

Full wwPDB X-ray Structure Validation Report (i)

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PDB ID	:	9EWA
Title	:	The sTeLIC pentameric Ligand-Gated Ion Channel (wild-type) in complex
		with 4-Bromophenethylamine
Authors	:	Fourati, Z.; Delarue, M.
Deposited on	:	2024-04-03
Resolution	:	3.01 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 as 541 be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7(2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.5

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.01 Å.

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



Motrie	Whole archive	Similar resolution		
	$(\# { m Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$		
R _{free}	164625	2511 (3.00-3.00)		
Clashscore	180529	2866 (3.00-3.00)		
Ramachandran outliers	177936	2778 (3.00-3.00)		
Sidechain outliers	177891	2781 (3.00-3.00)		
RSRZ outliers	164620	2523 (3.00-3.00)		

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	320	64%	31% ••					
1	BBB	320	65%	30% ••					
1	CCC	320	% 66%	30% ••					
1	DDD	320	% 67%	27% ••					
1	EEE	320	2% 57%	33% 7% •					



9 EWA

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 13062 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

Mol	Chain	Residues		Atoms					AltConf	Trace
1	A A A	210	Total	С	Ν	0	\mathbf{S}	0	1	0
1	ААА	310	2574	1696	424	449	5	0	1	0
1	BBB	310	Total	С	Ν	0	S	0	0	0
1		510	2566	1690	423	448	5	0	0	0
1	CCC	310	Total	С	Ν	Ο	\mathbf{S}	0	0	0
1			2566	1690	423	448	5	0	0	
1	מממ	310	Total	С	Ν	0	S	0	0	0
1		510	2566	1690	423	448	5	0	0	0
1	1 EEE	E 312	Total	С	Ν	0	S	0	0	0
			2576	1696	425	450	5	0	U	U

• Molecule 1 is a protein called Cys-loop ligand-gated ion channel.

• Molecule 2 is nonyl beta-D-glucopyranoside (three-letter code: BNG) (formula: $C_{15}H_{30}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	AAA	1	Total 21	C 15	O 6	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	BBB	1	Total C O 21 15 6	0	0
2	BBB	1	Total C O 21 15 6	0	0
2	DDD	1	Total C O 21 15 6	0	0
2	DDD	1	Total C O 21 15 6	0	0

• Molecule 3 is 2-(4-bromophenyl)ethanamine (three-letter code: VMT) (formula: $C_8H_{10}BrN$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
3	ΛΛΛ	1	Total	Br	С	Ν	0	0	
0	ллл	1	10	1	8	1	0	0	
3	BBB	1	Total	Br	С	Ν	0	0	
0	DDD	1	10	1	8	1	0	0	
2	CCC	1	Total	Br	С	Ν	0	0	
0		1	10	1	8	1	0	0	
2	מממ	1	Total	Br	С	Ν	0	0	
0	עעע	1	10	1	8	1	0	0	
3	FFF	1	Total	Br	С	Ν	0	0	
5	עניי	1	10	1	8	1		0	

• Molecule 4 is water.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	AAA	13	Total O 13 13	0	0
4	BBB	12	Total O 12 12	0	0
4	CCC	12	Total O 12 12	0	0
4	DDD	18	Total O 18 18	0	0
4	EEE	4	Total O 4 4	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: Cys-loop ligand-gated ion channel









4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants	143.21Å 112.34Å 210.80Å	Depositor
a, b, c, α , β , γ	90.00° 106.18° 90.00°	Depositor
Bosolution(A)	25.00 - 3.01	Depositor
Resolution (A)	25.00 - 3.01	EDS
% Data completeness	98.9 (25.00-3.01)	Depositor
(in resolution range)	98.9 (25.00-3.01)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.72 (at 2.99 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
D D.	0.241 , 0.281	Depositor
$\mathbf{n}, \mathbf{n}_{free}$	0.274 , 0.309	DCC
R_{free} test set	3202 reflections $(5.01%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	82.4	Xtriage
Anisotropy	0.385	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.27, 70.0	EDS
L-test for twinning ²	$ < L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	13062	wwPDB-VP
Average B, all atoms $(Å^2)$	105.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 6.00% of the height of the origin peak. No significant pseudotranslation is detected.

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: VMT, BNG

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

Mal	Chain	Bond	lengths	Bond angles	
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5
1	AAA	0.63	0/2647	0.79	0/3594
1	BBB	0.62	0/2639	0.79	0/3583
1	CCC	0.63	0/2639	0.80	0/3583
1	DDD	0.63	0/2639	0.78	0/3583
1	EEE	0.67	0/2649	0.84	0/3597
All	All	0.63	0/13213	0.80	0/17940

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AAA	2574	0	2549	116	2
1	BBB	2566	0	2539	85	0
1	CCC	2566	0	2539	77	0
1	DDD	2566	0	2539	100	0
1	EEE	2576	0	2549	132	0
2	AAA	21	0	30	2	0
2	BBB	42	0	60	11	0
2	DDD	42	0	60	8	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	AAA	10	0	0	0	0
3	BBB	10	0	0	0	0
3	CCC	10	0	0	1	0
3	DDD	10	0	0	2	0
3	EEE	10	0	0	0	0
4	AAA	13	0	0	2	0
4	BBB	12	0	0	2	0
4	CCC	12	0	0	2	2
4	DDD	18	0	0	1	0
4	EEE	4	0	0	1	0
All	All	13062	0	12865	448	2

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 17.

All (448) 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:AAA:310:THR:O	1:AAA:314:LEU:CD1	1.79	1.30
1:AAA:45:LEU:CD2	1:AAA:73:ILE:HD13	1.75	1.16
1:AAA:310:THR:O	1:AAA:314:LEU:HD12	1.52	1.09
1:BBB:146:GLU:HG3	1:BBB:171:LEU:HD11	1.27	1.08
1:EEE:254:THR:O	1:EEE:257:ASP:OD2	1.68	1.07
1:CCC:57:ARG:NE	1:DDD:72:GLN:NE2	2.03	1.06
1:DDD:146:GLU:HG3	1:DDD:171:LEU:HD11	1.38	1.06
1:CCC:49:HIS:HD2	1:CCC:98:GLU:OE1	1.38	1.06
1:EEE:124:PHE:CE1	1:EEE:195:LEU:CD1	2.39	1.05
1:EEE:7:GLU:HG2	1:EEE:8:PRO:HD3	1.10	1.04
1:DDD:63:THR:HG21	1:EEE:69:GLU:OE1	1.56	1.03
1:CCC:300:TYR:HB3	1:CCC:301:PRO:HD3	1.41	1.01
1:EEE:124:PHE:CD1	1:EEE:195:LEU:HD11	1.95	1.01
1:AAA:45:LEU:HD21	1:AAA:73:ILE:HD13	1.43	1.00
1:DDD:125:ASP:OD1	1:DDD:193:ARG:NH1	1.94	1.00
1:EEE:7:GLU:CG	1:EEE:8:PRO:HD3	1.93	0.98
1:DDD:90:GLN:CD	1:EEE:83:GLN:OE1	2.03	0.97
1:BBB:99:ASP:OD1	1:BBB:101:THR:OG1	1.81	0.97
1:DDD:47:PHE:CD1	1:DDD:57:ARG:CZ	2.49	0.96
1:DDD:99:ASP:OD1	1:DDD:101:THR:OG1	1.82	0.96
1:BBB:138:PRO:HG3	1:BBB:178:THR:HG21	1.48	0.94
1:AAA:99:ASP:OD1	1:AAA:101:THR:OG1	1.86	0.94
1:BBB:300:TYR:HB3	1:BBB:301:PRO:HD3	1.47	0.93



