

Full wwPDB X-ray Structure Validation Report (i)

Jan 14, 2024 - 04:54 am GMT

PDB ID	:	6YX7
Title	:	The high resolution structure of allophycocyanin from cyanobacterium Nostoc
		sp. WR13, the P21212 crystal form.
Authors	:	Patel, H.M.; Roszak, A.W.; Madamwar, D.; Cogdell, R.J.
Deposited on	:	2020-04-30
Resolution	:	1.42 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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.42 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive	Similar resolution
	$(\# { m Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$
R_{free}	130704	2579(1.44-1.40)
Clashscore	141614	2696 (1.44-1.40)
Ramachandran outliers	138981	2632(1.44-1.40)
Sidechain outliers	138945	2631 (1.44-1.40)
RSRZ outliers	127900	2528 (1.44-1.40)

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	AAA	160	.%	12%	
1	CCC	160	88%	12% •	
1	EEE	160	.% 89%	9% •	
1	GGG	160	83%	16% •	
1	III	160	91%	8% •	



Conti	Continueu from previous page								
Mol	Chain	Length	Quality of chain						
1	KKK	160	% 79%	19%	•				
2	BBB	161	% 	16%					
2	DDD	161	86%	14%	•				
2	\mathbf{FFF}	161	97%		•				
2	HHH	161	86%	14%					
2	JJJ	161	% • 93%	7%	6				
2	LLL	161	88%	12%					

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	P6G	CCC	202	-	-	-	Х
15	PGE	GGG	203	-	-	Х	-
15	PGE	LLL	204	-	-	-	Х
4	PG4	AAA	202	-	-	Х	-
4	PG4	CCC	203	-	-	Х	Х
4	PG4	FFF	204	-	-	-	Х
7	1PE	BBB	204	-	-	Х	-
8	PEG	BBB	205	-	-	Х	-
8	PEG	BBB	208	-	-	Х	-
8	PEG	CCC	204	-	-	Х	-
8	PEG	HHH	204	-	-	Х	-
8	PEG	JJJ	205	-	-	Х	-
9	EDO	KKK	203	-	-	Х	-
9	EDO	KKK	204	-	-	Х	-



2 Entry composition (i)

There are 17 unique types of molecules in this entry. The entry contains 19418 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1		160	Total	С	Ν	0	S	0	10	0
	ллл	100	1272	800	222	243	7	0	10	0
1	CCC	160	Total	С	Ν	0	S	0	15	0
	000	100	1292	820	223	243	6	0	10	0
1	FFF	160	Total	С	Ν	Ο	\mathbf{S}	0	12	0
		100	1285	808	226	245	6	0		0
1	CCC	160	Total	С	Ν	Ο	\mathbf{S}	0	13	0
	000	100	1272	803	220	243	6	0	10	0
1	TIT	160	Total	С	Ν	Ο	\mathbf{S}	0	8	0
L	111	100	1247	785	215	241	6	0	0	0
1	KKK	160	Total	С	Ν	0	S	0	16	0
		100	1319	830	230	252	7		10	U

• Molecule 1 is a protein called Allophycocyanin alpha.

• Molecule 2 is a protein called Allophycocyanin beta.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
2	BBB	161	Total	С	Ν	Ο	\mathbf{S}	0	15	0
	DDD	101	1303	831	213	253	6	Ŭ	10	U
2	מממ	161	Total	С	Ν	Ο	\mathbf{S}	0	10	0
	עעע	101	1309	837	210	256	6	0	19	0
0		161	Total	С	Ν	0	S	0	2	0
	ГГГ	101	1236	779	207	244	6	0	5	0
0	ипп	161	Total	С	Ν	0	S	0	12	0
	111111	101	1290	818	210	256	6	0	10	0
9	TTT	161	Total	С	Ν	Ο	S	0	0	0
	111	101	1258	797	209	246	6	0	9	0
9	ттт	161	Total	С	Ν	0	S	0	11	0
		101	1280	813	213	248	6	0		0

• Molecule 3 is PHYCOCYANOBILIN (three-letter code: CYC) (formula: $C_{33}H_{40}N_4O_6$) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	A	Aton	ns		ZeroOcc	AltConf
9	ΛΛΛ	1	Total	С	Ν	0	0	0
5	AAA	L	43	33	4	6	0	0
2	BBB	1	Total	С	Ν	0	0	0
0	DDD	L	43	33	4	6	0	0
3	CCC	1	Total	С	Ν	0	0	0
0		T	43	33	4	6	0	0
3	מחם	1	Total	С	Ν	0	0	0
0	DDD	I	43	33	4	6	0	0
3	$\mathbf{E}\mathbf{E}\mathbf{E}$	1	Total	С	Ν	Ο	0	0
0		I	43	33	4	6	0	0
3	FFF	1	Total	\mathbf{C}	Ν	Ο	0	0
	111	1	43	33	4	6	0	0
3	GGG	1	Total	С	Ν	Ο	0	0
		Ŧ	43	33	4	6	0	Ŭ
3	ннн	1	Total	С	Ν	Ο	0	0
		±	43	33	4	6	0	Ŭ
3	III	1	Total	С	Ν	Ο	0	0
		1	43	33	4	6	0	
3	TTT	1	Total	С	Ν	Ο	0	0
	000	1	43	33	4	6	0	0
3	ККК	1	Total	С	Ν	Ο	0	0
	11111	*	43	33	4	6	0	
3	LLL	1	Total	С	Ν	Ο	0	0
			43	33	4	6	U	

• Molecule 4 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	AAA	1	Total C O 13 8 5	0	0
4	CCC	1	Total C O 13 8 5	0	0
4	FFF	1	Total C O 13 8 5	0	0
4	JJJ	1	Total C O 13 8 5	0	0

• Molecule 5 is LYSINE (three-letter code: LYS) (formula: $C_6H_{15}N_2O_2$).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	BBB	1	Total C N O 16 11 3 2	0	1
5	III	1	Total C N O 10 6 2 2	0	0
5	KKK	1	Total C N O 10 6 2 2	0	0

• Molecule 6 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	BBB	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 8 & 6 & 2 \end{array}$	0	0
6	DDD	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 8 & 6 & 2 \end{array}$	0	0
6	EEE	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 8 6 2 \end{array}$	0	0
6	FFF	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 8 & 6 & 2 \end{array}$	0	0
6	HHH	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 8 & 6 & 2 \end{array}$	0	0
6	JJJ	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 8 & 6 & 2 \end{array}$	0	0
6	LLL	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 8 6 2 \end{array}$	0	0

• Molecule 7 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	BBB	1	Total 16	C 10	O 6	0	0

• Molecule 8 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	BBB	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 7 4 3 \end{array}$	0	0
8	BBB	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 7 4 3 \end{array}$	0	0
8	BBB	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 7 4 3 \end{array}$	0	0



Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	CCC	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 7 & 4 & 3 \end{array}$	0	0
8	GGG	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 7 & 4 & 3 \end{array}$	0	0
8	HHH	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 7 & 4 & 3 \end{array}$	0	0
8	JJJ	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 7 4 3 \end{array}$	0	0

• Molecule 9 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	BBB	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
9	CCC	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
9	CCC	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
9	KKK	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
9	KKK	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0

• Molecule 10 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: $C_{12}H_{26}O_7$).



P6G
CI CI CI CI CI CI CI CI CI CI CI CI CI C

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	CCC	1	Total 19	C 12	0 7	0	0



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	DDD	1	Total 10	С 5	N 1	0 4	0	0
11	ННН	1	Total 10	С 5	N 1	0 4	0	0

• Molecule 12 is GLYCINE (three-letter code: GLY) (formula: $C_2H_5NO_2$).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	EEE	1	Total 5	C 2	N 1	0 2	0	0

• Molecule 13 is ALANINE (three-letter code: ALA) (formula: $C_3H_7NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	FFF	1	Total 6	С 3	N 1	O 2	0	0

• Molecule 14 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula: $C_6H_{14}O_2$).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	GGG	1	Total 8	$\begin{array}{c} \mathrm{C} \\ \mathrm{6} \end{array}$	O 2	0	0

• Molecule 15 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	GGG	1	Total C O 10 6 4	0	0
15	GGG	1	Total C O 10 6 4	0	0
15	LLL	1	Total C O 10 6 4	0	0



• Molecule 16 is D-SERINE (three-letter code: DSN) (formula: C₃H₇NO₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	JJJ	1	Total C N O 7 3 1 3	0	0
16	LLL	1	$\begin{array}{ccccc} \text{Total} & \text{C} & \text{N} & \text{O} \\ 7 & 3 & 1 & 3 \end{array}$	0	0

• Molecule 17 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	AAA	230	Total O 230 230	0	0
17	BBB	281	Total O 281 281	0	0
17	CCC	299	Total O 299 299	0	0
17	DDD	303	Total O 303 303	0	0
17	EEE	246	Total O 246 246	0	0
17	FFF	286	Total O 286 286	0	0
17	GGG	241	Total O 241 241	0	0
17	ННН	284	Total O 284 284	0	0
17	III	252	Total O 252 252	0	0



Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	JJJ	284	Total O 284 284	0	0
17	KKK	238	Total O 238 238	0	0
17	LLL	264	Total O 264 264	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.



• Molecule 1: Allophycocyanin alpha

• Molecule 1: Allophycocyanin alpha



Chain KKK:	79%	19% •
81 12 12 12 12 12 12 12 12 12 12 12 14 14 14 14 14 14 14 14 14 14 14 14 14	866 866 177 177 177 177 186 188 103 103 103 1108 1108 1108 1108 110	v156 q160 ●
• Molecule 2: Allophycocyanin beta		
Chain BBB:	84%	16%
M1 15 15 15 124 124 124 124 155 135 135 135 135 135 135 165 165 165 165 165 165 165 165 165 16	VeV R90 R90 B106 V116 V116 V116 V116 Q131 Q131 Q131 Q131 C157 C157 S161	
• Molecule 2: Allophycocyanin beta		
Chain DDD:	86%	14% •
M1 22 22 21 21 21 21 21 21 22 21 22 24 24 24 24 24 24 24 24 24 25 24 25 26 3 26 3 26 3 26 3 26 26 26 26 26 26 26 27 21 16 27 21 20 21 20 21 20 20 20 20 20 20 20 20 20 20 20 20 20	N71 182 182 185 186 186 131 461 1130 1130 1130 1130 1130 1130 1130 11	
• Molecule 2: Allophycocyanin beta		
Chain FFF:	97%	•
M 124 K63 K63 R116 R134 K134 S161		
• Molecule 2: Allophycocyanin beta		
Chain HHH:	86%	14%
M1 16 16 17 14 127 127 123 128 143 143 143 143 143 143 143 143	D86 1115 1116 1130 1131 1130 1131 1140 1131 1140 1131 1140 1131 1140	
• Molecule 2: Allophycocyanin beta		
Chain JJJ:	93%	7%
N1 N1 015 N21 N21 N21 N21 N39 Y62 S63 Y78 Y78 Y78 Y78 Y116 Y78 Y131 U133 Q121 Q131 Q131 Q131 X134 X134 X134 Z161 X134 Z161		
• Molecule 2: Allophycocyanin beta		
Chain LLL:	88%	12%
M1 16 15 124 139 143 143 165 165 165 165 165 165 165 177 833 833 833 833 833 833 833 833 833 8	q128 A129 1130 1140 1140 1140 1143 2157 2157	



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants	123.69Å 177.73Å 106.37Å	Deperitor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Bosolution(A)	106.37 - 1.42	Depositor
Resolution (A)	106.37 - 1.42	EDS
% Data completeness	87.3 (106.37-1.42)	Depositor
(in resolution range)	87.3(106.37-1.42)	EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.54 (at 1.42 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
D D	0.126 , 0.175	Depositor
n, n_{free}	0.130 , 0.178	DCC
R_{free} test set	19133 reflections (4.99%)	wwPDB-VP
Wilson B-factor $(Å^2)$	20.1	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.32 , 48.7	EDS
L-test for $twinning^2$	$ < L >=0.49, < L^2>=0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	19418	wwPDB-VP
Average B, all atoms $(Å^2)$	28.0	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 48.78 % 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 8.1971e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

²Theoretical 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.



