

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

#### Nov 22, 2023 – 09:11 PM JST

PDB ID	:	7C8H
Title	:	Ambient temperature structure of Bifidobacterium longum phosphoketolase
		with thiamine diphosphate
Authors	:	Nakata, K.; Kashiwagi, T.; Nango, E.; Miyano, H.; Mizukoshi, T.; Iwata, S.
Deposited on	:	2020-06-01
Resolution	:	2.50  Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
$\mathrm{EDS}$	:	2.36
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

# 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.50 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
$R_{free}$	130704	$4661 \ (2.50-2.50)$
Clashscore	141614	$5346\ (2.50-2.50)$
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain		
1	А	831	% • • • • • • • • • • • • • • • • • • •	110/	
-		001	3%	1178	•
1	В	831	84%	13%	·
1	С	831	3%	19%	• •
	_		4%		
1	D	831	80%	17%	••
1	Е	831	5% 82%	14%	• •
			4%		_
1	F	831	80%	17%	••



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Mol	Chain	Length	Quality of chain		
1	G	831	% 83%	13%	•
1	Н	831	3% 82%	14%	••

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
4	LMR	В	902	-	-	-	Х
5	MLA	D	901	-	-	Х	-
5	MLA	D	902	-	-	-	Х
5	MLA	Е	901	-	-	-	Х
6	SIN	Е	904	-	-	-	Х
6	SIN	G	903	-	-	-	Х
6	SIN	Н	901	-	-	-	Х



# 2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 52781 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		А	toms			ZeroOcc	AltConf	Trace
1	Δ	807	Total	С	Ν	Ο	S	0	0	0
	Л	807	6418	4075	1094	1230	19	0	0	0
1	В	807	Total	С	Ν	Ο	$\mathbf{S}$	0	0	0
	D	001	6418	4075	1094	1230	19	0	0	0
1	С	807	Total	С	Ν	Ο	$\mathbf{S}$	0	0	0
L	U	001	6418	4075	1094	1230	19	0	0	0
1	П	808	Total	$\mathbf{C}$	Ν	Ο	$\mathbf{S}$	0	1	0
1	D	000	6433	4084	1097	1233	19	0	I	0
1	E	808	Total	$\mathbf{C}$	Ν	Ο	$\mathbf{S}$	0	1	0
		000	6436	4085	1098	1234	19	0	T	0
1	F	807	Total	$\mathbf{C}$	Ν	Ο	$\mathbf{S}$	0	0	0
	L	001	6418	4075	1094	1230	19	0	0	0
1	G	806	Total	$\mathbf{C}$	Ν	Ο	$\mathbf{S}$	0	2	0
1	ŭ	000	6427	4081	1096	1231	19	0	2	0
1	н	807	Total	$\mathbf{C}$	Ν	Ο	$\mathbf{S}$	0	1	0
	11	001	6428	4081	1097	1231	19		T	

• Molecule 1 is a protein called Xylulose-5-phosphate/fructose-6-phosphate phosphoketolase.

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	826	HIS	-	expression tag	UNP Q6R2Q7
А	827	HIS	-	expression tag	UNP Q6R2Q7
А	828	HIS	-	expression tag	UNP Q6R2Q7
А	829	HIS	-	expression tag	UNP Q6R2Q7
А	830	HIS	-	expression tag	UNP Q6R2Q7
А	831	HIS	-	expression tag	UNP Q6R2Q7
В	826	HIS	-	expression tag	UNP Q6R2Q7
В	827	HIS	-	expression tag	UNP Q6R2Q7
В	828	HIS	-	expression tag	UNP Q6R2Q7
В	829	HIS	-	expression tag	UNP Q6R2Q7
В	830	HIS	-	expression tag	UNP Q6R2Q7
В	831	HIS	-	expression tag	UNP Q6R2Q7
С	826	HIS	-	expression tag	UNP Q6R2Q7