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:CCC:138:PRO:HG3	1:CCC:178:THR:HG21	1.51	0.92
1:DDD:47:PHE:CE2	1:DDD:98:GLU:HA	2.04	0.92
1:AAA:310:THR:O	1:AAA:314:LEU:HD13	1.68	0.92
1:DDD:91:ASN:OD1	1:EEE:79:THR:OG1	1.87	0.91
1:EEE:13:ILE:HD11	1:EEE:144:PHE:CD1	2.05	0.91
1:EEE:138:PRO:HG3	1:EEE:178:THR:HG21	1.50	0.91
1:EEE:7:GLU:HG2	1:EEE:8:PRO:CD	2.00	0.91
1:BBB:240:ASN:HA	1:BBB:260:LEU:CD1	2.02	0.90
1:AAA:138:PRO:HG3	1:AAA:178:THR:HG21	1.54	0.90
1:DDD:138:PRO:HG3	1:DDD:178:THR:HG21	1.52	0.89
1:AAA:45:LEU:CD2	1:AAA:73:ILE:CD1	2.51	0.89
1:EEE:124:PHE:CD1	1:EEE:195:LEU:CD1	2.56	0.88
1:AAA:113:GLN:CD	1:EEE:19:GLN:OE1	2.12	0.87
1:CCC:49:HIS:CD2	1:CCC:98:GLU:OE1	2.27	0.87
1:DDD:90:GLN:CG	1:EEE:83:GLN:OE1	2.22	0.87
1:EEE:13:ILE:HD11	1:EEE:144:PHE:CG	2.09	0.87
1:DDD:146:GLU:CG	1:DDD:171:LEU:HD11	2.06	0.85
1:AAA:69:GLU:OE2	1:EEE:63:THR:OG1	1.93	0.85
1:DDD:47:PHE:HD1	1:DDD:57:ARG:CZ	1.87	0.85
1:DDD:300:TYR:HB3	1:DDD:301:PRO:HD3	1.57	0.85
1:AAA:45:LEU:HD23	1:AAA:73:ILE:HD13	1.58	0.85
1:BBB:214:TRP:HB2	1:BBB:300:TYR:CE2	2.12	0.84
1:AAA:125:ASP:OD1	1:AAA:193:ARG:NH1	2.09	0.84
1:CCC:214:TRP:HB2	1:CCC:300:TYR:CE2	2.13	0.84
1:EEE:124:PHE:CE1	1:EEE:195:LEU:HD13	2.11	0.83
1:AAA:69:GLU:OE1	1:EEE:63:THR:HG21	1.77	0.83
1:EEE:214:TRP:HB2	1:EEE:300:TYR:CE2	2.14	0.83
1:DDD:146:GLU:HG3	1:DDD:171:LEU:CD1	2.08	0.83
1:EEE:291:LYS:O	1:EEE:294:ILE:HG22	1.80	0.82
1:AAA:119:PHE:CD2	1:AAA:250:LEU:HD11	2.14	0.81
1:DDD:291:LYS:O	1:DDD:294:ILE:HG22	1.79	0.81
1:AAA:74:ARG:HG3	1:EEE:58:THR:HG21	1.64	0.80
1:BBB:125:ASP:CG	1:BBB:193:ARG:HH11	1.83	0.79
1:EEE:168:ASN:ND2	1:EEE:188:GLU:HB2	1.97	0.78
1:DDD:240:ASN:HA	1:DDD:260:LEU:CD1	2.13	0.78
1:AAA:45:LEU:HD21	1:AAA:73:ILE:CD1	2.12	0.78
1:EEE:240:ASN:HA	1:EEE:260:LEU:CD1	2.13	0.78
1:AAA:298:THR:HG22	4:AAA:512:HOH:O	1.83	0.78
1:CCC:57:ARG:HE	1:DDD:72:GLN:NE2	1.82	0.77
1:CCC:57:ARG:CZ	1:DDD:72:GLN:HE22	1.97	0.77
1:CCC:309:LEU:O	1:CCC:313:LEU:HG	1.84	0.77



Atom-1	Atom-2	Interatomic	Clash
	Atom-2	distance (Å)	overlap (Å)
1:EEE:124:PHE:HD1	1:EEE:195:LEU:HD11	1.47	0.76
1:EEE:146:GLU:HG3	1:EEE:171:LEU:HD11	1.68	0.75
1:DDD:125:ASP:CG	1:DDD:193:ARG:HH11	1.88	0.75
1:AAA:125:ASP:CG	1:AAA:193:ARG:HH11	1.89	0.75
1:EEE:55:LYS:HG3	1:EEE:98:GLU:HG3	1.68	0.74
1:BBB:295:TYR:HE1	4:BBB:504:HOH:O	1.71	0.74
1:CCC:57:ARG:CZ	1:DDD:72:GLN:NE2	2.51	0.74
1:CCC:57:ARG:NE	1:DDD:72:GLN:HE22	1.85	0.74
1:EEE:124:PHE:HE1	1:EEE:195:LEU:CD1	2.00	0.74
1:EEE:17:ILE:HD12	1:EEE:187:LEU:HD21	1.68	0.73
1:DDD:58:THR:HG21	1:EEE:74:ARG:HG3	1.71	0.73
1:CCC:170:HIS:HD2	1:CCC:186:VAL:HB	1.53	0.73
1:EEE:138:PRO:HG3	1:EEE:178:THR:CG2	2.21	0.71
1:EEE:146:GLU:CG	1:EEE:171:LEU:HD11	2.20	0.71
1:DDD:125:ASP:CG	1:DDD:193:ARG:NH1	2.42	0.71
1:DDD:19:GLN:OE1	1:EEE:113:GLN:HB2	1.92	0.69
1:DDD:47:PHE:CE1	1:DDD:57:ARG:NE	2.61	0.69
1:CCC:293:ASP:O	1:CCC:297:ILE:HD12	1.93	0.69
1:CCC:300:TYR:CB	1:CCC:301:PRO:HD3	2.22	0.68
1:CCC:170:HIS:CD2	1:CCC:186:VAL:HB	2.28	0.68
1:DDD:90:GLN:HG2	1:EEE:83:GLN:OE1	1.91	0.68
1:AAA:240:ASN:HA	1:AAA:260:LEU:CD1	2.23	0.68
1:DDD:63:THR:CG2	1:EEE:69:GLU:OE1	2.39	0.67
1:AAA:248:PRO:CG	1:AAA:250:LEU:HD21	2.24	0.67
1:DDD:294:ILE:HD12	1:DDD:294:ILE:O	1.95	0.67
1:CCC:240:ASN:HA	1:CCC:260:LEU:CD1	2.25	0.67
1:BBB:138:PRO:HG3	1:BBB:178:THR:CG2	2.24	0.66
1:EEE:37:ARG:NH2	1:EEE:147:MET:CE	2.59	0.66
1:EEE:168:ASN:HD22	1:EEE:188:GLU:HB2	1.60	0.66
1:CCC:138:PRO:HG3	1:CCC:178:THR:CG2	2.25	0.66
1:EEE:294:ILE:HD12	1:EEE:294:ILE:O	1.96	0.66
1:AAA:124:PHE:CE1	1:AAA:195:LEU:HD13	2.30	0.66
1:AAA:272:LEU:HD12	1:AAA:272:LEU:O	1.94	0.66
1:AAA:58:THR:HG21	1:BBB:74:ARG:HG3	1.76	0.66
1:BBB:294:ILE:O	1:BBB:294:ILE:HD12	1.95	0.65
1:EEE:171:LEU:HD12	1:EEE:171:LEU:N	2.11	0.65
1:AAA:113:GLN:NE2	1:EEE:19:GLN:OE1	2.30	0.65
1:DDD:47:PHE:HE2	1:DDD:98:GLU:HA	1.58	0.65
1:AAA:138:PRO:HG3	1:AAA:178:THR:CG2	2.26	0.64
1:BBB:300:TYR:CB	1:BBB:301:PRO:HD3	2.26	0.64
1:DDD:138:PRO:HG3	1:DDD:178:THR:CG2	2.26	0.64