¹Intensities 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: EDO, P6G, MRD, PEG, CYC, DSN, PG4, MPD, PGE, 1PE, MEN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 5 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mal	Chain	Bond lengths		Bond angles	
WIOI	Unain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	AAA	0.67	0/1320	0.79	1/1780~(0.1%)
1	CCC	0.70	0/1358	0.81	0/1831
1	EEE	0.69	0/1342	0.80	3/1808~(0.2%)
1	GGG	0.70	0/1326	0.84	2/1790~(0.1%)
1	III	0.71	0/1286	0.79	1/1735~(0.1%)
1	KKK	0.71	0/1358	0.84	2/1834~(0.1%)
2	BBB	0.67	0/1358	0.75	0/1836
2	DDD	0.73	0/1373	0.78	0/1857
2	FFF	0.67	0/1249	0.78	1/1689~(0.1%)
2	HHH	0.72	0/1333	0.76	0/1804
2	JJJ	0.65	0/1292	0.77	1/1746~(0.1%)
2	LLL	0.66	0/1317	0.76	1/1781~(0.1%)
All	All	0.69	0/15912	0.79	12/21491~(0.1%)

There are no bond length outliers.

All (12)	bond	angle	outliers	are	listed	below:	
----------	------	-------	----------	-----	--------	--------	--

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	\mathbf{FFF}	116	TYR	CB-CG-CD1	5.72	124.44	121.00
2	JJJ	116	TYR	CB-CG-CD1	5.52	124.31	121.00
1	III	35	ARG	CG-CD-NE	-5.36	100.56	111.80
2	LLL	94	TYR	CB-CG-CD1	5.34	124.21	121.00
1	EEE	35[A]	ARG	CG-CD-NE	-5.32	100.64	111.80
1	EEE	35[B]	ARG	CG-CD-NE	-5.32	100.64	111.80
1	GGG	86	TYR	CB-CG-CD1	5.31	124.19	121.00
1	AAA	86	TYR	CB-CG-CD1	5.30	124.18	121.00
1	KKK	58[A]	PHE	CB-CA-C	5.27	120.94	110.40
1	KKK	58[B]	PHE	CB-CA-C	5.27	120.94	110.40
1	EEE	86	TYR	CB-CG-CD1	5.17	124.10	121.00
1	GGG	82	ARG	CG-CD-NE	5.16	122.64	111.80



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	AAA	1272	0	1312	26	0
1	CCC	1292	0	1370	35	0
1	EEE	1285	0	1333	28	0
1	GGG	1272	0	1324	43	0
1	III	1247	0	1282	12	0
1	KKK	1319	0	1349	52	0
2	BBB	1303	0	1359	49	0
2	DDD	1309	0	1372	22	0
2	FFF	1236	0	1247	6	0
2	HHH	1290	0	1322	26	0
2	JJJ	1258	0	1292	13	0
2	LLL	1280	0	1322	17	0
3	AAA	43	0	37	4	0
3	BBB	43	0	37	3	0
3	CCC	43	0	37	3	0
3	DDD	43	0	37	2	0
3	EEE	43	0	37	3	0
3	FFF	43	0	37	2	0
3	GGG	43	0	37	3	0
3	HHH	43	0	37	3	0
3	III	43	0	37	3	0
3	JJJ	43	0	37	2	0
3	KKK	43	0	37	3	0
3	LLL	43	0	37	3	0
4	AAA	13	0	18	11	0
4	CCC	13	0	18	15	0
4	FFF	13	0	18	0	0
4	JJJ	13	0	18	2	0
5	BBB	16	0	24	0	0
5	III	10	0	12	0	0
5	KKK	10	0	12	1	0
6	BBB	8	0	14	0	0
6	DDD	8	0	14	0	0



01Λ	6	Y	2	ζ	7	
-------------	---	---	---	---	---	--

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	EEE	8	0	14	5	0
6	FFF	8	0	14	0	0
6	HHH	8	0	14	1	0
6	JJJ	8	0	14	0	0
6	LLL	8	0	14	0	0
7	BBB	16	0	22	8	0
8	BBB	21	0	30	28	0
8	CCC	7	0	10	4	0
8	GGG	7	0	10	0	0
8	HHH	7	0	10	4	0
8	JJJ	7	0	10	4	0
9	BBB	4	0	6	1	0
9	CCC	8	0	12	0	0
9	KKK	8	0	12	10	0
10	CCC	19	0	26	5	0
11	DDD	10	0	5	2	0
11	HHH	10	0	5	0	0
12	EEE	5	0	2	3	0
13	FFF	6	0	4	2	0
14	GGG	8	0	14	0	0
15	GGG	20	0	28	18	0
15	LLL	10	0	14	2	0
16	JJJ	7	0	6	1	0
16	LLL	7	0	6	0	0
17	AAA	230	0	0	5	0
17	BBB	281	0	0	17	0
17	CCC	299	0	0	7	0
17	DDD	303	0	0	11	0
17	EEE	246	0	0	7	0
17	FFF	286	0	0	2	0
17	GGG	241	0	0	18	0
17	HHH	284	0	0	13	0
17	III	252	0	0	5	1
17	JJJ	284	0	0	6	0
17	KKK	238	0	0	16	0
17	LLL	264	0	0	8	1
All	All	19418	0	16778	379	1

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 11.

All (379) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



Atom-1	Atom-2	Interatomic distance $(Å)$	Clash overlap (Å)
1·CCC·48[A]·ABG·NH2	4·CCC·203·PG4·H41	1.29	1.46
2:HHH:35[C]:GLU:HG3	17:HHH:301:HOH:O	1.37	1.24
2:LLL:131[B]:GLN:NE2	17:LLL:301:HOH:O	1.73	1.19
2:DDD:86[B]:ASP:0D1	17:DDD:302:HOH:O	1.60	1.18
2:DDD:15[B]:GLN:OE1	17:DDD:303:HOH:O	1.65	1.13
1:GGG:76[A]:MET:HE2	17:GGG:428:HOH:O	0.97	1.13
1:EEE:37[C]:ABG:CZ	17:EEE:303:HOH:O	1.97	1.12
2:DDD:15[B]:GLN:NE2	17:DDD:304:HOH:O	1.80	1.11
10:CCC:202:P6G:H122	4:CCC:203:PG4:H71	1.30	1.10
1:CCC:48[A]:ARG:HH22	4:CCC:203:PG4:C4	1.65	1.10
1:AAA:46[B]:ARG:HG3	1:AAA:46[B]:ARG:HH11	1.18	1.08
2:HHH:35[C]:GLU:CG	17:HHH:301:HOH:O	1.91	1.08
1:CCC:48[B]:ARG:NH2	4:CCC:203:PG4:H41	1.69	1.07
1:GGG:56[B]:GLN:NE2	17:GGG:303:HOH:O	1.90	1.04
1:CCC:4[B]:THR:HG21	17:CCC:368:HOH:O	1.57	1.04
1:CCC:48[A]:ARG:NH2	4:CCC:203:PG4:C4	2.21	1.03
10:CCC:202:P6G:H122	4:CCC:203:PG4:C7	1.88	1.03
1:EEE:147[B]:GLU:OE1	12:EEE:202:GLY:N	1.91	1.02
2:HHH:21[B]:ASN:OD1	17:HHH:303:HOH:O	1.79	1.01
2:BBB:39[B]:ARG:CD	8:BBB:208:PEG:O4	2.09	1.00
1:CCC:35[A]:ARG:NH1	17:CCC:302:HOH:O	1.84	1.00
9:KKK:203:EDO:H12	17:KKK:305:HOH:O	1.60	1.00
2:LLL:6[B]:THR:HG22	17:LLL:348:HOH:O	1.59	0.99
17:CCC:308:HOH:O	2:DDD:6[A]:THR:HG22	1.63	0.98
2:BBB:117[B]:ASN:OD1	17:BBB:302:HOH:O	1.81	0.97
2:DDD:54[B]:GLU:OE2	17:DDD:305:HOH:O	1.83	0.97
8:BBB:208:PEG:O4	17:BBB:303:HOH:O	1.85	0.95
2:BBB:39[B]:ARG:HD2	8:BBB:208:PEG:O4	1.67	0.94
2:BBB:39[B]:ARG:CZ	8:BBB:208:PEG:H31	1.97	0.94
1:GGG:133:LYS:HE2	15:GGG:203:PGE:H3	1.49	0.93
1:GGG:76[A]:MET:HE1	17:GGG:505:HOH:O	1.66	0.93
11:DDD:202:GLU:HG2	11:DDD:202:GLU:OXT	1.66	0.93
8:BBB:208:PEG:C2	15:GGG:203:PGE:H32	2.00	0.92
2:LLL:6[B]:THR:CG2	17:LLL:348:HOH:O	2.14	0.91
2:BBB:39[B]:ARG:CZ	8:BBB:208:PEG:C3	2.48	0.91
8:BBB:208:PEG:H21	15:GGG:203:PGE:H32	1.53	0.90
10:CCC:202:P6G:C12	4:CCC:203:PG4:H71	2.03	0.89
2:DDD:45[B]:SER:OG	17:DDD:306:HOH:O	1.89	0.88
3:KKK:201:CYC:HMA1	3:KKK:201:CYC:HB	1.38	0.88
2:JJJ:15[B]:GLN:CD	17:JJJ:302:HOH:O	2.12	0.87
1:AAA:48[A]:ARG:HH21	1:AAA:139:LEU:HD21	1.38	0.87
2:JJJ:15[B]:GLN:OE1	17:JJJ:302:HOH:O	1.92	0.86



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:EEE:201:CYC:HB	3:EEE:201:CYC:HMA1	1.39	0.86
2:HHH:35[C]:GLU:CD	17:HHH:301:HOH:O	2.08	0.86
1:EEE:37[B]:ARG:HG2	1:EEE:37[B]:ARG:HH11	1.39	0.86
2:HHH:35[A]:GLU:OE1	17:HHH:304:HOH:O	1.92	0.86
3:III:201:CYC:HB	3:III:201:CYC:HMA1	1.40	0.85
1:GGG:134[A]:SER:HA	15:GGG:203:PGE:H6	1.56	0.85
2:HHH:86[B]:ASP:OD2	17:HHH:305:HOH:O	1.93	0.85
1:KKK:61[A]:ARG:NH1	1:KKK:63[A]:ASP:OD1	2.10	0.85
3:GGG:201:CYC:HMA1	3:GGG:201:CYC:HB	1.40	0.85
1:AAA:27:SER:OG	1:GGG:24[B]:ARG:CZ	2.25	0.84
1:GGG:134[B]:SER:HA	15:GGG:203:PGE:H6	1.56	0.84
3:AAA:201:CYC:HB	3:AAA:201:CYC:HMA1	1.40	0.84
2:BBB:39[B]:ARG:NH1	8:BBB:208:PEG:H31	1.91	0.84
2:BBB:39[B]:ARG:NH1	17:BBB:304:HOH:O	2.10	0.83
1:KKK:156:VAL:O	1:KKK:160:GLN:HG3	1.78	0.83
1:EEE:60:LYS:O	9:KKK:204:EDO:H22	1.80	0.82
2:DDD:14[B]:VAL:HG23	17:DDD:368:HOH:O	1.78	0.82
3:CCC:201:CYC:HMA1	3:CCC:201:CYC:HB	1.43	0.82
1:CCC:48[B]:ARG:HH22	4:CCC:203:PG4:H41	1.42	0.81
2:DDD:86[B]:ASP:OD2	17:DDD:308:HOH:O	1.99	0.80
2:DDD:86[B]:ASP:OD2	17:DDD:307:HOH:O	1.98	0.80
6:EEE:203:MPD:O2	17:EEE:302:HOH:O	1.99	0.80
8:BBB:208:PEG:H21	15:GGG:203:PGE:C3	2.12	0.79
1:AAA:11:ASP:OD2	4:AAA:202:PG4:H11	1.83	0.79
2:JJJ:15[B]:GLN:NE2	17:JJJ:302:HOH:O	2.15	0.78
4:AAA:202:PG4:H72	2:BBB:87:TYR:CE1	2.19	0.77
1:GGG:133:LYS:HE2	15:GGG:203:PGE:H5	1.67	0.77
1:CCC:34[B]:GLN:HG3	1:CCC:37[B]:ARG:HH12	1.49	0.77
1:EEE:37[B]:ARG:HH11	1:EEE:37[B]:ARG:CG	1.98	0.75
1:KKK:61[A]:ARG:HH11	1:KKK:61[A]:ARG:HB3	1.48	0.75
2:HHH:21[B]:ASN:ND2	17:HHH:308:HOH:O	2.19	0.75
2:BBB:131[A]:GLN:OE1	2:BBB:134:LYS:HE2	1.88	0.74
1:GGG:28:PHE:CE1	1:GGG:35[A]:ARG:NH2	2.55	0.74
1:GGG:76[A]:MET:CE	17:GGG:428:HOH:O	1.76	0.74
1:EEE:147[B]:GLU:OE1	12:EEE:202:GLY:CA	2.35	0.74
1:CCC:48[A]:ARG:HH22	4:CCC:203:PG4:H41	0.93	0.73
1:GGG:2:ILE:HD11	1:GGG:24[B]:ARG:HB3	1.70	0.73
8:HHH:204:PEG:H41	17:HHH:318:HOH:O	1.88	0.73
1:EEE:37[C]:ARG:NH2	17:EEE:303:HOH:O	2.11	0.73
11:DDD:202:GLU:OXT	11:DDD:202:GLU:CG	2.35	0.73
8:BBB:208:PEG:H41	17:BBB:307:HOH:O	1.88	0.72



