	В	477	21/21	0.98	0.10	14,16,18,19	0
3	MG	В	476	1/1	0.99	0.07	14,14,14,14	0
3	MG	F	476	1/1	0.99	0.09	13,13,13,13	0
4	CAP	Н	477	21/21	0.99	0.10	14,16,17,19	0
3	MG	G	476	1/1	0.99	0.16	14,14,14,14	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.





















# 4.5 Other polymers (i)

There are no such residues in this entry.