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:EEE:16:LYS:HA	1:EEE:152:GLY:O	1.97	0.64
1:EEE:68:LEU:HD22	1:EEE:73:ILE:HB	1.79	0.64
1:AAA:248:PRO:HB2	1:AAA:250:LEU:CD2	2.28	0.64
1:CCC:57:ARG:NH2	1:DDD:72:GLN:HE22	1.96	0.64
1:AAA:119:PHE:CD2	1:AAA:250:LEU:CD1	2.81	0.63
1:AAA:214:TRP:HB2	1:AAA:300:TYR:CE2	2.33	0.63
1:AAA:248:PRO:HB2	1:AAA:250:LEU:HD23	1.79	0.63
1:EEE:7:GLU:CG	1:EEE:8:PRO:CD	2.67	0.63
1:EEE:214:TRP:HB2	1:EEE:300:TYR:HE2	1.61	0.63
1:EEE:298:THR:O	1:EEE:301:PRO:HD2	1.97	0.63
1:AAA:266:ILE:HG21	1:AAA:304:TYR:CE2	2.33	0.63
1:CCC:208:LEU:HD21	1:DDD:264:PHE:HB3	1.80	0.63
1:AAA:251:GLY:HA3	1:EEE:194:HIS:ND1	2.14	0.63
1:EEE:124:PHE:HE1	1:EEE:195:LEU:HD12	1.64	0.63
1:AAA:81:HIS:HA	1:EEE:107:ARG:NH2	2.13	0.62
1:BBB:230:GLY:HA3	2:BBB:401:BNG:H5'2	1.81	0.62
1:DDD:47:PHE:HD1	1:DDD:57:ARG:NH2	1.96	0.62
1:AAA:63:THR:HG21	1:BBB:69:GLU:OE1	2.00	0.62
1:EEE:254:THR:HB	1:EEE:257:ASP:H	1.65	0.62
1:CCC:57:ARG:NE	1:DDD:72:GLN:HE21	1.97	0.62
1:AAA:119:PHE:HD2	1:AAA:250:LEU:CD1	2.11	0.61
1:AAA:82:ASN:ND2	1:AAA:130:PHE:O	2.34	0.61
1:BBB:214:TRP:CD1	1:BBB:300:TYR:CD2	2.89	0.61
1:CCC:272:LEU:O	1:CCC:272:LEU:HD12	1.99	0.61
1:EEE:240:ASN:HA	1:EEE:260:LEU:HD12	1.81	0.60
1:CCC:218:PHE:O	1:DDD:279:ARG:NH1	2.35	0.60
1:DDD:240:ASN:HA	1:DDD:260:LEU:HD13	1.83	0.60
1:AAA:300:TYR:HB3	1:AAA:301:PRO:HD3	1.83	0.60
1:DDD:82:ASN:ND2	1:DDD:130:PHE:O	2.34	0.60
1:EEE:135:SER:HB3	1:EEE:144:PHE:CZ	2.36	0.60
1:CCC:82:ASN:ND2	1:CCC:130:PHE:O	2.33	0.60
1:AAA:291:LYS:O	1:AAA:294:ILE:HG22	2.02	0.60
1:AAA:271:VAL:HG11	1:EEE:212:VAL:HG13	1.83	0.60
1:BBB:295:TYR:CE1	4:BBB:504:HOH:O	2.50	0.60
1:DDD:17:ILE:HD12	1:DDD:153:LEU:HD11	1.84	0.60
1:AAA:314:LEU:HD12	1:AAA:314:LEU:H	1.65	0.59
1:CCC:63:THR:HG21	1:DDD:69:GLU:OE1	2.01	0.59
1:CCC:228:LEU:HD11	2:DDD:401:BNG:H6'1	1.84	0.59
1:BBB:171:LEU:HD12	1:BBB:171:LEU:N	2.17	0.59
1:EEE:37:ARG:HB3	1:EEE:37:ARG:CZ	2.31	0.59
1:AAA:81:HIS:HA	1:EEE:107:ARG:HH22	1.66	0.59



A + a 1		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:BBB:63:THR:HG21	1:CCC:69:GLU:OE1	2.03	0.59
1:BBB:82:ASN:ND2	1:BBB:130:PHE:O	2.35	0.59
1:AAA:113:GLN:HB2	1:EEE:19:GLN:OE1	2.02	0.59
1:CCC:214:TRP:CD1	1:CCC:300:TYR:CD2	2.91	0.58
1:AAA:144:PHE:O	1:AAA:171:LEU:CD1	2.52	0.58
1:DDD:125:ASP:OD2	1:DDD:193:ARG:NH1	2.36	0.58
1:DDD:214:TRP:HB2	1:DDD:300:TYR:CE2	2.38	0.58
1:AAA:124:PHE:HD1	1:AAA:195:LEU:HD11	1.69	0.58
1:BBB:125:ASP:OD2	1:BBB:193:ARG:NH1	2.36	0.58
1:EEE:67:LEU:HD12	1:EEE:67:LEU:O	2.02	0.58
1:AAA:250:LEU:HD23	1:AAA:250:LEU:N	2.19	0.58
1:EEE:83:GLN:HE21	1:EEE:87:MET:HB2	1.68	0.57
1:BBB:228:LEU:HD11	2:BBB:402:BNG:H6'1	1.85	0.57
1:CCC:64:PHE:CE2	1:CCC:68:LEU:HD11	2.40	0.57
1:EEE:135:SER:CB	1:EEE:144:PHE:CZ	2.87	0.57
1:AAA:64:PHE:CE2	1:AAA:68:LEU:HD11	2.39	0.57
2:BBB:402:BNG:H1'1	2:BBB:402:BNG:H9'3	1.87	0.57
1:EEE:7:GLU:CB	1:EEE:8:PRO:CD	2.83	0.57
2:BBB:402:BNG:H1'2	1:CCC:230:GLY:HA3	1.86	0.57
1:BBB:266:ILE:HG21	1:BBB:304:TYR:CE2	2.40	0.57
1:BBB:254:THR:HB	1:BBB:257:ASP:H	1.70	0.57
1:EEE:37:ARG:NH2	1:EEE:147:MET:HE3	2.20	0.56
1:DDD:64:PHE:CE2	1:DDD:68:LEU:HD11	2.39	0.56
1:AAA:228:LEU:HD11	2:BBB:401:BNG:H6'1	1.87	0.56
1:AAA:240:ASN:HA	1:AAA:260:LEU:HD13	1.87	0.56
1:AAA:254:THR:HB	1:AAA:257:ASP:H	1.69	0.56
1:CCC:266:ILE:HG21	1:CCC:304:TYR:CZ	2.41	0.56
1:AAA:125:ASP:CG	1:AAA:193:ARG:NH1	2.55	0.56
1:BBB:64:PHE:CE2	1:BBB:68:LEU:HD11	2.40	0.56
1:BBB:240:ASN:HA	1:BBB:260:LEU:HD12	1.82	0.56
1:BBB:261:VAL:O	1:BBB:264:PHE:HB2	2.05	0.56
1:BBB:293:ASP:OD1	1:BBB:297:ILE:HD11	2.06	0.56
1:AAA:314:LEU:HD12	1:AAA:314:LEU:N	2.21	0.56
1:DDD:146:GLU:CG	1:DDD:171:LEU:CD1	2.77	0.56
1:AAA:248:PRO:HG2	1:AAA:250:LEU:HD21	1.88	0.56
1:DDD:254:THR:HB	1:DDD:257:ASP:H	1.71	0.56
1:DDD:266:ILE:HG21	1:DDD:304:TYR:CZ	2.41	0.55
1:AAA:208:LEU:HD21	1:BBB:264:PHE:HB3	1.88	0.55
1:CCC:254:THR:HB	1:CCC:257:ASP:H	1.71	0.55
1:EEE:42:GLN:OE1	1:EEE:43:PRO:HD2	2.05	0.55
1:AAA:266:ILE:HG21	1:AAA:304:TYR:CZ	2.41	0.55