Atom 1	-1 Atom-2 Interatomic		Clash
Atom-1	Atom-2	$\frac{\text{distance (Å)}}{1.80} = 0.72$	
9:KKK:204:EDO:H21	17:KKK:327:HOH:O	1.89	0.72
2:BBB:39[B]:ARG:HD2	8:BBB:208:PEG:HO4	1.55	0.72
1:CCC:48[A]:ARG:HH21	4:CCC:203:PG4:H41	1.45	0.72
1:GGG:137:ALA:HB2	15:GGG:203:PGE:H22	1.72	0.71
1:CCC:28:PHE:CE1	1:CCC:35[A]:ARG:NH2	2.58	0.71
1:KKK:37[A]:ARG:NH1	17:KKK:304:HOH:O	2.23	0.71
1:GGG:24[B]:ARG:NE	1:GGG:24[B]:ARG:HA	2.06	0.70
1:KKK:48[C]:ARG:HH11	1:KKK:48[C]:ARG:HB3	1.54	0.70
1:AAA:96[B]:VAL:HG11	2:BBB:27:LEU:HD13	1.73	0.70
1:GGG:56[B]:GLN:NE2	17:GGG:302:HOH:O	1.79	0.70
1:EEE:56:GLN:O	1:EEE:60:LYS:HD3	1.92	0.69
1:GGG:51[A]:LYS:NZ	17:GGG:306:HOH:O	2.26	0.69
1:GGG:2:ILE:HD11	1:GGG:24[A]:ARG:HB3	1.74	0.69
1:KKK:48[C]:ARG:HH11	1:KKK:48[C]:ARG:CB	2.07	0.68
1:EEE:37[C]:ARG:NE	17:EEE:303:HOH:O	2.17	0.68
1:EEE:40:GLN:HE22	2:FFF:24:LEU:HD11	1.59	0.67
1:III:37:ARG:HH21	1:III:40[A]:GLN:NE2	1.92	0.67
6:EEE:203:MPD:C1	6:EEE:203:MPD:H53	2.23	0.67
6:EEE:203:MPD:H53	6:EEE:203:MPD:H13	1.76	0.67
8:BBB:208:PEG:C4	17:BBB:303:HOH:O	2.40	0.67
2:BBB:35:GLU:OE1	2:BBB:39[B]:ARG:CG	2.43	0.66
2:BBB:65[B]:ILE:HG13	17:BBB:488:HOH:O	1.95	0.66
1:EEE:24:ARG:HG2	17:III:496:HOH:O	1.95	0.66
3:GGG:201:CYC:HMD2	3:GGG:201:CYC:HC	1.60	0.66
3:III:201:CYC:HMD2	3:III:201:CYC:HC	1.60	0.66
3:AAA:201:CYC:HMD2	3:AAA:201:CYC:HC	1.60	0.66
1:CCC:2[B]:ILE:HD11	1:CCC:24:ARG:NH1	2.10	0.66
2:BBB:39[B]:ARG:CZ	8:BBB:208:PEG:H32	2.26	0.66
3:KKK:201:CYC:HC	3:KKK:201:CYC:HMD2	1.61	0.66
3:EEE:201:CYC:HC	3:EEE:201:CYC:HMD2	1.61	0.65
1:GGG:35[A]:ARG:NH1	17:GGG:305:HOH:O	2.23	0.65
2:BBB:143:PRO:HA	7:BBB:204:1PE:C12	2.27	0.65
2:BBB:143:PRO:HA	7:BBB:204:1PE:H121	1.79	0.65
1:EEE:37[B]:ARG:HG2	1:EEE:37[B]:ARG:NH1	2.11	0.65
2:BBB:5[A]:ILE:HD12	2:BBB:27:LEU:HD22	1.79	0.64
2:HHH:116:TYR:OH	17:HHH:306:HOH:O	2.14	0.64
2:DDD:2[A]:GLN:NE2	17:DDD:301:HOH:O	2.29	0.64
1:KKK:57:LEU:O	1:KKK:61[B]:ARG:HB2	1.97	0.64
2:BBB:39[A]:ARG:HH22	8:BBB:205:PEG:H11	1.62	0.64
1:KKK:23[B]:ASP:OD2	17:KKK:301:HOH:O	2.15	0.64
1:EEE:40:GLN:NE2	2:FFF:24:LEU:CD1	2.61	0.64



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
6:EEE:203:MPD:H4	17:EEE:384:HOH:O	1.98	0.64
9:BBB:207:EDO:H12	17:BBB:443:HOH:O	1.97	0.63
2:LLL:39[B]:ARG:NH2	15:LLL:204:PGE:O4	2.31	0.63
2:DDD:21[B]:ASN:ND2	17:DDD:312:HOH:O	2.27	0.63
1:III:48[A]:ARG:NH2	1:III:139:LEU:HD21	2.13	0.63
1:EEE:40:GLN:NE2	2:FFF:24:LEU:HD11	2.14	0.63
1:AAA:46[B]:ARG:HG3	1:AAA:46[B]:ARG:NH1	1.97	0.63
1:GGG:24[A]:ARG:NH2	17:GGG:307:HOH:O	2.31	0.62
2:DDD:43:THR:CG2	2:DDD:140[B]:LEU:HG	2.29	0.62
1:GGG:52:GLN:NE2	17:GGG:308:HOH:O	2.32	0.62
3:DDD:201:CYC:HMD2	3:DDD:201:CYC:HC	1.65	0.62
1:KKK:56:GLN:O	1:KKK:60[B]:LYS:HB3	1.98	0.62
1:KKK:66[A]:SER:HB2	9:KKK:204:EDO:O1	1.99	0.61
15:GGG:203:PGE:H62	17:GGG:438:HOH:O	2.00	0.61
1:AAA:2:ILE:HG12	1:AAA:24[A]:ARG:HG3	1.82	0.61
1:KKK:64[A]:VAL:HG12	1:KKK:121:PRO:HG3	1.81	0.61
1:KKK:63[A]:ASP:HB2	9:KKK:204:EDO:H21	1.82	0.61
3:LLL:201:CYC:HMD2	3:LLL:201:CYC:HC	1.65	0.61
1:AAA:27:SER:OG	1:GGG:24[B]:ARG:NE	2.33	0.60
1:GGG:112[B]:ARG:HH22	1:GGG:160:GLN:C	2.05	0.60
1:KKK:59[B]:GLN:NE2	17:KKK:306:HOH:O	2.34	0.60
1:CCC:112[B]:ARG:NH2	1:CCC:160:GLN:O	2.34	0.60
3:CCC:201:CYC:HMD2	3:CCC:201:CYC:HC	1.67	0.60
1:GGG:137:ALA:HB2	15:GGG:203:PGE:C2	2.31	0.59
2:LLL:65[B]:ILE:HG13	17:LLL:481:HOH:O	2.02	0.59
1:GGG:51[A]:LYS:HE2	1:GGG:51[A]:LYS:HA	1.85	0.59
1:KKK:40:GLN:HE22	2:LLL:24:LEU:HD11	1.67	0.59
1:III:56[A]:GLN:NE2	17:III:305:HOH:O	2.31	0.59
3:BBB:201:CYC:HC	3:BBB:201:CYC:HMD2	1.67	0.59
1:AAA:48[B]:ARG:CB	1:AAA:48[B]:ARG:CZ	2.82	0.58
1:KKK:123:ASP:CG	17:KKK:303:HOH:O	2.42	0.58
1:III:37:ARG:HH21	1:III:40[A]:GLN:HE21	1.49	0.58
2:BBB:131[A]:GLN:OE1	2:BBB:134:LYS:CE	2.52	0.58
1:CCC:24:ARG:NH2	1:KKK:23[B]:ASP:OD2	2.35	0.58
2:HHH:6[A]:THR:HG23	17:HHH:390:HOH:O	2.03	0.58
2:BBB:143:PRO:HD3	7:BBB:204:1PE:H132	1.85	0.58
2:BBB:35:GLU:OE1	2:BBB:39[B]:ARG:HG3	2.04	0.58
1:III:112:ARG:NH2	1:III:158:ALA:O	2.36	0.58
2:JJJ:78:TYR:CG	1:KKK:114[B]:MET:HE2	2.38	0.57
2:HHH:86[B]:ASP:OD1	17:HHH:307:HOH:O	2.17	0.57
3:AAA:201:CYC:HMA1	3:AAA:201:CYC:NB	2.16	0.57



Atom 1	Atom-2 Interatomic Clas		Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:HHH:201:CYC:HC	3:HHH:201:CYC:HMD2	1.68	0.57
1:KKK:65[B]:VAL:HB	9:KKK:203:EDO:O1	2.05	0.57
8:BBB:208:PEG:H22	15:GGG:203:PGE:H32	1.85	0.56
2:BBB:39[A]:ARG:NH2	8:BBB:205:PEG:H11	2.20	0.56
2:BBB:106[B]:GLU:HG3	17:BBB:344:HOH:O	2.04	0.56
2:DDD:21[B]:ASN:OD1	17:DDD:309:HOH:O	2.18	0.56
2:BBB:5[A]:ILE:HD12	2:BBB:27:LEU:CD2	2.35	0.56
2:JJJ:21[B]:ASN:ND2	17:JJJ:303:HOH:O	2.39	0.56
1:III:48[A]:ARG:HH22	1:III:139:LEU:HD21	1.71	0.56
1:AAA:2:ILE:HG12	1:AAA:24[B]:ARG:HG3	1.87	0.56
2:HHH:7[A]:SER:OG	8:HHH:204:PEG:H11	2.06	0.56
1:GGG:17:LEU:O	17:GGG:304:HOH:O	2.17	0.55
2:BBB:35:GLU:OE1	2:BBB:39[B]:ARG:HG2	2.05	0.55
3:GGG:201:CYC:HMA1	3:GGG:201:CYC:NB	2.17	0.55
1:GGG:96[B]:VAL:HG11	2:HHH:27:LEU:HD13	1.87	0.55
2:HHH:14[A]:VAL:HG13	17:HHH:458:HOH:O	2.06	0.55
3:III:201:CYC:HMA1	3:III:201:CYC:NB	2.17	0.55
1:AAA:14:ALA:HB2	4:AAA:202:PG4:H52	1.88	0.55
1:CCC:96[B]:VAL:HG11	2:DDD:27:LEU:HD13	1.89	0.55
1:CCC:48[A]:ARG:NH1	17:CCC:305:HOH:O	2.40	0.54
1:CCC:48[B]:ARG:HH22	4:CCC:203:PG4:C4	2.19	0.54
1:CCC:2[B]:ILE:HG21	1:CCC:28:PHE:CG	2.43	0.53
1:EEE:60:LYS:O	9:KKK:204:EDO:C2	2.54	0.53
1:AAA:36:LEU:HD23	1:AAA:96[B]:VAL:HG22	1.91	0.53
4:AAA:202:PG4:H22	4:AAA:202:PG4:O3	2.09	0.53
1:EEE:31:GLY:C	1:EEE:35[B]:ARG:HH12	2.11	0.53
3:KKK:201:CYC:HMA1	3:KKK:201:CYC:NB	2.16	0.53
2:BBB:39[B]:ARG:NH2	8:BBB:208:PEG:H31	2.23	0.53
13:FFF:202:ALA:N	17:FFF:303:HOH:O	2.40	0.53
8:BBB:208:PEG:C3	17:BBB:307:HOH:O	2.57	0.53
17:CCC:308:HOH:O	2:DDD:6[A]:THR:CG2	2.39	0.53
2:LLL:143:PRO:HD3	15:LLL:204:PGE:H12	1.90	0.53
3:JJJ:201:CYC:HMD2	3:JJJ:201:CYC:HC	1.74	0.52
2:BBB:39[B]:ARG:NH2	8:BBB:208:PEG:C3	2.72	0.52
2:HHH:43:THR:CG2	2:HHH:140[B]:LEU:HG	2.40	0.52
1:KKK:50:VAL:HG22	1:KKK:132[B]:MET:HE1	1.92	0.52
2:BBB:39[B]:ARG:NE	8:BBB:208:PEG:O4	2.42	0.52
1:KKK:57:LEU:O	1:KKK:61[B]:ARG:N	2.43	0.52
1:AAA:11:ASP:OD2	4:AAA:202:PG4:C1	2.56	0.52
2:HHH:33:THR:HB	6:HHH:203:MPD:HM3	1.92	0.52
1:CCC:34[B]:GLN:CG	1:CCC:37[B]:ARG:HH12	2.22	0.51