Chain	Residue	Modelled	Actual	Comment	Reference
С	827	HIS	-	expression tag	UNP Q6R2Q7
С	828	HIS	_	expression tag	UNP Q6R2Q7
С	829	HIS	_	expression tag	UNP Q6R2Q7
С	830	HIS	-	expression tag	UNP Q6R2Q7
С	831	HIS	_	expression tag	UNP Q6R2Q7
D	826	HIS	-	expression tag	UNP Q6R2Q7
D	827	HIS	-	expression tag	UNP Q6R2Q7
D	828	HIS	-	expression tag	UNP Q6R2Q7
D	829	HIS	-	expression tag	UNP Q6R2Q7
D	830	HIS	_	expression tag	UNP Q6R2Q7
D	831	HIS	-	expression tag	UNP Q6R2Q7
Е	826	HIS	-	expression tag	UNP Q6R2Q7
Е	827	HIS	-	expression tag	UNP Q6R2Q7
Е	828	HIS	-	expression tag	UNP Q6R2Q7
Е	829	HIS	-	expression tag	UNP Q6R2Q7
Е	830	HIS	-	expression tag	UNP Q6R2Q7
Е	831	HIS	-	expression tag	UNP Q6R2Q7
F	826	HIS	-	expression tag	UNP Q6R2Q7
F	827	HIS	-	expression tag	UNP Q6R2Q7
F	828	HIS	-	expression tag	UNP Q6R2Q7
F	829	HIS	-	expression tag	UNP Q6R2Q7
F	830	HIS	-	expression tag	UNP Q6R2Q7
F	831	HIS	-	expression tag	UNP Q6R2Q7
G	826	HIS	-	expression tag	UNP Q6R2Q7
G	827	HIS	-	expression tag	UNP Q6R2Q7
G	828	HIS	-	expression tag	UNP Q6R2Q7
G	829	HIS	-	expression tag	UNP Q6R2Q7
G	830	HIS	-	expression tag	UNP Q6R2Q7
G	831	HIS	-	expression tag	UNP Q6R2Q7
Н	826	HIS	-	expression tag	UNP Q6R2Q7
H	827	HIS	-	expression tag	$\overline{\text{UNP Q6R2Q7}}$
Н	828	HIS	-	expression tag	UNP Q6R2Q7
Н	829	HIS	-	expression tag	UNP Q6R2Q7
Н	830	HIS	-	expression tag	UNP Q6R2Q7
Н	831	HIS	-	expression tag	UNP Q6R2Q7

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• Molecule 2 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula:  $C_{12}H_{19}N_4O_7P_2S$ ) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues		Α	tom	IS			ZeroOcc	AltConf									
0	Λ	1	Total	С	Ν	0	Р	S	0	0									
	A	L L	26	12	4	7	2	1	0	0									
0	B	1	Total	С	Ν	0	Р	S	0	0									
	D	1	26	12	4	7	2	1	0	0									
0	C	1	Total	С	Ν	0	Р	S	0	0									
	C		U	U	0	U	U	U	U	1	26	12	4	7	2	1	0	0	
0	Л	1	Total	С	Ν	0	Р	S	0	0									
	D	1	26	12	4	7	2	1	0										
0	F	F	F	F	1	Total	С	Ν	0	Р	S	0	0						
	Ľ	1	26	12	4	7	2	1	0	0									
9	F	1	Total	С	Ν	0	Р	S	0	0									
	Ľ	1	26	12	4	7	2	1	0	0									
9	C	C	C	C	1	Total	С	Ν	0	Р	S	0	0						
	G		26	12	4	7	2	1		0									
9	Ц	1	Total	С	Ν	Ο	Р	S	0	0									
	11		26	12	4	7	2	1		0									

#### • Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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



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

• Molecule 4 is (2S)-2-hydroxy butanedioic acid (three-letter code: LMR) (formula:  $C_4H_6O_5$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 9 & 4 & 5 \end{array}$	0	0
4	В	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 9  4  5 \end{array}$	0	0





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 7 & 3 & 4 \end{array}$	0	0
5	D	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 7  3  4 \end{array}$	0	0
5	Е	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 7 & 3 & 4 \end{array}$	0	0



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	Ε	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 8 & 4 & 4 \end{array}$	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	G	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 8 & 4 & 4 \end{array}$	0	0
6	Н	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 8 & 4 & 4 \end{array}$	0	0

• Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	А	211	Total         O           211         211	0	0
7	В	215	Total         O           215         215	0	0
7	С	92	Total         O           92         92	0	0
7	D	77	Total O 77 77	0	0
7	Е	126	Total O 126 126	0	0
7	F	93	Total O 93 93	0	0
7	G	160	Total O 160 160	0	0
7	Н	132	Total O 132 132	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.

 $\bullet$  Molecule 1: Xylulose-5-phosphate/fructose-6-phosphate phosphoketolase







 $<sup>\</sup>bullet$  Molecule 1: Xylulose-5-phosphate/fructose-6-phosphate phosphoketolase









## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	144.62Å 185.80Å 162.89Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $99.61^{\circ}$ $90.00^{\circ}$	Depositor
Bosolution(Å)	46.80 - 2.50	Depositor
Resolution (A)	46.76 - 1.90	EDS
% Data completeness	$100.0 \ (46.80-2.50)$	Depositor
(in resolution range)	62.8 (46.76 - 1.90)	EDS
R <sub>merge</sub>	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$16.17 (at 1.90 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
D D .	0.161 , $0.218$	Depositor
$\Lambda, \Lambda_{free}$	0.169 , $0.219$	DCC
$R_{free}$ test set	21065  reflections  (5.02%)	wwPDB-VP
Wilson B-factor $(Å^2)$	53.8	Xtriage
Anisotropy	0.090	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.29, 27.2	EDS
L-test for $twinning^2$	$ \langle L  \rangle = 0.50, \langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	52781	wwPDB-VP
Average B, all atoms $(Å^2)$	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.16% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 5 Model quality (i)