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:DDD:402:BNG:H5'2	1:EEE:230:GLY:HA3	1.89	0.55
1:EEE:37:ARG:HH21	1:EEE:147:MET:CE	2.19	0.55
1:BBB:266:ILE:HG21	1:BBB:304:TYR:CZ	2.41	0.55
1:CCC:17:ILE:HD12	1:CCC:153:LEU:HD11	1.89	0.55
1:CCC:240:ASN:HA	1:CCC:260:LEU:HD13	1.89	0.55
1:DDD:144:PHE:O	1:DDD:171:LEU:CD2	2.55	0.55
1:DDD:146:GLU:O	1:DDD:148:GLN:NE2	2.40	0.55
1:CCC:61:LEU:HD11	3:CCC:401:VMT:C05	2.38	0.54
1:EEE:261:VAL:O	1:EEE:264:PHE:HB2	2.07	0.54
1:EEE:64:PHE:CG	1:EEE:94:ILE:HD12	2.42	0.54
1:DDD:47:PHE:CD1	1:DDD:57:ARG:NE	2.75	0.54
1:EEE:266:ILE:HG21	1:EEE:304:TYR:CZ	2.43	0.54
1:CCC:44:LEU:N	1:CCC:44:LEU:HD23	2.22	0.54
1:DDD:47:PHE:CD2	1:DDD:98:GLU:HA	2.43	0.54
1:EEE:19:GLN:HA	1:EEE:157:LEU:HA	1.90	0.54
1:AAA:68:LEU:HD13	1:AAA:75:TRP:HB3	1.90	0.54
1:AAA:125:ASP:OD2	1:AAA:193:ARG:NH1	2.41	0.54
1:AAA:218:PHE:O	1:BBB:279:ARG:NH1	2.42	0.53
1:AAA:248:PRO:HD2	1:AAA:250:LEU:HD21	1.91	0.53
1:AAA:113:GLN:HE22	1:EEE:19:GLN:HB2	1.74	0.53
1:DDD:47:PHE:CD2	1:DDD:47:PHE:N	2.77	0.53
1:EEE:300:TYR:HB3	1:EEE:301:PRO:HD3	1.89	0.53
1:AAA:248:PRO:CD	1:AAA:250:LEU:HD21	2.39	0.53
1:AAA:230:GLY:HA3	2:AAA:401:BNG:H5'2	1.91	0.53
1:AAA:201:ARG:HA	1:BBB:240:ASN:HD21	1.73	0.53
1:DDD:47:PHE:N	1:DDD:47:PHE:HD2	2.06	0.53
1:DDD:173:THR:HA	1:DDD:182:ALA:O	2.09	0.53
1:AAA:113:GLN:NE2	1:EEE:19:GLN:HB2	2.24	0.53
1:AAA:124:PHE:CD1	1:AAA:195:LEU:CD1	2.92	0.52
1:CCC:298:THR:HG22	4:CCC:506:HOH:O	2.08	0.52
1:CCC:68:LEU:HD13	1:CCC:75:TRP:HB3	1.91	0.52
1:BBB:125:ASP:OD1	1:BBB:193:ARG:NH1	2.31	0.52
1:CCC:58:THR:HG21	1:DDD:74:ARG:HG3	1.91	0.52
1:EEE:173:THR:HA	1:EEE:182:ALA:O	2.09	0.52
1:BBB:119:PHE:CD2	1:BBB:250:LEU:HD11	2.44	0.52
1:BBB:272:LEU:HD12	1:BBB:272:LEU:O	2.10	0.52
1:BBB:173:THR:HA	1:BBB:182:ALA:O	2.10	0.52
1:CCC:313:LEU:N	1:CCC:313:LEU:HD23	2.24	0.52
1:AAA:171:LEU:N	1:AAA:171:LEU:HD23	2.25	0.52
1:DDD:243:ILE:HG21	1:DDD:256:MET:HG2	1.91	0.52
1:BBB:293:ASP:OD1	1:BBB:297:ILE:CD1	2.58	0.52



Atom-1	Atom-2	Interatomic distance (\hat{A})	Clash
1.CCC·173·THB·HA	1.CCC:182.ALA.O	2.09	$\frac{0.52}{0.52}$
1:DDD:25:GLN:OE1	1.000.102.1111.0	2.03	0.52
1.DDD.266.ILE.HG21	1.DDD:304·TYB·CE2	2.45	0.52
1.AAA.173.THB.HA	$\frac{1.2223.001.1110.022}{1.4 \text{ A} \text{ A} \cdot 182 \cdot \text{ A} \text{ L} \text{ A} \cdot \text{O}}$	2.10	0.52
1.CCC:57:ABG:HG2	1.DDD:72:GLN:HG2	1.92	0.52
1.EEE.64.PHE.C	1.EEE.64.PHE.CD2	2.83	0.52
1.BBB·240·ASN·CA	1.BBB.260.LEU.CD1	2.83	0.51
1.BBB·12·PHE·CD1	1.BBB:145:GLN:HB2	2.45	0.51
1.BBB:68:LEU:HD13	1.BBB·75·TRP·HB3	1.92	0.51
1.CCC·266·ILE·HG21	$1 \cdot CCC \cdot 304 \cdot TYB \cdot CE2$	2.45	0.51
1.BBB·293·ASP·0	1.BBB:297:ILE:HD12	2.10	0.51
1:EEE·23·ILE·HD12	1.EEE.162.TRP.CD1	2.46	0.51
1:EEE:41:ABG:HA	1.EEE:101.THR.HA	1.91	0.51
1:EEE:122:PHE:HB3	1·EEE·254·THR·HG23	1.91	0.51
1·CCC·305·LEU·HD21	4·CCC·507·HOH·O	2.11	0.51
1.DDD·47.PHE·HD2	1.DDD·47.PHE·H	1.58	0.51
1.DDD.68.LEU.HD13	1.DDD.75.TRP.HB3	1.92	0.51
1:EEE:82:ASN:HD21	1:EEE:131:ILE:HA	1.76	0.51
1:AAA:25:GLN:OE1	1:AAA:193:ARG:NH2	2.45	0.50
1:BBB:12:PHE:HD1	1:BBB:145:GLN:HB2	1.76	0.50
1:CCC:231:GLY:HA3	2:DDD:401:BNG:O4	2.10	0.50
1:EEE:12:PHE:CD1	1:EEE:145:GLN:HB2	2.46	0.50
1:CCC:119:PHE:CD2	1:CCC:250:LEU:HD11	2.47	0.50
1:BBB:58:THR:HG21	1:CCC:74:ARG:HG3	1.94	0.50
1:BBB:230:GLY:HA3	2:BBB:401:BNG:H1'2	1.94	0.50
1:DDD:47:PHE:HE2	1:DDD:98:GLU:CA	2.22	0.50
1:EEE:243:ILE:HG21	1:EEE:256:MET:HG2	1.93	0.50
1:DDD:300:TYR:HB3	1:DDD:301:PRO:CD	2.35	0.50
1:EEE:68:LEU:CD1	1:EEE:75:TRP:HB3	2.41	0.50
1:EEE:37:ARG:HH21	1:EEE:147:MET:HE3	1.75	0.50
1:AAA:215:PHE:CE2	1:BBB:272:LEU:HB2	2.47	0.50
1:EEE:67:LEU:HD12	1:EEE:67:LEU:C	2.32	0.50
1:EEE:240:ASN:CA	1:EEE:260:LEU:CD1	2.89	0.49
1:BBB:216:THR:HG21	2:BBB:402:BNG:H4'2	1.94	0.49
1:DDD:42:GLN:OE1	1:DDD:43:PRO:HD2	2.12	0.49
1:EEE:44:LEU:HD23	1:EEE:44:LEU:N	2.26	0.49
1:BBB:218:PHE:O	1:CCC:279:ARG:NH1	2.45	0.49
1:DDD:208:LEU:HD21	1:EEE:264:PHE:HB3	1.95	0.49
1:EEE:9:SER:HB3	4:EEE:503:HOH:O	2.12	0.49
1:DDD:12:PHE:CD1	1:DDD:145:GLN:HB2	2.48	0.49
1:EEE:298:THR:C	1:EEE:301:PRO:HD2	2.33	0.49