Atom-1	Atom-2		Clash	
		distance (A)	overlap (A)	
1:GGG:143:GLU:CD	1:GGG:143:GLU:H	2.12	0.51	
1:AAA:76[C]:MET:HG2	17:AAA:402:HOH:0	2.10	0.51	
15:GGG:203:PGE:H22	15:GGG:203:PGE:H52	1.93	0.51	
1:GGG:24[B]:ARG:NH1	17:GGG:307:HOH:O	2.42	0.51	
1:EEE:160:GLN:HE21	1:EEE:160:GLN:HA	1.76	0.51	
3:CCC:201:CYC:HMA1	3:CCC:201:CYC:NB	2.20	0.51	
1:EEE:40:GLN:HE22	2:FFF:24:LEU:CD1	2.21	0.51	
2:BBB:143:PRO:CA	7:BBB:204:1PE:H121	2.39	0.51	
3:EEE:201:CYC:HMA1	3:EEE:201:CYC:NB	2.16	0.51	
8:BBB:208:PEG:C4	17:BBB:307:HOH:O	2.55	0.51	
2:HHH:7[A]:SER:OG	8:HHH:204:PEG:C1	2.58	0.51	
2:BBB:131[A]:GLN:CD	17:BBB:314:HOH:O	2.49	0.50	
8:CCC:204:PEG:H42	17:KKK:301:HOH:O	2.10	0.50	
3:FFF:201:CYC:HMD2	3:FFF:201:CYC:HC	1.76	0.50	
1:GGG:2:ILE:HD12	1:GGG:24[A]:ARG:NH1	2.26	0.50	
2:DDD:43:THR:HG22	2:DDD:140[B]:LEU:HG	1.93	0.50	
10:CCC:202:P6G:C12	4:CCC:203:PG4:C7	2.74	0.50	
1:KKK:88:LEU:HB2	1:KKK:132[B]:MET:HE1	1.93	0.50	
1:CCC:51[B]:LYS:HE2	17:CCC:420:HOH:O	2.11	0.50	
2:LLL:117[B]:ASN:OD1	17:LLL:302:HOH:O	2.18	0.50	
1:GGG:24[B]:ARG:HD3	17:GGG:307:HOH:O	2.12	0.49	
2:JJJ:78:TYR:CB	1:KKK:114[B]:MET:HE2	2.41	0.49	
2:JJJ:128:GLN:OE1	8:JJJ:205:PEG:H11	2.13	0.49	
1:EEE:160:GLN:HG3	1:KKK:116:LYS:HE3	1.94	0.49	
2:DDD:131:GLN:HE22	2:DDD:134[A]:LYS:NZ	2.10	0.49	
3:JJJ:201:CYC:HMA1	16:JJJ:202:DSN:HB2	1.93	0.49	
1:CCC:2[C]:ILE:HG12	1:CCC:98:GLY:O	2.13	0.49	
2:DDD:56:VAL:HG21	2:DDD:82[B]:ILE:HD12	1.95	0.49	
1:EEE:31:GLY:C	1:EEE:35[B]:ARG:NH1	2.66	0.49	
2:LLL:77[B]:ARG:NH1	17:LLL:305:HOH:O	2.44	0.49	
1:AAA:104:GLU:HA	1:AAA:108:ILE:HB	1.95	0.49	
2:BBB:15[B]:GLN:NE2	17:BBB:310:HOH:O	2.45	0.49	
2:HHH:26:LYS:HE2	8:HHH:204:PEG:H21	1.94	0.48	
2:HHH:131:GLN:HE22	2:HHH:134:LYS:NZ	2.11	0.48	
1:KKK:50:VAL:HG22	1:KKK:132[B]:MET:CE	2.43	0.48	
1:KKK:102:PRO:HD3	17:KKK:308:HOH:O	2.11	0.48	
1:GGG:24[A]:ARG:CZ	17:GGG:307:HOH:O	2.61	0.48	
2:DDD:85[A]:LEU:HD13	3:DDD:201:CYC:HBC1	1.96	0.48	
2:BBB:39[A]:ARG:HH12	8:BBB:205:PEG:C1	2.26	0.48	
1:EEE:5:LYS:HE2				
	17:EEE:325:HOH:O	2.13	0.48	



Atom 1	Atom 2	Interatomic	Clash	
Atom-1	Atom-2 distance (Å)		overlap (Å)	
1:CCC:71:ALA:HA	1:CCC:76[B]:MET:HB3	1.96	0.47	
1:KKK:61[A]:ARG:HH12	1:KKK:63[A]:ASP:CG	2.18	0.47	
17:BBB:366:HOH:O	1:CCC:76[B]:MET:CE	2.62	0.47	
1:KKK:66[A]:SER:HB2	9:KKK:204:EDO:HO1	1.79	0.47	
1:KKK:49:ILE:HG22	1:KKK:132[B]:MET:CE	2.44	0.47	
1:AAA:48[B]:ARG:CZ	1:AAA:48[B]:ARG:HB2	2.45	0.47	
1:AAA:123:ASP:OD2	17:AAA:302:HOH:O	2.20	0.47	
1:KKK:104:GLU:HA	1:KKK:108:ILE:HB	1.95	0.47	
1:CCC:51[A]:LYS:HE3	17:CCC:506:HOH:O	2.15	0.47	
1:GGG:71:ALA:HA	1:GGG:76[A]:MET:HB3	1.96	0.47	
2:JJJ:131:GLN:HE22	2:JJJ:134:LYS:NZ	2.13	0.47	
1:KKK:65[B]:VAL:CG1	9:KKK:203:EDO:O1	2.63	0.47	
2:BBB:39[B]:ARG:HD3	8:BBB:208:PEG:O4	2.08	0.47	
2:JJJ:63:SER:HB2	8:JJJ:205:PEG:H31	1.96	0.47	
1:KKK:61[A]:ARG:NH1	1:KKK:63[A]:ASP:CG	2.68	0.47	
1:KKK:88:LEU:HB2	1:KKK:132[B]:MET:CE	2.45	0.46	
1:AAA:48[A]:ARG:NH2	1:AAA:139:LEU:HD21	2.19	0.46	
1:GGG:48:ARG:HH11	1:GGG:139:LEU:HD11	1.80	0.46	
2:BBB:143:PRO:HA	7:BBB:204:1PE:H122	1.94	0.46	
6:EEE:203:MPD:C1	6:EEE:203:MPD:C5	2.91	0.46	
1:III:71:ALA:HA	1:III:76[B]:MET:HB3	1.97	0.46	
4:JJJ:204:PG4:H41	17:JJJ:461:HOH:O	2.15	0.45	
1:KKK:40:GLN:NE2	2:LLL:24:LEU:HD11	2.31	0.45	
1:GGG:145:ALA:HB1	15:GGG:203:PGE:H2	1.98	0.45	
15:GGG:203:PGE:H3	15:GGG:203:PGE:H5	1.52	0.45	
1:CCC:2[A]:ILE:HG21	1:CCC:28:PHE:CG	2.51	0.45	
1:EEE:147[B]:GLU:OE1	12:EEE:202:GLY:C	2.55	0.45	
1:KKK:76:MET:HG2	17:KKK:424:HOH:O	2.17	0.45	
4:AAA:202:PG4:C6	2:BBB:90:ARG:HH22	2.30	0.45	
4:AAA:202:PG4:H61	2:BBB:90:ARG:HH22	1.80	0.45	
1:EEE:2:ILE:HG21	1:EEE:28:PHE:CG	2.52	0.45	
1:KKK:64[A]:VAL:HA	17:KKK:349:HOH:O	2.16	0.45	
4:CCC:203:PG4:H41	4:CCC:203:PG4:H22	1.69	0.45	
1:GGG:133:LYS:HG3	15:GGG:203:PGE:H1	1.98	0.45	
8:JJJ:205:PEG:H31	17:JJJ:480:HOH:O	2.17	0.45	
1:KKK:66[A]:SER:CB	17:KKK:403:HOH:O	2.64	0.45	
2:DDD:130:ILE:HG21	2:DDD:157:CYS:SG	2.57	0.45	
1:KKK:55:ASP:O	1:KKK:59[A]:GLN:OE1	2.35	0.45	
1:KKK:63[A]:ASP:C	17:KKK:327:HOH:O	2.54	0.45	
1:GGG:60:LYS:NZ	17:GGG:320:HOH:O	2.49	0.45	
2:HHH:58:LYS:HD2	17:HHH:309:HOH:O	2.16	0.45	



Atom 1	Atom 2	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:AAA:59:GLN:HG2	17:AAA:440:HOH:O	2.16	0.45	
8:JJJ:205:PEG:H42	8:JJJ:205:PEG:H21	1.62	0.45	
1:KKK:65[B]:VAL:CG1	9:KKK:203:EDO:HO1	2.30	0.45	
1:GGG:96[B]:VAL:CG1	2:HHH:27:LEU:HD13	2.46	0.44	
1:KKK:24:ARG:NE	17:KKK:317:HOH:O	2.50	0.44	
1:KKK:49:ILE:HG22	1:KKK:132[B]:MET:HE2	1.99	0.44	
1:EEE:60:LYS:N	1:EEE:60:LYS:CD	2.80	0.44	
2:HHH:130:ILE:HG21	2:HHH:157:CYS:SG	2.57	0.44	
1:CCC:2[C]:ILE:HD11	1:CCC:98:GLY:O	2.18	0.44	
1:CCC:24:ARG:HA	8:CCC:204:PEG:H41	2.00	0.44	
2:BBB:63:SER:OG	2:BBB:65[A]:ILE:HG22	2.17	0.44	
1:CCC:27:SER:CB	8:CCC:204:PEG:H22	2.48	0.44	
1:EEE:71:ALA:HA	1:EEE:76[B]:MET:HB3	1.97	0.44	
1:GGG:56[B]:GLN:HG2	17:GGG:303:HOH:O	2.18	0.44	
1:AAA:11:ASP:CG	4:AAA:202:PG4:H11	2.38	0.44	
2:DDD:63:SER:OG	2:DDD:65[B]:ILE:HG22	2.17	0.43	
2:FFF:131:GLN:HE22	2:FFF:134:LYS:NZ	2.16	0.43	
1:GGG:112[A]:ARG:CZ	17:GGG:393:HOH:O	2.66	0.43	
1:AAA:71:ALA:HA	1:AAA:76[A]:MET:HB3	1.98	0.43	
2:BBB:39[B]:ARG:NH1	8:BBB:208:PEG:C3	2.67	0.43	
1:GGG:104:GLU:HA	1:GGG:108:ILE:HB	1.99	0.43	
2:JJJ:62:TYR:CE2	5:KKK:202:LYS:HA	2.53	0.43	
1:KKK:47[B]:GLU:HG2	17:KKK:486:HOH:O	2.18	0.43	
2:HHH:115:THR:HG21	3:HHH:201:CYC:HMA2	1.99	0.43	
2:JJJ:39:ARG:HH12	4:JJJ:204:PG4:H12	1.82	0.43	
2:BBB:39[A]:ARG:HH22	8:BBB:205:PEG:C1	2.30	0.43	
2:BBB:83:ARG:NH1	3:BBB:201:CYC:O1A	2.52	0.43	
1:AAA:11:ASP:O	4:AAA:202:PG4:C5	2.66	0.43	
7:BBB:204:1PE:OH7	8:BBB:206:PEG:O4	2.13	0.42	
1:CCC:23:ASP:OD2	8:CCC:204:PEG:C1	2.66	0.42	
1:CCC:104:GLU:HA	1:CCC:108:ILE:HB	2.00	0.42	
1:EEE:51[A]:LYS:HE2	1:EEE:51[A]:LYS:HB3	1.76	0.42	
2:BBB:39[B]:ARG:NH2	8:BBB:208:PEG:H32	2.33	0.42	
2:HHH:83:ARG:NH1	3:HHH:201:CYC:O1A	2.51	0.42	
1:KKK:60[B]:LYS:O	1:KKK:60[B]:LYS:HG3	2.19	0.42	
10:CCC:202:P6G:H112	10:CCC:202:P6G:H141	1.65	0.42	
3:FFF:201:CYC:HAB2	13:FFF:202:ALA:HB3	2.02	0.42	
1:KKK:61[A]:ARG:HH11	1:KKK:61[A]:ARG:CB	2.24	0.42	
2:BBB:77[A]:ARG:NH1	17:BBB:316:HOH:O	2.52	0.42	
1:GGG:134[A]:SER:CA	15:GGG:203:PGE:H6	2.39	0.42	
4:AAA:202:PG4:O3	4:AAA:202:PG4:C2	2.67	0.42	



Atom 1	Atom 2	Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
1:KKK:64[A]:VAL:HG12	1:KKK:121:PRO:CG	2.48	0.42	
2:LLL:63:SER:OG	2:LLL:65[A]:ILE:HG22	2.20	0.42	
1:AAA:40:GLN:HE22	2:BBB:24:LEU:HD11	1.84	0.42	
1:CCC:2[C]:ILE:CG1	1:CCC:98:GLY:O	2.68	0.42	
2:LLL:115:THR:HG21	3:LLL:201:CYC:HMA2	2.01	0.42	
1:EEE:37[B]:ARG:HH11	1:EEE:37[B]:ARG:CB	2.33	0.42	
4:CCC:203:PG4:H62	4:CCC:203:PG4:H81	1.16	0.42	
17:BBB:366:HOH:O	1:CCC:76[B]:MET:HE3	2.20	0.42	
1:AAA:46[B]:ARG:NH2	17:AAA:315:HOH:O	2.52	0.41	
2:BBB:39[B]:ARG:HD2	2:BBB:39[B]:ARG:HA	1.86	0.41	
2:BBB:53:LYS:NZ	17:BBB:317:HOH:O	2.53	0.41	
1:GGG:48:ARG:NH2	1:GGG:52:GLN:HE22	2.18	0.41	
1:KKK:2:ILE:HB	17:KKK:460:HOH:O	2.20	0.41	
1:AAA:27:SER:OG	1:GGG:24[B]:ARG:NH1	2.52	0.41	
1:CCC:48[A]:ARG:NH2	4:CCC:203:PG4:H22	2.35	0.41	
2:LLL:43:THR:CG2	2:LLL:140[B]:LEU:HG	2.50	0.41	
1:KKK:58[B]:PHE:CZ	1:KKK:77:THR:HG23	2.54	0.41	
2:LLL:117[B]:ASN:CG	17:LLL:302:HOH:O	2.58	0.41	
4:AAA:202:PG4:H62	4:AAA:202:PG4:H82	1.67	0.41	
2:BBB:130:ILE:HG21	2:BBB:157:CYS:SG	2.61	0.41	
7:BBB:204:1PE:H152	7:BBB:204:1PE:H162	1.77	0.41	
1:III:59[A]:GLN:HG3	17:III:382:HOH:O	2.20	0.41	
2:LLL:15[B]:GLN:NE2	17:LLL:312:HOH:O	2.53	0.41	
2:JJJ:78:TYR:CD1	1:KKK:114[A]:MET:HG3	2.55	0.41	
2:LLL:130:ILE:HG21	2:LLL:157:CYS:SG	2.61	0.41	
3:AAA:201:CYC:HMD2	3:AAA:201:CYC:NC	2.31	0.41	
2:JJJ:130:ILE:HG21	2:JJJ:157:CYS:SG	2.61	0.41	
2:LLL:83:ARG:NH1	3:LLL:201:CYC:O1A	2.53	0.41	
1:AAA:46[B]:ARG:NH2	17:AAA:316:HOH:O	2.53	0.41	
2:HHH:43:THR:HG22	2:HHH:140[B]:LEU:HG	2.01	0.41	
1:III:76[A]:MET:CE	17:III:327:HOH:O	2.69	0.41	
1:CCC:2[B]:ILE:CD1	1:CCC:24:ARG:NH1	2.83	0.41	
2:BBB:26:LYS:NZ	17:BBB:308:HOH:O	2.44	0.41	
1:CCC:34[B]:GLN:HG3	1:CCC:37[B]:ARG:NH1	2.27	0.41	
2:FFF:53:LYS:NZ	17:FFF:306:HOH:O	2.50	0.41	
2:HHH:58:LYS:HB3	2:HHH:58:LYS:HE3	1.89	0.41	
1:III:40[B]:GLN:NE2	17:III:310:HOH:O	2.44	0.41	
1:KKK:65[B]:VAL:HG12	1:KKK:77:THR:OG1	2.21	0.41	
2:BBB:115:THR:HG21	3:BBB:201:CYC:HMA2	2.01	0.41	
$1:KKK:50:VAL:CG\overline{2}$	1:KKK:132[B]:MET:HE1	2.51	0.41	
15:GGG:203:PGE:C6	17:GGG:438:HOH:O	2.63	0.40	



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:BBB:204:1PE:H262	8:BBB:205:PEG:H41	2.03	0.40
1:GGG:133:LYS:CE	15:GGG:203:PGE:H3	2.35	0.40
1:KKK:5:LYS:HG3	17:KKK:309:HOH:O	2.21	0.40
2:BBB:25:GLU:OE2	2:BBB:28:LYS:NZ	2.50	0.40
2:DDD:43:THR:HG22	2:DDD:140[B]:LEU:CD2	2.51	0.40
2:HHH:63:SER:OG	2:HHH:65[B]:ILE:HG22	2.21	0.40
1:EEE:59:GLN:NE2	17:EEE:304:HOH:O	2.12	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:III:428:HOH:O	17:LLL:475:HOH:O[4_454]	2.19	0.01

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	ntiles
1	AAA	170/160~(106%)	169 (99%)	1 (1%)	0	100	100
1	CCC	176/160~(110%)	176 (100%)	0	0	100	100
1	EEE	172/160~(108%)	172 (100%)	0	0	100	100
1	GGG	172/160~(108%)	172 (100%)	0	0	100	100
1	III	167/160~(104%)	167 (100%)	0	0	100	100
1	KKK	175/160~(109%)	175 (100%)	0	0	100	100
2	BBB	174/161~(108%)	172 (99%)	2(1%)	0	100	100
2	DDD	177/161~(110%)	175~(99%)	2(1%)	0	100	100
2	\mathbf{FFF}	161/161~(100%)	159 (99%)	2(1%)	0	100	100
2	HHH	172/161~(107%)	170 (99%)	2(1%)	0	100	100



	J						
Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	\mathbf{n} tiles
2	JJJ	167/161~(104%)	164 (98%)	3~(2%)	0	100	100
2	LLL	169/161~(105%)	167~(99%)	2(1%)	0	100	100
All	All	2052/1926~(106%)	2038~(99%)	14 (1%)	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 sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
1	AAA	134/122~(110%)	132~(98%)	2(2%)	65	36
1	CCC	140/122~(115%)	136~(97%)	4 (3%)	42	10
1	EEE	136/122~(112%)	135~(99%)	1 (1%)	84	65
1	GGG	136/122~(112%)	132~(97%)	4 (3%)	42	10
1	III	131/122~(107%)	126~(96%)	5(4%)	33	5
1	KKK	139/122~(114%)	135~(97%)	4 (3%)	42	10
2	BBB	141/125~(113%)	140~(99%)	1 (1%)	84	65
2	DDD	144/125~(115%)	139~(96%)	5 (4%)	36	7
2	\mathbf{FFF}	128/125~(102%)	128 (100%)	0	100	100
2	HHH	139/125~(111%)	139 (100%)	0	100	100
2	JJJ	133/125~(106%)	133 (100%)	0	100	100
2	LLL	136/125~(109%)	135 (99%)	1 (1%)	84	65
All	All	1637/1482~(110%)	1610 (98%)	27 (2%)	71	32

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	134	SER
1	AAA	140	LEU
2	BBB	36	LEU
1	CCC	2[A]	ILE



Mol	Chain	Res	Type
1	CCC	2[B]	ILE
1	CCC	2[C]	ILE
1	CCC	60	LYS
2	DDD	11[A]	SER
2	DDD	11[B]	SER
2	DDD	58	LYS
2	DDD	85[A]	LEU
2	DDD	85[B]	LEU
1	EEE	160	GLN
1	GGG	23[A]	ASP
1	GGG	23[B]	ASP
1	GGG	46	ARG
1	GGG	143	GLU
1	III	23	ASP
1	III	51	LYS
1	III	60[A]	LYS
1	III	60[B]	LYS
1	III	60[C]	LYS
1	KKK	59[A]	GLN
1	KKK	59[B]	GLN
1	KKK	61[A]	ARG
1	KKK	61[B]	ARG
2	LLL	128	GLN

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)

6 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	Link	B	Bond lengths			Bond angles		
WIOI	туре	Unam	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2	
2	MEN	HHH	71	2	7,8,9	1.32	1 (14%)	6,9,11	0.84	0	
2	MEN	FFF	71	2	7,8,9	0.52	0	6,9,11	0.45	0	
2	MEN	BBB	71	2	7,8,9	0.81	0	6,9,11	0.92	0	
2	MEN	DDD	71	2	7,8,9	1.29	1 (14%)	6,9,11	0.68	0	
2	MEN	JJJ	71	2	7,8,9	0.38	0	6,9,11	0.45	0	
2	MEN	LLL	71	2	7,8,9	1.03	0	6,9,11	1.15	1 (16%)	

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	MEN	HHH	71	2	-	2/7/8/10	-
2	MEN	FFF	71	2	-	2/7/8/10	-
2	MEN	BBB	71	2	-	2/7/8/10	-
2	MEN	DDD	71	2	-	2/7/8/10	-
2	MEN	JJJ	71	2	-	2/7/8/10	-
2	MEN	LLL	71	2	-	2/7/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
2	DDD	71	MEN	OD1-CG	2.56	1.28	1.23
2	HHH	71	MEN	CE2-ND2	2.48	1.50	1.45

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	LLL	71	MEN	OD1-CG-CB	2.57	125.26	121.50

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	BBB	71	MEN	CA-CB-CG-OD1
2	DDD	71	MEN	CA-CB-CG-OD1
2	FFF	71	MEN	CA-CB-CG-OD1
2	JJJ	71	MEN	CA-CB-CG-OD1



Mol	Chain	Res	Type	Atoms
2	HHH	71	MEN	CA-CB-CG-OD1
2	LLL	71	MEN	CA-CB-CG-OD1
2	BBB	71	MEN	CA-CB-CG-ND2
2	DDD	71	MEN	CA-CB-CG-ND2
2	FFF	71	MEN	CA-CB-CG-ND2
2	HHH	71	MEN	CA-CB-CG-ND2
2	JJJ	71	MEN	CA-CB-CG-ND2
2	LLL	71	MEN	CA-CB-CG-ND2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