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:AAA:81:HIS:CA	1:EEE:107:ARG:HH22	2.26	0.49
1:BBB:266:ILE:O	1:BBB:269:LEU:HB2	2.13	0.49
1:EEE:13:ILE:CD1	1:EEE:144:PHE:CG	2.91	0.48
1:EEE:25:GLN:OE1	1:EEE:193:ARG:NH2	2.46	0.48
1:AAA:240:ASN:HD21	1:EEE:201:ARG:HA	1.78	0.48
1:BBB:243:ILE:HG21	1:BBB:256:MET:HG2	1.95	0.48
1:AAA:124:PHE:CD1	1:AAA:195:LEU:HD11	2.48	0.48
1:CCC:201:ARG:HA	1:DDD:240:ASN:HD21	1.77	0.48
1:DDD:58:THR:HG21	1:EEE:74:ARG:HH11	1.78	0.48
1:EEE:171:LEU:HD12	1:EEE:171:LEU:H	1.78	0.48
1:DDD:240:ASN:CA	1:DDD:260:LEU:HD13	2.44	0.48
1:EEE:19:GLN:CG	1:EEE:33:VAL:HB	2.44	0.48
1:EEE:254:THR:O	1:EEE:257:ASP:CG	2.49	0.48
1:AAA:243:ILE:HG21	1:AAA:256:MET:HG2	1.95	0.48
1:AAA:310:THR:C	1:AAA:314:LEU:HD13	2.33	0.48
1:BBB:201:ARG:HA	1:CCC:240:ASN:HD21	1.79	0.48
2:BBB:402:BNG:H5'2	1:CCC:230:GLY:HA3	1.96	0.48
1:CCC:289:ALA:O	1:CCC:293:ASP:N	2.45	0.48
1:BBB:208:LEU:HD21	1:CCC:264:PHE:HB3	1.96	0.47
1:EEE:214:TRP:CD1	1:EEE:300:TYR:CD2	3.02	0.47
1:AAA:57:ARG:HG2	1:BBB:72:GLN:HG2	1.95	0.47
1:AAA:272:LEU:HD12	1:AAA:272:LEU:C	2.34	0.47
1:CCC:12:PHE:CD1	1:CCC:145:GLN:HB2	2.49	0.47
1:AAA:272:LEU:O	1:AAA:275:VAL:HB	2.14	0.47
1:BBB:215:PHE:CE2	1:CCC:272:LEU:HB2	2.50	0.47
1:BBB:291:LYS:O	1:BBB:294:ILE:HG22	2.15	0.47
1:CCC:300:TYR:HB3	1:CCC:301:PRO:CD	2.29	0.47
1:EEE:37:ARG:NH2	1:EEE:147:MET:HE1	2.29	0.47
1:EEE:309:LEU:O	1:EEE:313:LEU:HG	2.14	0.47
1:BBB:168:ASN:N	1:BBB:168:ASN:OD1	2.48	0.47
1:DDD:40:TRP:HE3	3:DDD:403:VMT:BR01	2.53	0.47
1:BBB:42:GLN:OE1	1:BBB:43:PRO:HD2	2.15	0.47
1:EEE:266:ILE:HG21	1:EEE:304:TYR:CE2	2.50	0.46
1:AAA:12:PHE:CD1	1:AAA:145:GLN:HB2	2.49	0.46
1:BBB:230:GLY:HA3	2:BBB:401:BNG:C1'	2.45	0.46
1:BBB:14:GLY:HA2	1:BBB:151:SER:OG	2.15	0.46
1:CCC:18:ASP:OD2	1:CCC:107:ARG:NH1	2.49	0.46
1:CCC:42:GLN:OE1	1:CCC:43:PRO:HD2	2.15	0.46
2:DDD:401:BNG:H2'1	2:DDD:401:BNG:C6'	2.46	0.46
1:AAA:113:GLN:CG	1:EEE:19:GLN:OE1	2.63	0.46
1:EEE:7:GLU:CB	1:EEE:8:PRO:HD3	2.45	0.46



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:EEE:8:PRO:HG3	1:EEE:140:HIS:O	2.16	0.46
1:CCC:122:PHE:HB3	1:CCC:254:THR:HG23	1.98	0.46
1:DDD:12:PHE:HD1	1:DDD:145:GLN:HB2	1.81	0.46
1:AAA:113:GLN:CB	1:EEE:19:GLN:OE1	2.63	0.46
1:CCC:293:ASP:OD1	1:CCC:297:ILE:HD11	2.16	0.46
1:EEE:82:ASN:ND2	1:EEE:130:PHE:O	2.49	0.46
1:DDD:201:ARG:HA	1:EEE:240:ASN:HD21	1.80	0.45
1:BBB:293:ASP:O	1:BBB:297:ILE:CD1	2.64	0.45
1:DDD:47:PHE:CD1	1:DDD:57:ARG:NH1	2.84	0.45
1:EEE:119:PHE:CD2	1:EEE:250:LEU:HD11	2.52	0.45
1:EEE:24:ASN:ND2	1:EEE:27:GLU:HB2	2.31	0.45
1:EEE:214:TRP:CD1	1:EEE:300:TYR:HD2	2.35	0.45
1:AAA:161:GLU:HG2	1:AAA:193:ARG:HG3	1.98	0.45
1:BBB:122:PHE:HB3	1:BBB:254:THR:HG23	1.99	0.45
1:CCC:47:PHE:CE2	1:CCC:57:ARG:HD2	2.52	0.45
1:DDD:144:PHE:O	1:DDD:171:LEU:HD23	2.16	0.45
1:DDD:47:PHE:CE1	1:DDD:57:ARG:CD	3.00	0.45
1:AAA:214:TRP:HB2	1:AAA:300:TYR:HE2	1.81	0.45
1:AAA:291:LYS:HD2	1:AAA:291:LYS:HA	1.53	0.45
1:AAA:298:THR:HG23	4:AAA:511:HOH:O	2.17	0.45
1:EEE:18:ASP:OD2	1:EEE:107:ARG:NH1	2.49	0.45
1:AAA:18:ASP:OD2	1:AAA:107:ARG:NH1	2.50	0.45
1:EEE:19:GLN:HG3	1:EEE:33:VAL:HB	1.98	0.45
1:AAA:45:LEU:HB3	1:AAA:96:LEU:HD11	1.97	0.44
1:AAA:146:GLU:HG2	1:AAA:171:LEU:HD21	1.99	0.44
1:DDD:309:LEU:O	1:DDD:313:LEU:HG	2.16	0.44
1:BBB:18:ASP:OD2	1:BBB:107:ARG:NH1	2.50	0.44
1:DDD:18:ASP:OD2	1:DDD:107:ARG:NH1	2.49	0.44
1:EEE:17:ILE:HD12	1:EEE:187:LEU:CD2	2.41	0.44
1:AAA:261:VAL:O	1:AAA:264:PHE:HB2	2.18	0.44
1:AAA:122:PHE:HB3	1:AAA:254:THR:HG23	1.99	0.44
2:DDD:401:BNG:H2'2	2:DDD:401:BNG:H1	1.71	0.44
1:AAA:124:PHE:HE1	1:AAA:195:LEU:HD13	1.82	0.44
1:CCC:293:ASP:CG	1:CCC:297:ILE:HD11	2.38	0.44
1:DDD:40:TRP:CE3	3:DDD:403:VMT:BR01	3.26	0.44
1:BBB:55:LYS:HG3	1:BBB:98:GLU:CD	2.38	0.44
1:AAA:216:THR:HG21	2:BBB:401:BNG:H4'2	2.00	0.44
1:DDD:122:PHE:HB3	1:DDD:254:THR:HG23	1.98	0.44
1:DDD:214:TRP:HB2	1:DDD:300:TYR:CD2	2.53	0.44
1:EEE:164:VAL:HG13	1:EEE:189:PHE:HD2	1.82	0.44
1:BBB:238:ALA:O	1:BBB:241:PHE:N	2.51	0.43