51 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	Tuno	Chain	Dog	Link	Bo	ond leng	$_{\rm sths}$	B	ond ang	les
	Type	Ullaili	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
3	CYC	EEE	201	1	42,46,46	1.23	1 (2%)	$50,\!67,\!67$	1.37	7 (14%)
3	CYC	CCC	201	1	42,46,46	1.24	1 (2%)	$50,\!67,\!67$	1.37	8 (16%)
3	CYC	III	201	1	42,46,46	1.32	1 (2%)	$50,\!67,\!67$	1.32	9 (18%)
11	GLU	DDD	202	-	8,9,9	0.97	1 (12%)	10,11,11	1.09	0
6	MPD	JJJ	203	-	7,7,7	0.20	0	9,10,10	0.50	0
3	CYC	KKK	201	1	42,46,46	1.12	1 (2%)	$50,\!67,\!67$	1.32	7 (14%)
8	PEG	BBB	205	-	$6,\!6,\!6$	0.19	0	$5,\!5,\!5$	0.24	0
5	LYS	BBB	202[B]	-	$8,\!9,\!9$	0.81	1 (12%)	$9,\!10,\!10$	1.31	2 (22%)
13	ALA	FFF	202	-	$5,\!5,\!5$	1.12	1 (20%)	$6,\!6,\!6$	0.88	0
3	CYC	DDD	201	2	42,46,46	1.13	1 (2%)	50,67,67	0.96	1 (2%)



	m		Ъ	т· 1	Bo	ond leng	ths	В	ond ang	les
NIOI	Type	Chain	Res	Link	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
15	PGE	GGG	203	-	$9,\!9,\!9$	0.26	0	8,8,8	0.24	0
8	PEG	HHH	204	-	$6,\!6,\!6$	0.27	0	$5,\!5,\!5$	0.16	0
14	MRD	GGG	202	-	7,7,7	0.37	0	$9,\!10,\!10$	0.58	0
3	CYC	LLL	201	2	42,46,46	1.34	1 (2%)	$50,\!67,\!67$	1.05	2 (4%)
3	CYC	HHH	201	2	42,46,46	1.22	1 (2%)	50,67,67	1.04	2 (4%)
7	1PE	BBB	204	-	$15,\!15,\!15$	0.76	0	14,14,14	0.77	0
9	EDO	KKK	203	-	3,3,3	0.26	0	2,2,2	0.34	0
16	DSN	JJJ	202	-	$5,\!6,\!6$	1.16	1 (20%)	5,7,7	0.99	0
5	LYS	III	202	-	8,9,9	0.71	0	9,10,10	0.95	0
5	LYS	KKK	202	-	8,9,9	0.76	1 (12%)	9,10,10	1.15	1 (11%)
12	GLY	EEE	202	-	4,4,4	0.98	0	3,4,4	1.53	0
4	PG4	AAA	202	-	12,12,12	0.15	0	11,11,11	0.33	0
8	PEG	CCC	204	-	$6,\!6,\!6$	0.17	0	$5,\!5,\!5$	0.18	0
16	DSN	LLL	202	-	$5,\!6,\!6$	1.07	1 (20%)	5,7,7	1.99	2 (40%)
4	PG4	FFF	204	-	12,12,12	0.14	0	11,11,11	0.16	0
3	CYC	GGG	201	1	42,46,46	1.36	1 (2%)	50,67,67	1.40	8 (16%)
5	LYS	BBB	202[A]	-	8,9,9	0.80	1 (12%)	9,10,10	1.32	2 (22%)
3	CYC	JJJ	201	2	42,46,46	1.44	2 (4%)	50,67,67	1.12	5 (10%)
6	MPD	FFF	203	-	7,7,7	0.23	0	9,10,10	0.38	0
6	MPD	HHH	203	-	7,7,7	0.43	0	$9,\!10,\!10$	0.53	0
3	CYC	AAA	201	1	42,46,46	1.47	1 (2%)	50,67,67	1.35	8 (16%)
8	PEG	JJJ	205	-	6,6,6	0.50	0	$5,\!5,\!5$	0.36	0
4	PG4	JJJ	204	-	12,12,12	0.15	0	11,11,11	0.17	0
9	EDO	CCC	206	-	3,3,3	0.30	0	2,2,2	0.69	0
15	PGE	GGG	204	-	9,9,9	0.18	0	8,8,8	0.19	0
6	MPD	BBB	203	-	7,7,7	0.15	0	$9,\!10,\!10$	0.36	0
3	CYC	BBB	201	2	42,46,46	1.38	2 (4%)	$50,\!67,\!67$	1.12	3 (6%)
6	MPD	DDD	203	-	7,7,7	0.35	0	9,10,10	0.42	0
6	MPD	EEE	203	-	7,7,7	0.18	0	$9,\!10,\!10$	0.48	0
11	GLU	HHH	202	-	$8,\!9,\!9$	1.07	1 (12%)	10, 11, 11	1.26	2 (20%)
4	PG4	CCC	203	-	12,12,12	0.16	0	11,11,11	0.10	0
8	PEG	BBB	208	_	$6,\!6,\!6$	0.29	0	$5,\!5,\!5$	0.29	0
6	MPD	LLL	203	-	7,7,7	0.23	0	9,10,10	0.30	0
8	PEG	BBB	206	-	$6,\!6,\!6$	0.13	0	$5,\!5,\!5$	0.10	0
3	CYC	FFF	201	2	42,46,46	1.51	2(4%)	$50,\!67,\!67$	1.12	3 (6%)
9	EDO	CCC	205	-	3,3,3	0.10	0	$2,\!2,\!2$	0.70	0
9	EDO	KKK	204	_	3,3,3	0.16	0	2,2,2	0.61	0
15	PGE	LLL	204	-	9,9,9	0.16	0	8,8,8	0.13	0
9	EDO	BBB	207	-	$3,\!3,\!3$	0.26	0	2,2,2	0.57	0
10	P6G	CCC	202	-	$18,\!18,\!18$	0.85	1(5%)	$17,\!17,\!17$	0.84	1 (5%)



Mol Type	Type	Chain	Dog	Link	Bond lengths			Bond angles		
	Type		nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
8	PEG	GGG	205	-	$6,\!6,\!6$	0.18	0	$5,\!5,\!5$	0.09	0

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
3	CYC	EEE	201	1	-	8/25/74/74	0/4/4/4
3	CYC	CCC	201	1	-	5/25/74/74	0/4/4/4
3	CYC	III	201	1	-	7/25/74/74	0/4/4/4
11	GLU	DDD	202	-	_	1/9/9/9	-
6	MPD	JJJ	203	-	-	0/5/5/5	-
3	CYC	KKK	201	1	-	6/25/74/74	0/4/4/4
8	PEG	BBB	205	-	-	2/4/4/4	-
5	LYS	BBB	202[B]	-	-	7/9/9/9	-
13	ALA	FFF	202	-	-	3/4/4/4	-
3	CYC	DDD	201	2	-	8/25/74/74	0/4/4/4
15	PGE	GGG	203	-	-	5/7/7/7	-
8	PEG	HHH	204	-	-	3/4/4/4	-
14	MRD	GGG	202	-	-	0/5/5/5	-
3	CYC	LLL	201	2	-	8/25/74/74	0/4/4/4
3	CYC	HHH	201	2	-	8/25/74/74	0/4/4/4
7	1PE	BBB	204	-	-	9/13/13/13	-
9	EDO	KKK	203	-	-	1/1/1/1	-
16	DSN	JJJ	202	-	-	4/6/6/6	-
5	LYS	III	202	-	-	5/9/9/9	-
5	LYS	KKK	202	-	-	2/9/9/9	-
12	GLY	EEE	202	-	-	0/2/2/2	-
4	PG4	AAA	202	-	-	4/10/10/10	-
8	PEG	CCC	204	-	-	3/4/4/4	-
16	DSN	LLL	202	-	-	2/6/6/6	-
4	PG4	FFF	204	-	-	4/10/10/10	-
3	CYC	GGG	201	1	-	5/25/74/74	0/4/4/4
5	LYS	BBB	202[A]	-	-	6/9/9/9	-
3	CYC	JJJ	201	2	-	8/25/74/74	0/4/4/4
6	MPD	FFF	203	_	-	0/5/5/5	-



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MPD	HHH	203	-	-	0/5/5/5	-
3	CYC	AAA	201	1	-	8/25/74/74	0/4/4/4
8	PEG	JJJ	205	-	-	2/4/4/4	-
4	PG4	JJJ	204	-	-	6/10/10/10	-
9	EDO	CCC	206	-	-	1/1/1/1	-
15	PGE	GGG	204	-	-	5/7/7/7	-
6	MPD	BBB	203	-	-	0/5/5/5	-
3	CYC	BBB	201	2	-	8/25/74/74	0/4/4/4
6	MPD	DDD	203	-	-	0/5/5/5	-
6	MPD	EEE	203	-	-	1/5/5/5	-
11	GLU	HHH	202	-	-	5/9/9/9	-
4	PG4	CCC	203	-	-	10/10/10/10	-
8	PEG	BBB	208	-	-	1/4/4/4	-
6	MPD	LLL	203	-	-	0/5/5/5	-
8	PEG	BBB	206	-	-	3/4/4/4	-
3	CYC	\mathbf{FFF}	201	2	-	8/25/74/74	0/4/4/4
9	EDO	CCC	205	-	-	1/1/1/1	-
9	EDO	KKK	204	-	-	0/1/1/1	-
15	PGE	LLL	204	-	-	4/7/7/7	-
9	EDO	BBB	207	-	-	1/1/1/1	-
10	P6G	CCC	202	-	-	11/16/16/16	-
8	PEG	GGG	205	-	-	3/4/4/4	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	FFF	201	CYC	CHA-C1A	8.49	1.42	1.35
3	JJJ	201	CYC	CHA-C1A	8.08	1.41	1.35
3	AAA	201	CYC	CHA-C1A	8.05	1.41	1.35
3	BBB	201	CYC	CHA-C1A	7.55	1.41	1.35
3	GGG	201	CYC	CHA-C1A	7.52	1.41	1.35
3	LLL	201	CYC	CHA-C1A	7.44	1.41	1.35
3	III	201	CYC	CHA-C1A	6.99	1.41	1.35
3	HHH	201	CYC	CHA-C1A	6.76	1.40	1.35
3	EEE	201	CYC	CHA-C1A	6.74	1.40	1.35
3	CCC	201	CYC	CHA-C1A	6.73	1.40	1.35
3	DDD	201	CYC	CHA-C1A	5.89	1.40	1.35
3	KKK	201	CYC	CHA-C1A	5.62	1.39	1.35
10	CCC	202	P6G	O10-C11	3.03	1.55	1.42
3	FFF	201	CYC	O2D-CGD	-2.50	1.22	1.30
						Continued on	next page



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	JJJ	202	DSN	OXT-C	-2.49	1.22	1.30
3	JJJ	201	CYC	O2D-CGD	-2.35	1.22	1.30
5	BBB	202[A]	LYS	OXT-C	-2.23	1.23	1.30
5	BBB	202[B]	LYS	OXT-C	-2.23	1.23	1.30
3	BBB	201	CYC	C1B-C2B	-2.20	1.41	1.45
16	LLL	202	DSN	OXT-C	-2.17	1.23	1.30
13	\mathbf{FFF}	202	ALA	OXT-C	-2.17	1.23	1.30
11	HHH	202	GLU	OXT-C	-2.17	1.23	1.30
11	DDD	202	GLU	OXT-C	-2.10	1.23	1.30
5	KKK	202	LYS	OXT-C	-2.07	1.23	1.30

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
3	CCC	201	CYC	C1B-CHB-C4A	4.10	138.10	128.08
3	EEE	201	CYC	C1B-CHB-C4A	3.93	137.68	128.08
3	III	201	CYC	C1B-CHB-C4A	3.88	137.57	128.08
3	KKK	201	CYC	C1B-CHB-C4A	3.85	137.48	128.08
3	GGG	201	CYC	CMB-C2B-C1B	3.72	128.81	124.17
3	AAA	201	CYC	C1B-CHB-C4A	3.68	137.06	128.08
3	EEE	201	CYC	CMB-C2B-C1B	3.66	128.74	124.17
3	GGG	201	CYC	C1B-CHB-C4A	3.65	137.01	128.08
3	BBB	201	CYC	CMB-C2B-C1B	3.41	128.42	124.17
16	LLL	202	DSN	OXT-C-CA	3.29	124.59	113.38
5	BBB	202[A]	LYS	OXT-C-O	-3.02	117.22	124.09
5	BBB	202[B]	LYS	OXT-C-O	-3.02	117.22	124.09
3	AAA	201	CYC	CHB-C1B-C2B	-2.98	121.04	126.95
3	KKK	201	CYC	CMA-C3A-C4A	2.89	129.52	125.06
3	CCC	201	CYC	CHB-C4A-NA	-2.86	118.95	124.93
3	AAA	201	CYC	CMA-C3A-C4A	2.84	129.43	125.06
3	GGG	201	CYC	CMA-C3A-C4A	2.83	129.42	125.06
3	CCC	201	CYC	CMB-C2B-C1B	2.79	127.65	124.17
3	CCC	201	CYC	CHB-C4A-C3A	2.77	132.02	124.90
3	CCC	201	CYC	C4D-CHA-C1A	2.75	132.09	128.81
5	KKK	202	LYS	OXT-C-O	-2.74	117.87	124.09
3	KKK	201	CYC	CMB-C2B-C1B	2.66	127.49	124.17
16	LLL	202	DSN	OXT-C-O	-2.64	118.11	124.09
11	HHH	202	GLU	OXT-C-O	-2.62	118.14	124.09
3	KKK	201	CYC	CHB-C4A-NA	-2.60	119.50	124.93
3	III	201	CYC	CHB-C4A-C3A	2.59	131.56	124.90
3	HHH	201	CYC	CHA-C1A-NA	-2.59	125.24	128.83
3	AAA	201	CYC	CMB-C2B-C1B	2.58	127.38	124.17



6	YX7	
U	T T T I	

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	GGG	201	CYC	CHA-C1A-NA	-2.52	125.33	128.83
3	FFF	201	CYC	CMB-C2B-C1B	2.52	127.31	124.17
3	AAA	201	CYC	C2C-C3C-C4C	2.48	105.06	101.34
3	AAA	201	CYC	CHA-C1A-NA	-2.47	125.40	128.83
3	JJJ	201	CYC	CHD-C4C-NC	2.46	128.13	125.20
3	FFF	201	CYC	CHA-C1A-NA	-2.45	125.42	128.83
3	LLL	201	CYC	CMB-C2B-C1B	2.44	127.21	124.17
3	JJJ	201	CYC	C2C-C3C-C4C	2.44	104.99	101.34
3	EEE	201	CYC	CHB-C4A-C3A	2.43	131.16	124.90
3	HHH	201	CYC	C4D-CHA-C1A	2.43	131.71	128.81
3	GGG	201	CYC	CHB-C4A-C3A	2.41	131.10	124.90
5	BBB	202[A]	LYS	OXT-C-CA	2.39	121.52	113.38
5	BBB	202[B]	LYS	OXT-C-CA	2.39	121.52	113.38
3	DDD	201	CYC	C4D-CHA-C1A	2.38	131.65	128.81
10	CCC	202	P6G	O10-C9-C8	-2.38	99.68	110.39
3	EEE	201	CYC	CHB-C4A-NA	-2.37	119.98	124.93
3	EEE	201	CYC	CHA-C1A-NA	-2.36	125.55	128.83
3	BBB	201	CYC	CHA-C1A-NA	-2.35	125.57	128.83
3	FFF	201	CYC	CAC-C3C-C4C	2.34	118.69	112.67
3	KKK	201	CYC	CHB-C4A-C3A	2.31	130.85	124.90
3	CCC	201	CYC	C2C-C3C-C4C	2.31	104.80	101.34
3	GGG	201	CYC	CHB-C1B-C2B	-2.30	122.39	126.95
3	III	201	CYC	CMB-C2B-C1B	2.29	127.03	124.17
3	III	201	CYC	CMA-C3A-C4A	2.29	128.58	125.06
3	III	201	CYC	CHB-C4A-NA	-2.28	120.15	124.93
3	KKK	201	CYC	CHB-C1B-C2B	-2.28	122.44	126.95
3	KKK	201	CYC	C2C-C3C-C4C	2.27	104.73	101.34
3	CCC	201	CYC	CHA-C1A-NA	-2.25	125.71	128.83
3	JJJ	201	CYC	CHA-C1A-NA	-2.23	125.73	128.83
3	JJJ	201	CYC	CMB-C2B-C1B	2.22	126.94	124.17
3	GGG	201	CYC	$C2C-\overline{C3C}-C4C$	2.22	104.66	101.34
3	EEE	201	CYC	CMA-C3A-C4A	2.20	128.45	125.06
3	III	201	CYC	CHA-C1A-NA	-2.20	125.78	128.83
3	JJJ	201	CYC	OC-C1C-C2C	-2.18	124.44	126.17
3	EEE	201	CYC	C2C-C3C-C4C	2.17	104.58	101.34
3	CCC	201	CYC	CMA-C3A-C4A	2.16	128.40	125.06
3	BBB	201	CYC	CHD-C4C-NC	2.15	127.76	125.20
3	LLL	201	CYC	CHA-C1A-NA	-2.13	125.87	128.83
3	GGG	201	CYC	CHB-C4A-NA	-2.12	120.49	124.93
3	AAA	201	CYC	CHB-C1B-NB	2.10	130.57	126.06
3	III	201	CYC	CHB-C1B-C2B	-2.08	122.83	126.95
3	AAA	201	CYC	CHB-C4A-NA	-2.06	120.62	124.93



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	III	201	CYC	C4D-CHA-C1A	2.02	131.22	128.81
11	HHH	202	GLU	OXT-C-CA	2.02	120.26	113.38
3	III	201	CYC	O1A-CGA-CBA	-2.01	116.63	123.08

There are no chirality outliers.

All (202) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	AAA	201	CYC	ND-C1D-CHD-C4C
3	AAA	201	CYC	C2D-C1D-CHD-C4C
3	BBB	201	CYC	NA-C4A-CHB-C1B
3	BBB	201	CYC	C3A-C4A-CHB-C1B
3	BBB	201	CYC	ND-C1D-CHD-C4C
3	BBB	201	CYC	C2D-C1D-CHD-C4C
3	CCC	201	CYC	NA-C4A-CHB-C1B
3	CCC	201	CYC	C3A-C4A-CHB-C1B
3	CCC	201	CYC	ND-C1D-CHD-C4C
3	DDD	201	CYC	NA-C4A-CHB-C1B
3	DDD	201	CYC	C3A-C4A-CHB-C1B
3	DDD	201	CYC	ND-C1D-CHD-C4C
3	DDD	201	CYC	C2D-C1D-CHD-C4C
3	EEE	201	CYC	NA-C4A-CHB-C1B
3	EEE	201	CYC	C3A-C4A-CHB-C1B
3	EEE	201	CYC	ND-C1D-CHD-C4C
3	EEE	201	CYC	C2D-C1D-CHD-C4C
3	FFF	201	CYC	NA-C4A-CHB-C1B
3	FFF	201	CYC	C3A-C4A-CHB-C1B
3	FFF	201	CYC	ND-C1D-CHD-C4C
3	FFF	201	CYC	C2D-C1D-CHD-C4C
3	GGG	201	CYC	C3A-C4A-CHB-C1B
3	GGG	201	CYC	ND-C1D-CHD-C4C
3	HHH	201	CYC	NA-C4A-CHB-C1B
3	HHH	201	CYC	C3A-C4A-CHB-C1B
3	HHH	201	CYC	ND-C1D-CHD-C4C
3	HHH	201	CYC	C2D-C1D-CHD-C4C
3	III	201	CYC	C3A-C4A-CHB-C1B
3	III	201	CYC	ND-C1D-CHD-C4C
3	JJJ	201	CYC	NA-C4A-CHB-C1B
3	JJJ	201	CYC	C3A-C4A-CHB-C1B
3	JJJ	201	CYC	ND-C1D-CHD-C4C
3	JJJ	201	CYC	C2D-C1D-CHD-C4C
3	KKK	201	CYC	NA-C4A-CHB-C1B



Mol	Chain	Res	Type	Atoms
3	KKK	201	CYC	C3A-C4A-CHB-C1B
3	KKK	201	CYC	ND-C1D-CHD-C4C
3	KKK	201	CYC	C2D-C1D-CHD-C4C
3	LLL	201	CYC	NA-C4A-CHB-C1B
3	LLL	201	CYC	C3A-C4A-CHB-C1B
3	LLL	201	CYC	ND-C1D-CHD-C4C
3	LLL	201	CYC	C2D-C1D-CHD-C4C
5	BBB	202[A]	LYS	O-C-CA-N
5	BBB	202[B]	LYS	O-C-CA-N
5	III	202	LYS	O-C-CA-N
11	DDD	202	GLU	C-CA-CB-CG
16	JJJ	202	DSN	O-C-CA-N
16	JJJ	202	DSN	N-CA-CB-OG
16	JJJ	202	DSN	C-CA-CB-OG
4	CCC	203	PG4	C8-C7-O4-C6
8	JJJ	205	PEG	C4-C3-O2-C2
15	LLL	204	PGE	C3-C4-O3-C5
7	BBB	204	1PE	C16-C26-OH6-C15
4	AAA	202	PG4	O1-C1-C2-O2
8	HHH	204	PEG	O1-C1-C2-O2
15	GGG	203	PGE	C3-C4-O3-C5
4	CCC	203	PG4	C4-C3-O2-C2
4	FFF	204	PG4	O2-C3-C4-O3
15	GGG	203	PGE	O2-C3-C4-O3
4	FFF	204	PG4	O3-C5-C6-O4
7	BBB	204	1PE	OH4-C13-C23-OH3
15	LLL	204	PGE	O2-C3-C4-O3
16	JJJ	202	DSN	OXT-C-CA-N
4	CCC	203	PG4	O3-C5-C6-O4
15	GGG	203	PGE	C4-C3-O2-C2
10	CCC	202	P6G	C11-C12-O13-C14
8	GGG	205	PEG	O2-C3-C4-O4
10	CCC	202	P6G	O16-C17-C18-O19
3	GGG	201	CYC	NA-C4A-CHB-C1B
4	AAA	202	PG4	C8-C7-O4-C6
5	BBB	$202[\overline{A}]$	LYS	OXT-C-CA-N
5	BBB	202[B]	LYS	OXT-C-CA-N
5	III	202	LYS	OXT-C-CA-N
4	AAA	202	PG4	O4-C7-C8-O5
4	JJJ	204	PG4	O1-C1-C2-O2
8	CCC	204	PEG	O2-C3-C4-O4
8	GGG	205	PEG	O1-C1-C2-O2

Continued from previous page...



Mol	Chain	Res	Type	Atoms
8	JJJ	205	PEG	O1-C1-C2-O2
15	GGG	203	PGE	O3-C5-C6-O4
15	LLL	204	PGE	O3-C5-C6-O4
3	AAA	201	CYC	NA-C4A-CHB-C1B
3	III	201	CYC	NA-C4A-CHB-C1B
3	AAA	201	CYC	C3A-C4A-CHB-C1B
5	BBB	202[A]	LYS	CE-CD-CG-CB
8	BBB	205	PEG	O2-C3-C4-O4
8	BBB	206	PEG	O2-C3-C4-O4
9	BBB	207	EDO	O1-C1-C2-O2
9	CCC	205	EDO	O1-C1-C2-O2
15	LLL	204	PGE	O1-C1-C2-O2
5	III	202	LYS	CA-CB-CG-CD
4	CCC	203	PG4	O1-C1-C2-O2
8	BBB	205	PEG	O1-C1-C2-O2
13	FFF	202	ALA	O-C-CA-CB
13	FFF	202	ALA	OXT-C-CA-CB
4	CCC	203	PG4	O4-C7-C8-O5
4	FFF	204	PG4	O1-C1-C2-O2
8	HHH	204	PEG	O2-C3-C4-O4
15	GGG	204	PGE	O1-C1-C2-O2
4	AAA	202	PG4	O2-C3-C4-O3
4	FFF	204	PG4	O4-C7-C8-O5
4	JJJ	204	PG4	C1-C2-O2-C3
10	CCC	202	P6G	C6-C5-O4-C3
5	BBB	202[B]	LYS	CE-CD-CG-CB
10	CCC	202	P6G	C8-C9-O10-C11
8	HHH	204	PEG	C4-C3-O2-C2
4	JJJ	204	PG4	O2-C3-C4-O3
8	GGG	205	PEG	C1-C2-O2-C3
11	HHH	202	GLU	CA-CB-CG-CD
8	BBB	206	PEG	C1-C2-O2-C3
4	JJJ	204	PG4	O3-C5-C6-O4
15	GGG	204	PGE	C3-C4-O3-C5
5	BBB	202[B]	LYS	OXT-C-CA-CB
11	HHH	202	GLU	OXT-C-CA-CB
10	CCC	202	P6G	O1-C2-C3-O4
7	BBB	204	1PE	C14-C24-OH4-C13
10	CCC	202	P6G	C2-C3-O4-C5
7	BBB	204	1PE	С13-С23-ОН3-С22
10	CCC	202	P6G	C18-C17-O16-C15
15	GGG	204	PGE	C1-C2-O2-C3

Continued from previous page...