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:DDD:171:LEU:N	1:DDD:171:LEU:HD12	2.33	0.43
1:DDD:197:TYR:CG	1:EEE:249:ARG:HD3	2.53	0.43
1:EEE:238:ALA:O	1:EEE:241:PHE:N	2.51	0.43
1:BBB:146:GLU:CG	1:BBB:171:LEU:HD11	2.20	0.43
1:CCC:261:VAL:O	1:CCC:264:PHE:HB2	2.18	0.43
1:CCC:46:ALA:HB2	1:CCC:99:ASP:O	2.18	0.43
1:DDD:238:ALA:O	1:DDD:241:PHE:N	2.51	0.43
1:DDD:298:THR:O	1:DDD:302:LEU:HG	2.19	0.43
1:AAA:45:LEU:HD23	1:AAA:45:LEU:N	2.34	0.43
1:AAA:85:GLY:H	1:EEE:109:THR:HG21	1.83	0.43
2:AAA:401:BNG:H6'1	1:EEE:228:LEU:HD11	2.00	0.43
1:DDD:279:ARG:HD3	4:DDD:506:HOH:O	2.19	0.43
1:CCC:12:PHE:HD1	1:CCC:145:GLN:HB2	1.83	0.43
1:DDD:58:THR:CG2	1:EEE:74:ARG:NH1	2.82	0.43
1:AAA:23:ILE:HD12	1:AAA:162:TRP:CD1	2.54	0.43
1:AAA:238:ALA:O	1:AAA:241:PHE:N	2.52	0.43
1:BBB:212:VAL:HG13	1:CCC:271:VAL:HG11	2.00	0.43
1:AAA:124:PHE:CD1	1:AAA:195:LEU:HD13	2.54	0.43
1:CCC:164:VAL:HG13	1:CCC:189:PHE:HD2	1.83	0.43
1:DDD:23:ILE:HD12	1:DDD:162:TRP:CD1	2.54	0.43
1:DDD:64:PHE:CD1	1:DDD:94:ILE:HG21	2.54	0.43
1:DDD:261:VAL:O	1:DDD:264:PHE:HB2	2.18	0.42
1:CCC:293:ASP:O	1:CCC:297:ILE:CD1	2.66	0.42
1:DDD:161:GLU:HG2	1:DDD:193:ARG:HG3	2.01	0.42
1:AAA:164:VAL:HG13	1:AAA:189:PHE:HD2	1.84	0.42
1:BBB:25:GLN:OE1	1:BBB:193:ARG:NH2	2.45	0.42
1:AAA:64:PHE:CD1	1:AAA:94:ILE:HG21	2.54	0.42
1:AAA:124:PHE:CE1	1:AAA:195:LEU:CD1	3.00	0.42
1:CCC:23:ILE:HD12	1:CCC:162:TRP:CD1	2.54	0.42
1:CCC:291:LYS:O	1:CCC:294:ILE:HG22	2.19	0.42
1:BBB:23:ILE:HD12	1:BBB:162:TRP:CD1	2.55	0.42
1:DDD:228:LEU:HD11	2:DDD:402:BNG:H6'1	2.01	0.42
1:AAA:144:PHE:O	1:AAA:171:LEU:HD12	2.19	0.42
1:AAA:194:HIS:ND1	1:BBB:251:GLY:HA3	2.35	0.42
1:BBB:230:GLY:CA	2:BBB:401:BNG:H5'2	2.48	0.42
1:EEE:281:GLU:HG2	1:EEE:286:GLN:HG3	2.02	0.42
1:AAA:42:GLN:OE1	1:AAA:43:PRO:HD2	2.19	0.42
1:AAA:174:HIS:CE1	1:AAA:176:GLU:HB2	2.55	0.42
1:AAA:212:VAL:HG13	1:BBB:271:VAL:HG11	2.02	0.42
1:BBB:164:VAL:HG13	1:BBB:189:PHE:HD2	1.84	0.42
1:CCC:64:PHE:CD1	1:CCC:94:ILE:HG21	2.54	0.42



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:DDD:45:LEU:HD11	1:DDD:68:LEU:HD21	2.00	0.42
1:DDD:60:THR:HG23	1:EEE:69:GLU:OE2	2.20	0.42
1:DDD:153:LEU:HD22	1:DDD:167:VAL:CG1	2.50	0.42
1:AAA:44:LEU:HD12	1:AAA:44:LEU:N	2.35	0.42
1:AAA:249:ARG:HB2	1:EEE:161:GLU:HB2	2.01	0.42
1:BBB:74:ARG:HD3	1:BBB:137:PHE:CE2	2.55	0.42
1:AAA:264:PHE:HB3	1:EEE:208:LEU:HD21	2.01	0.41
1:AAA:306[B]:LEU:HA	1:AAA:306[B]:LEU:HD12	1.82	0.41
1:AAA:248:PRO:CB	1:AAA:250:LEU:CD2	2.97	0.41
1:BBB:291:LYS:HD3	1:BBB:291:LYS:HA	1.65	0.41
1:BBB:293:ASP:CG	1:BBB:297:ILE:HD11	2.41	0.41
1:CCC:12:PHE:HB2	1:CCC:39:ASP:HB2	2.02	0.41
1:DDD:174:HIS:CE1	1:DDD:176:GLU:HB2	2.56	0.41
1:EEE:17:ILE:CD1	1:EEE:187:LEU:HD21	2.46	0.41
1:AAA:74:ARG:NH1	1:EEE:58:THR:CG2	2.84	0.41
1:EEE:204:ILE:HB	1:EEE:205:PRO:HD3	2.02	0.41
1:AAA:214:TRP:CD1	1:AAA:300:TYR:CD2	3.08	0.41
1:BBB:17:ILE:HD12	1:BBB:153:LEU:HD11	2.02	0.41
1:CCC:238:ALA:O	1:CCC:241:PHE:N	2.52	0.41
1:EEE:68:LEU:HD23	1:EEE:68:LEU:HA	1.78	0.41
1:BBB:12:PHE:HB2	1:BBB:39:ASP:HB2	2.01	0.41
2:DDD:401:BNG:H2'1	2:DDD:401:BNG:H7'2	2.02	0.41
1:EEE:129:PHE:HD2	1:EEE:189:PHE:CE2	2.38	0.41
1:BBB:137:PHE:HA	1:BBB:138:PRO:HD3	1.93	0.41
1:DDD:164:VAL:HG13	1:DDD:189:PHE:HD2	1.85	0.41
1:AAA:12:PHE:O	1:AAA:38:ILE:HA	2.21	0.41
1:AAA:215:PHE:CD2	1:BBB:272:LEU:HB2	2.56	0.41
1:AAA:271:VAL:HG11	1:EEE:212:VAL:CG1	2.50	0.41
1:BBB:161:GLU:HG2	1:BBB:193:ARG:HG2	2.03	0.41
1:DDD:235:LEU:O	1:DDD:238:ALA:HB3	2.20	0.41
1:AAA:12:PHE:HD1	1:AAA:145:GLN:HB2	1.85	0.41
1:AAA:135:SER:HB2	1:AAA:144:PHE:CZ	2.56	0.41
1:BBB:174:HIS:CE1	1:BBB:176:GLU:HB2	2.56	0.41
1:BBB:204:ILE:HB	1:BBB:205:PRO:HD3	2.03	0.41
1:BBB:235:LEU:O	1:BBB:238:ALA:HB3	2.21	0.41
1:CCC:12:PHE:O	1:CCC:38:ILE:HA	2.21	0.41
1:CCC:41:ARG:HA	1:CCC:101:THR:HA	2.03	0.41
1:CCC:243:ILE:HG21	1:CCC:256:MET:HG2	2.02	0.41
1:EEE:121:LEU:HD13	1:EEE:316:PHE:CE2	2.56	0.41
1:BBB:64:PHE:CD1	1:BBB:94:ILE:HG21	2.56	0.41
1:BBB:138:PRO:CG	1:BBB:178:THR:HG21	2.34	0.41