Mol	Chain	Res	Type	Atoms
4	CCC	203	PG4	C3-C4-O3-C5
10	CCC	202	P6G	O13-C14-C15-O16
8	CCC	204	PEG	C4-C3-O2-C2
16	LLL	202	DSN	N-CA-CB-OG
5	BBB	202[A]	LYS	O-C-CA-CB
5	BBB	202[A]	LYS	OXT-C-CA-CB
5	BBB	202[B]	LYS	O-C-CA-CB
11	HHH	202	GLU	O-C-CA-CB
7	BBB	204	1PE	OH7-C16-C26-OH6
9	CCC	206	EDO	O1-C1-C2-O2
4	CCC	203	PG4	O2-C3-C4-O3
7	BBB	204	1PE	C25-C15-OH6-C26
3	JJJ	201	CYC	CAA-CBA-CGA-O2A
3	BBB	201	CYC	CAA-CBA-CGA-O1A
3	DDD	201	CYC	CAA-CBA-CGA-O1A
3	HHH	201	CYC	CAA-CBA-CGA-O2A
3	JJJ	201	CYC	CAA-CBA-CGA-O1A
5	KKK	202	LYS	CE-CD-CG-CB
4	CCC	203	PG4	C1-C2-O2-C3
3	FFF	201	CYC	CAD-CBD-CGD-O1D
3	DDD	201	CYC	CAA-CBA-CGA-O2A
3	FFF	201	CYC	CAD-CBD-CGD-O2D
3	HHH	201	CYC	CAD-CBD-CGD-O1D
4	CCC	203	PG4	C5-C6-O4-C7
3	HHH	201	CYC	CAA-CBA-CGA-O1A
3	DDD	201	CYC	CAD-CBD-CGD-O1D
3	LLL	201	CYC	CAA-CBA-CGA-O1A
3	LLL	201	CYC	CAD-CBD-CGD-O1D
3	BBB	201	CYC	CAD-CBD-CGD-O2D
3	FFF	201	CYC	CAA-CBA-CGA-OIA
3	HHH	201	CYC	CAD-CBD-CGD-O2D
7	BBB	204	1PE	C23-C13-OH4-C24
3	BBB	201	CYC	CAD-CBD-CGD-O1D
3	FFF	201	CYC	CAA-CBA-CGA-O2A
3	GGG	201	CYC	CAA-CBA-CGA-OIA
3	JJJ	201	CYC	CAD-CBD-CGD-O1D
3	LLL	201	CYC	CAD-CBD-CGD-O2D
8	BBB	206	PEG	C4-C3-O2-C2
3	BBB	201	CYC	CAA-CBA-CGA-O2A
3	LLL	201	CYC	CAA-CBA-CGA-O2A
3	CCC	201	CYC	CAA-CBA-CGA-O1A
3	GGG	201	CYC	CAA-CBA-CGA-O2A

Continued from previous page...



Mol	Chain	Res	Type	Atoms
3	JJJ	201	CYC	CAD-CBD-CGD-O2D
3	KKK	201	CYC	CAA-CBA-CGA-O1A
3	KKK	201	CYC	CAA-CBA-CGA-O2A
5	III	202	LYS	OXT-C-CA-CB
10	CCC	202	P6G	O7-C8-C9-O10
3	AAA	201	CYC	CAA-CBA-CGA-O1A
5	BBB	202[A]	LYS	CA-CB-CG-CD
3	AAA	201	CYC	CAA-CBA-CGA-O2A
3	DDD	201	CYC	CAD-CBD-CGD-O2D
3	EEE	201	CYC	CAA-CBA-CGA-O2A
3	III	201	CYC	CAA-CBA-CGA-O1A
3	III	201	CYC	CAA-CBA-CGA-O2A
3	CCC	201	CYC	CAA-CBA-CGA-O2A
3	EEE	201	CYC	CAA-CBA-CGA-O1A
11	HHH	202	GLU	OE1-CD-CG-CB
4	JJJ	204	PG4	C5-C6-O4-C7
5	BBB	202[B]	LYS	CA-CB-CG-CD
15	GGG	203	PGE	C1-C2-O2-C3
9	KKK	203	EDO	O1-C1-C2-O2
7	BBB	204	1PE	OH5-C14-C24-OH4
3	III	201	CYC	CAD-CBD-CGD-O1D
11	HHH	202	GLU	OE2-CD-CG-CB
5	III	202	LYS	O-C-CA-CB
4	JJJ	204	PG4	O4-C7-C8-O5
16	LLL	202	DSN	OXT-C-CA-CB
3	EEE	201	CYC	CAD-CBD-CGD-O1D
10	CCC	202	P6G	O10-C11-C12-O13
4	CCC	203	PG4	C6-C5-O3-C4
8	BBB	208	PEG	O2-C3-C4-O4
15	GGG	204	PGE	O3-C5-C6-O4
6	EEE	203	MPD	C2-C3-C4-C5
15	GGG	204	PGE	C6-C5-O3-C4
3	AAA	201	CYC	CAD-CBD-CGD-O2D
10	CCC	202	P6G	O4-C5-C6-O7
8	CCC	204	PEG	C1-C2-O2-C3
13	\mathbf{FFF}	202	ALA	OXT-C-CA-N
3	III	201	CYC	CAD-CBD-CGD-O2D
5	BBB	202[B]	LYS	CG-CD-CE-NZ
5	KKK	202	LYS	CG-CD-CE-NZ
3	AAA	201	CYC	CAD-CBD-CGD-O1D
3	EEE	201	CYC	CAD-CBD-CGD-O2D
7	BBB	204	1PE	OH6-C15-C25-OH5

Continued from previous page...



There are no ring outliers.

35 monomers are involved in 149 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	EEE	201	CYC	3	0
3	CCC	201	CYC	3	0
3	III	201	CYC	3	0
11	DDD	202	GLU	2	0
3	KKK	201	CYC	3	0
8	BBB	205	PEG	5	0
13	FFF	202	ALA	2	0
3	DDD	201	CYC	2	0
15	GGG	203	PGE	18	0
8	HHH	204	PEG	4	0
3	LLL	201	CYC	3	0
3	HHH	201	CYC	3	0
7	BBB	204	1PE	8	0
9	KKK	203	EDO	4	0
16	JJJ	202	DSN	1	0
5	KKK	202	LYS	1	0
12	EEE	202	GLY	3	0
4	AAA	202	PG4	11	0
8	CCC	204	PEG	4	0
3	GGG	201	CYC	3	0
3	JJJ	201	CYC	2	0
6	HHH	203	MPD	1	0
3	AAA	201	CYC	4	0
8	JJJ	205	PEG	4	0
4	JJJ	204	PG4	2	0
3	BBB	201	CYC	3	0
6	EEE	203	MPD	5	0
4	CCC	203	PG4	15	0
8	BBB	208	PEG	22	0
8	BBB	206	PEG	1	0
3	FFF	201	CYC	2	0
9	KKK	204	EDO	6	0
15	LLL	204	PGE	2	0
9	BBB	207	EDO	1	0
10	CCC	202	P6G	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.



Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



























5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ $>$	#RSRZ>2	$OWAB(Å^2)$	Q < 0.9
1	AAA	160/160~(100%)	-0.55	1 (0%) 89 88	19,31,55,71	0
1	CCC	160/160~(100%)	-0.60	0 100 100	14, 23, 36, 50	0
1	EEE	160/160~(100%)	-0.60	1 (0%) 89 88	14, 23, 36, 57	0
1	GGG	160/160~(100%)	-0.53	0 100 100	15, 22, 39, 48	0
1	III	160/160~(100%)	-0.55	0 100 100	15, 25, 38, 60	0
1	KKK	160/160~(100%)	-0.45	1 (0%) 89 88	16, 29, 44, 65	0
2	BBB	160/161~(99%)	-0.64	1 (0%) 89 88	14, 23, 39, 69	0
2	DDD	160/161~(99%)	-0.68	0 100 100	15, 21, 35, 62	0
2	\mathbf{FFF}	160/161~(99%)	-0.66	0 100 100	17, 22, 35, 58	0
2	HHH	160/161 (99%)	-0.66	0 100 100	16, 21, 37, 60	0
2	JJJ	160/161~(99%)	-0.62	1 (0%) 89 88	14, 21, 35, 56	0
2	LLL	160/161 (99%)	-0.63	0 100 100	15, 22, 35, 65	0
All	All	1920/1926 (99%)	-0.60	5 (0%) 94 93	14, 23, 40, 71	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	160	GLN	2.5
1	KKK	160	GLN	2.4
1	EEE	160	GLN	2.2
2	BBB	161	SER	2.1
2	JJJ	161	SER	2.1

6.2 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,



Mol	Type	Chain	\mathbf{Res}	Atoms	RSCC	\mathbf{RSR}	$B-factors(A^2)$	$Q{<}0.9$
2	MEN	LLL	71	9/10	0.96	0.06	$16,\!18,\!21,\!22$	0
2	MEN	DDD	71	9/10	0.97	0.05	20,21,26,28	0
2	MEN	HHH	71	9/10	0.97	0.06	21,24,30,30	0
2	MEN	BBB	71	9/10	0.97	0.06	15,17,20,22	0
2	MEN	JJJ	71	9/10	0.98	0.05	13,14,17,20	0
2	MEN	\mathbf{FFF}	71	9/10	0.99	0.05	14,15,18,18	0

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.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
12	GLY	EEE	202	5/5	0.20	0.24	30,31,33,34	5
8	PEG	BBB	206	7/7	0.55	0.23	35,36,37,38	7
11	GLU	HHH	202	10/10	0.61	0.23	37,43,47,47	10
8	PEG	BBB	205	7/7	0.62	0.26	28,34,38,39	7
15	PGE	LLL	204	10/10	0.62	0.49	32,38,40,42	10
15	PGE	GGG	204	10/10	0.63	0.27	35,38,43,43	10
6	MPD	EEE	203	8/8	0.63	0.26	28,30,31,32	8
11	GLU	DDD	202	10/10	0.66	0.25	35,38,40,41	10
10	P6G	CCC	202	19/19	0.67	0.43	33,37,39,41	19
5	LYS	III	202	10/10	0.69	0.19	35,37,40,43	10
4	PG4	CCC	203	13/13	0.72	0.88	30,32,34,34	13
14	MRD	GGG	202	8/8	0.73	0.17	28,29,32,36	8
4	PG4	\mathbf{FFF}	204	13/13	0.74	0.86	20,27,33,37	13
8	PEG	BBB	208	7/7	0.76	0.36	32,33,35,37	7
8	PEG	JJJ	205	7/7	0.77	0.19	24,25,30,32	7
8	PEG	GGG	205	7/7	0.77	0.17	30,32,37,38	7
4	PG4	JJJ	204	13/13	0.80	0.19	28,34,41,43	13
7	1PE	BBB	204	16/16	0.80	0.17	$2\overline{5,38,43,44}$	16
15	PGE	GGG	203	10/10	0.81	0.20	$2\overline{4,31,34,36}$	10
16	DSN	JJJ	202	7/7	0.82	0.20	34,37,39,40	7



6	YX7	

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B -factors($Å^2$)	Q<0.9
4	PG4	AAA	202	13/13	0.84	0.22	25,29,34,36	13
8	PEG	HHH	204	7/7	0.85	0.19	25,29,32,34	7
9	EDO	CCC	205	4/4	0.86	0.18	29,29,30,31	4
5	LYS	KKK	202	10/10	0.87	0.20	21,33,40,43	10
6	MPD	BBB	203	8/8	0.88	0.28	24,27,32,33	8
5	LYS	BBB	202[A]	10/10	0.88	0.27	26,36,39,39	10
13	ALA	\mathbf{FFF}	202	6/6	0.88	0.24	37,37,40,43	6
5	LYS	BBB	202[B]	10/10	0.88	0.27	25,36,39,39	10
8	PEG	CCC	204	7/7	0.89	0.32	28,34,37,38	7
16	DSN	LLL	202	7/7	0.89	0.22	33,36,37,38	7
6	MPD	DDD	203	8/8	0.90	0.12	26,29,34,37	8
9	EDO	KKK	204	4/4	0.91	0.14	27,27,27,28	4
9	EDO	BBB	207	4/4	0.92	0.10	28,32,33,33	4
6	MPD	HHH	203	8/8	0.93	0.14	26,29,35,36	8
6	MPD	LLL	203	8/8	0.93	0.31	23,26,32,33	8
9	EDO	CCC	206	4/4	0.93	0.22	24,26,27,27	4
9	EDO	KKK	203	4/4	0.93	0.12	28,29,31,33	4
6	MPD	JJJ	203	8/8	0.94	0.08	23,26,29,34	0
6	MPD	\mathbf{FFF}	203	8/8	0.96	0.07	26,29,31,36	8
3	CYC	LLL	201	43/43	0.96	0.06	14,18,31,40	0
3	CYC	EEE	201	43/43	0.96	0.06	14,16,22,28	0
3	CYC	\mathbf{FFF}	201	43/43	0.96	0.06	14,21,35,39	0
3	CYC	HHH	201	43/43	0.96	0.06	20,25,36,43	0
3	CYC	III	201	43/43	0.96	0.06	14,17,23,28	0
3	CYC	JJJ	201	43/43	0.96	0.06	14,22,36,40	0
3	CYC	AAA	201	43/43	0.97	0.06	17,19,26,31	0
3	CYC	KKK	201	43/43	0.97	0.06	14,18,26,29	0
3	CYC	BBB	201	43/43	0.97	0.06	14,19,34,43	0
3	CYC	GGG	201	43/43	0.97	0.06	13,15,21,25	0
3	CYC	CCC	201	43/43	0.97	0.06	13,15,22,25	0
3	CYC	DDD	201	43/43	0.97	0.06	17,22,33,37	0

Continued from previous page...

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.