Atom_1	Atom_2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:DDD:146:GLU:HG2	1:DDD:171:LEU:HD11	1.98	0.40
2:DDD:402:BNG:H5'2	2:DDD:402:BNG:H1'1	2.03	0.40
1:AAA:235:LEU:O	1:AAA:238:ALA:HB3	2.21	0.40
1:EEE:174:HIS:CE1	1:EEE:176:GLU:HB2	2.55	0.40
1:DDD:19:GLN:OE1	1:EEE:113:GLN:CB	2.66	0.40
1:EEE:235:LEU:O	1:EEE:238:ALA:HB3	2.21	0.40
1:AAA:204:ILE:HB	1:AAA:205:PRO:HD3	2.03	0.40
1:BBB:135:SER:HB2	1:BBB:144:PHE:CZ	2.56	0.40
1:BBB:240:ASN:CA	1:BBB:260:LEU:HD13	2.50	0.40
1:DDD:161:GLU:HB2	1:EEE:249:ARG:HB2	2.03	0.40
1:EEE:128:LEU:HD13	1:EEE:190:HIS:CE1	2.56	0.40
1:EEE:253:ILE:HG23	1:EEE:257:ASP:HB2	2.03	0.40
1:CCC:204:ILE:HB	1:CCC:205:PRO:HD3	2.02	0.40
1:CCC:281:GLU:HG2	1:CCC:286:GLN:HG3	2.03	0.40
1:DDD:135:SER:HB2	1:DDD:144:PHE:CZ	2.56	0.40

All (2) 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)	
1:AAA:49:HIS:NE2	4:CCC:501:HOH:O[4_455]	1.78	0.42	
1:AAA:98:GLU:OE1	4:CCC:501:HOH:O[4_455]	2.04	0.16	

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	309/320~(97%)	295~(96%)	14 (4%)	0	100	100
1	BBB	308/320~(96%)	294 (96%)	14 (4%)	0	100	100
1	CCC	308/320~(96%)	293 (95%)	15 (5%)	0	100	100
1	DDD	308/320~(96%)	291 (94%)	17 (6%)	0	100	100



Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
1	EEE	310/320~(97%)	295~(95%)	14 (4%)	1 (0%)	37	70
All	All	1543/1600~(96%)	1468 (95%)	74 (5%)	1 (0%)	48	81

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	EEE	7	GLU

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	\mathbf{P}	erc	entiles
1	AAA	276/282~(98%)	253~(92%)	23~(8%)		9	34
1	BBB	275/282~(98%)	252~(92%)	23~(8%)		9	33
1	CCC	275/282~(98%)	254 (92%)	21 (8%)		11	37
1	DDD	275/282~(98%)	250~(91%)	25~(9%)		7	30
1	EEE	275/282~(98%)	232~(84%)	43 (16%)		2	11
All	All	1376/1410 (98%)	1241 (90%)	135 (10%)		6	26

All (135) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	35	SER
1	AAA	42	GLN
1	AAA	45	LEU
1	AAA	66	LYS
1	AAA	90	GLN
1	AAA	95	SER
1	AAA	99	ASP
1	AAA	117	PHE
1	AAA	121	LEU
1	AAA	126	ASN
1	AAA	140	HIS



Mol	Chain	Res	Type
1	AAA	141	LEU
1	AAA	166	GLU
1	AAA	167	VAL
1	AAA	168	ASN
1	AAA	171	LEU
1	AAA	193	ARG
1	AAA	244	SER
1	AAA	267	THR
1	AAA	290	ARG
1	AAA	291	LYS
1	AAA	306[A]	LEU
1	AAA	306[B]	LEU
1	BBB	35	SER
1	BBB	42	GLN
1	BBB	66	LYS
1	BBB	90	GLN
1	BBB	95	SER
1	BBB	99	ASP
1	BBB	117	PHE
1	BBB	126	ASN
1	BBB	140	HIS
1	BBB	141	LEU
1	BBB	166	GLU
1	BBB	167	VAL
1	BBB	168	ASN
1	BBB	244	SER
1	BBB	259	PHE
1	BBB	267	THR
1	BBB	269	LEU
1	BBB	290	ARG
1	BBB	291	LYS
1	BBB	294	ILE
1	BBB	302	LEU
1	BBB	306	LEU
1	BBB	314	LEU
1	CCC	35	SER
1	CCC	42	GLN
1	CCC	66	LYS
1	CCC	90	GLN
1	CCC	95	SER
1	CCC	99	ASP
1	CCC	117	PHE



Mol	Chain	Res	Type
1	CCC	126	ASN
1	CCC	140	HIS
1	CCC	141	LEU
1	CCC	166	GLU
1	CCC	167	VAL
1	CCC	168	ASN
1	CCC	170	HIS
1	CCC	193	ARG
1	CCC	244	SER
1	CCC	259	PHE
1	CCC	267	THR
1	CCC	290	ARG
1	CCC	306	LEU
1	CCC	314	LEU
1	DDD	35	SER
1	DDD	42	GLN
1	DDD	47	PHE
1	DDD	66	LYS
1	DDD	90	GLN
1	DDD	95	SER
1	DDD	99	ASP
1	DDD	117	PHE
1	DDD	121	LEU
1	DDD	126	ASN
1	DDD	140	HIS
1	DDD	141	LEU
1	DDD	166	GLU
1	DDD	167	VAL
1	DDD	168	ASN
1	DDD	193	ARG
1	DDD	195	LEU
1	DDD	244	SER
1	DDD	259	PHE
1	DDD	267	THR
1	DDD	290	ARG
1	DDD	291	LYS
1	DDD	294	ILE
1	DDD	306	LEU
1	DDD	314	LEU
1	EEE	13	ILE
1	EEE	16	LYS
1	EEE	25	GLN



Mol	Chain	Res	Type
1	EEE	26	LYS
1	EEE	32	VAL
1	EEE	35	SER
1	EEE	37	ARG
1	EEE	42	GLN
1	EEE	44	LEU
1	EEE	45	LEU
1	EEE	48	GLU
1	EEE	55	LYS
1	EEE	63	THR
1	EEE	66	LYS
1	EEE	67	LEU
1	EEE	74	ARG
1	EEE	79	THR
1	EEE	90	GLN
1	EEE	93	LEU
1	EEE	95	SER
1	EEE	96	LEU
1	EEE	99	ASP
1	EEE	101	THR
1	EEE	107	ARG
1	EEE	121	LEU
1	EEE	126	ASN
1	EEE	135	SER
1	EEE	141	LEU
1	EEE	166	GLU
1	EEE	167	VAL
1	EEE	168	ASN
1	EEE	171	LEU
1	EEE	193	ARG
1	EEE	244	SER
1	EEE	249	ARG
1	EEE	257	ASP
1	EEE	259	PHE
1	EEE	267	THR
1	EEE	290	ARG
1	EEE	294	ILE
1	EEE	302	LEU
1	EEE	306	LEU
1	EEE	314	LEU

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



5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

10 ligands are modelled in this entry.

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

Mal	Turne	no Chain Bos Link		Tink	Bo	ond leng	ths	Bond angles		
INIOI	туре	Unain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	VMT	DDD	403	-	9,10,10	0.63	0	11,12,12	0.59	0
3	VMT	EEE	401	-	9,10,10	0.43	0	11,12,12	0.95	0
2	BNG	DDD	402	-	21,21,21	0.89	1 (4%)	26,26,26	1.10	3 (11%)
3	VMT	CCC	401	-	9,10,10	0.72	0	11,12,12	1.24	0
2	BNG	AAA	401	-	21,21,21	0.76	1 (4%)	26,26,26	1.10	2 (7%)
3	VMT	AAA	402	-	9,10,10	0.55	0	11,12,12	1.04	1 (9%)
2	BNG	DDD	401	-	21,21,21	0.69	1 (4%)	26,26,26	0.88	1 (3%)
2	BNG	BBB	402	-	21,21,21	1.00	1 (4%)	26,26,26	1.29	3 (11%)
2	BNG	BBB	401	-	21,21,21	0.66	0	26,26,26	1.52	5 (19%)
3	VMT	BBB	403	-	9,10,10	0.34	0	11,12,12	0.77	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	VMT	DDD	403	-	-	0/3/3/3	0/1/1/1
3	VMT	EEE	401	-	-	2/3/3/3	0/1/1/1
2	BNG	DDD	402	-	-	10/12/32/32	0/1/1/1
3	VMT	CCC	401	-	-	3/3/3/3	0/1/1/1
2	BNG	AAA	401	-	-	11/12/32/32	0/1/1/1
3	VMT	AAA	402	-	-	0/3/3/3	0/1/1/1
2	BNG	DDD	401	-	-	6/12/32/32	0/1/1/1
2	BNG	BBB	402	-	-	10/12/32/32	0/1/1/1
2	BNG	BBB	401	-	-	8/12/32/32	0/1/1/1
3	VMT	BBB	403	-	-	0/3/3/3	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	$\mathrm{Ideal}(\mathrm{\AA})$
2	BBB	402	BNG	O1-C1	3.14	1.45	1.40
2	DDD	402	BNG	O1-C1	2.85	1.45	1.40
2	AAA	401	BNG	O1-C1	2.49	1.44	1.40
2	DDD	401	BNG	01-C1	2.29	1.44	1.40

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	BBB	401	BNG	C1-C2-C3	-3.30	103.12	110.00
2	BBB	402	BNG	C1-O5-C5	2.97	119.51	113.69
2	BBB	401	BNG	O1-C1'-C2'	2.68	118.94	109.56
3	AAA	402	VMT	C08-C07-C04	-2.55	107.00	112.85
2	DDD	402	BNG	C1'-O1-C1	2.44	117.88	113.84
2	BBB	401	BNG	C1-O5-C5	-2.42	108.94	113.69
2	BBB	401	BNG	O1-C1-C2	2.37	112.01	108.30
2	DDD	401	BNG	C4-C3-C2	-2.34	106.74	110.82
2	BBB	401	BNG	O2-C2-C1	2.33	115.71	110.05
2	BBB	402	BNG	O1-C1-C2	2.32	111.93	108.30
2	BBB	402	BNG	O1-C1'-C2'	2.24	117.42	109.56
2	AAA	401	BNG	O5-C5-C6	2.24	112.00	106.44
2	DDD	402	BNG	O1-C1'-C2'	2.24	117.41	109.56
2	AAA	401	BNG	C1-C2-C3	2.23	114.63	110.00
2	DDD	402	BNG	O5-C5-C6	2.16	111.80	106.44

There are no chirality outliers.

All (50) torsion outliers are listed below:



Mol	Chain	Res	Type	Atoms
2	BBB	401	BNG	C2-C1-O1-C1'
2	BBB	401	BNG	O5-C1-O1-C1'
2	BBB	401	BNG	C2'-C1'-O1-C1
2	BBB	402	BNG	C2-C1-O1-C1'
2	BBB	402	BNG	O5-C1-O1-C1'
2	DDD	401	BNG	C2'-C1'-O1-C1
2	DDD	402	BNG	C2-C1-O1-C1'
3	CCC	401	VMT	C04-C07-C08-N01
2	DDD	402	BNG	C4-C5-C6-O6
2	DDD	402	BNG	O5-C5-C6-O6
2	BBB	402	BNG	O5-C5-C6-O6
2	AAA	401	BNG	O5-C5-C6-O6
2	BBB	402	BNG	C4-C5-C6-O6
2	AAA	401	BNG	C4-C5-C6-O6
2	DDD	402	BNG	O5-C1-O1-C1'
2	BBB	402	BNG	C3'-C4'-C5'-C6'
2	AAA	401	BNG	C2-C1-O1-C1'
2	AAA	401	BNG	C5'-C6'-C7'-C8'
2	DDD	401	BNG	C4'-C5'-C6'-C7'
2	DDD	402	BNG	C5'-C6'-C7'-C8'
2	BBB	401	BNG	C3'-C4'-C5'-C6'
2	DDD	401	BNG	O1-C1'-C2'-C3'
2	BBB	402	BNG	C4'-C5'-C6'-C7'
2	AAA	401	BNG	O5-C1-O1-C1'
2	DDD	402	BNG	C3'-C4'-C5'-C6'
2	DDD	401	BNG	C3'-C4'-C5'-C6'
2	BBB	402	BNG	C6'-C7'-C8'-C9'
2	AAA	401	BNG	C2'-C1'-O1-C1
2	BBB	402	BNG	C2'-C1'-O1-C1
2	DDD	402	BNG	C2'-C1'-O1-C1
2	AAA	401	BNG	C6'-C7'-C8'-C9'
3	EEE	401	VMT	C05-C04-C07-C08
2	DDD	401	BNG	C6'-C7'-C8'-C9'
3	EEE	401	VMT	C03-C04-C07-C08
2	DDD	402	BNG	C6'-C7'-C8'-C9'
2	AAA	401	BNG	C3'-C4'-C5'-C6'
2	AAA	401	BNG	C4'-C5'-C6'-C7'
3	CCC	401	VMT	C05-C04-C07-C08
2	DDD	402	BNG	C4'-C5'-C6'-C7'
2	DDD	401	BNG	C4-C5-C6-O6
2	BBB	401	BNG	C1'-C2'-C3'-C4'
3	CCC	401	VMT	C03-C04-C07-C08
2	AAA	401	BNG	C2'-C3'-C4'-C5'



Mol	Chain	Res	Type	Atoms
2	BBB	402	BNG	C5'-C6'-C7'-C8'
2	DDD	402	BNG	C1'-C2'-C3'-C4'
2	AAA	401	BNG	C1'-C2'-C3'-C4'
2	BBB	401	BNG	C6'-C7'-C8'-C9'
2	BBB	402	BNG	C2'-C3'-C4'-C5'
2	BBB	401	BNG	C4'-C5'-C6'-C7'
2	BBB	401	BNG	O5-C5-C6-O6

There are no ring outliers.

7 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	DDD	403	VMT	2	0
2	DDD	402	BNG	3	0
3	CCC	401	VMT	1	0
2	AAA	401	BNG	2	0
2	DDD	401	BNG	5	0
2	BBB	402	BNG	5	0
2	BBB	401	BNG	6	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	310/320~(96%)	0.08	1 (0%) 90 81	54, 100, 133, 160	1 (0%)
1	BBB	310/320~(96%)	-0.07	0 100 100	66, 98, 131, 214	0
1	CCC	310/320~(96%)	0.02	3 (0%) 79 60	63, 96, 128, 157	0
1	DDD	310/320~(96%)	0.11	4 (1%) 74 54	64, 102, 148, 212	0
1	EEE	312/320~(97%)	-0.00	8 (2%) 57 35	74, 113, 156, 202	0
All	All	1552/1600~(97%)	0.03	16 (1%) 79 60	54, 101, 142, 214	1 (0%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	DDD	152	GLY	6.4
1	AAA	306[A]	LEU	5.1
1	CCC	152	GLY	4.3
1	EEE	155	ASP	2.9
1	CCC	98	GLU	2.6
1	CCC	180	GLY	2.6
1	EEE	78	PHE	2.5
1	EEE	152	GLY	2.5
1	EEE	43	PRO	2.5
1	DDD	72	GLN	2.4
1	EEE	103	MET	2.4
1	DDD	148	GLN	2.2
1	DDD	151	SER	2.1
1	EEE	95	SER	2.1
1	EEE	75	TRP	2.1
1	EEE	194	HIS	2.1



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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(Å^2)$	Q<0.9
3	VMT	DDD	403	10/10	0.80	0.34	134,144,153,247	0
3	VMT	AAA	402	10/10	0.82	0.29	113,139,156,194	0
3	VMT	CCC	401	10/10	0.83	0.26	116,131,159,159	0
2	BNG	AAA	401	21/21	0.87	0.15	77,125,150,167	0
2	BNG	BBB	402	21/21	0.88	0.13	62,114,134,143	0
3	VMT	EEE	401	10/10	0.88	0.27	113,183,194,196	0
2	BNG	BBB	401	21/21	0.89	0.14	76,129,139,147	0
2	BNG	DDD	401	21/21	0.90	0.14	75,118,158,166	0
2	BNG	DDD	402	21/21	0.90	0.14	78,118,128,130	0
3	VMT	BBB	403	10/10	0.94	0.15	92,117,123,151	0

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































6.5 Other polymers (i)

There are no such residues in this entry.