## 5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: LMR, CA, TPP, SIN, MLA

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

Mal	Chain	Bo	ond lengths	Bo	ond angles
MIOI	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	А	0.70	0/6595	0.86	0/8970
1	В	0.71	1/6595~(0.0%)	0.89	0/8970
1	С	0.72	0/6595	0.86	0/8970
1	D	0.72	0/6614	0.85	0/8996
1	Е	0.70	0/6614	0.85	0/8996
1	F	0.69	0/6595	0.85	1/8970~(0.0%)
1	G	0.71	0/6608	0.88	1/8987~(0.0%)
1	H	0.69	0/6606	0.86	1/8985~(0.0%)
All	All	0.70	1/52822~(0.0%)	0.86	3/71844~(0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
1	В	589	GLU	CD-OE1	7.17	1.33	1.25

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	Н	218	LYS	CB-CA-C	5.25	120.90	110.40
1	G	781	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	F	218	LYS	CB-CA-C	5.05	120.50	110.40

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



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	6418	0	6108	49	0
1	В	6418	0	6108	62	0
1	С	6418	0	6108	94	0
1	D	6433	0	6119	79	0
1	Е	6436	0	6118	78	0
1	F	6418	0	6108	78	0
1	G	6427	0	6113	69	0
1	Н	6428	0	6114	86	0
2	А	26	0	16	5	0
2	В	26	0	16	4	0
2	С	26	0	16	6	0
2	D	26	0	16	7	0
2	Е	26	0	16	5	0
2	F	26	0	16	1	0
2	G	26	0	16	5	0
2	Н	26	0	16	6	0
3	А	1	0	0	0	0
3	В	1	0	0	0	0
3	С	1	0	0	0	0
3	D	1	0	0	0	0
3	Е	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	Н	1	0	0	0	0
4	В	18	0	8	1	0
5	D	14	0	4	6	0
5	Е	7	0	2	1	0
6	Е	8	0	4	0	0
6	G	8	0	4	0	0
6	Н	8	0	4	0	0
7	А	211	0	0	3	0
7	В	215	0	0	3	0
7	С	92	0	0	1	0
7	D	77	0	0	4	0
7	Е	126	0	0	4	0
7	F	93	0	0	2	0
7	G	160	0	0	3	0
7	Н	132	0	0	3	0
All	All	52781	0	49050	573	0

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.

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 6.

All (573) 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:E:442:ARG:HA	1:E:444:GLN:HE22	1.21	1.00
1:D:441:ASN:HD22	1:D:499:SER:HB2	1.22	0.99
1:D:772:ASP:HA	7:D:1070:HOH:O	1.68	0.91
2:D:903:TPP:H2	2:D:903:TPP:HN42	1.35	0.90
1:E:441:ASN:HD22	1:E:499:SER:HB2	1.37	0.89
1:F:442:ARG:HA	1:F:444:GLN:HE22	1.37	0.88
1:E:442:ARG:HA	1:E:444:GLN:NE2	1.90	0.84
1:C:442:ARG:HA	1:C:444:GLN:HE22	1.44	0.83
1:E:444:GLN:H	1:E:444:GLN:HE21	1.25	0.81
1:G:140:PRO:HA	1:H:740:THR:CG2	2.09	0.81
1:A:442:ARG:HA	1:A:444:GLN:HE22	1.45	0.81
1:F:444:GLN:H	1:F:444:GLN:HE21	1.27	0.80
1:C:444:GLN:H	1:C:444:GLN:HE21	1.30	0.77
1:B:144:ALA:HB1	1:B:145:PRO:HD2	1.67	0.74
1:H:547:ASP:O	1:H:740:THR:HA	1.87	0.74
2:H:902:TPP:H2	2:H:902:TPP:HN42	1.52	0.74
1:H:442:ARG:HA	1:H:444:GLN:HE22	1.52	0.73
1:E:638:ASP:HB2	7:E:1108:HOH:O	1.89	0.72
1:A:589:GLU:OE2	7:A:1001:HOH:O	2.07	0.71
1:E:568[A]:HIS:O	1:E:568[A]:HIS:CD2	2.43	0.71
1:A:547:ASP:OD2	1:B:60:ARG:NH2	2.22	0.71
1:D:441:ASN:ND2	1:D:499:SER:HB2	2.03	0.70
1:D:547:ASP:O	1:D:740:THR:HA	1.91	0.70
1:H:390:ASN:HD22	1:H:392:GLU:HG2	1.55	0.70
1:G:740:THR:HG21	1:H:140:PRO:HA	1.74	0.69
1:F:230:ASP:OD1	1:F:246:GLU:OE2	2.11	0.69
1:G:552:SER:OG	1:G:553:HIS:ND1	2.24	0.68
2:H:902:TPP:HN42	2:H:902:TPP:C2	2.06	0.68
1:C:140:PRO:HA	1:D:740:THR:CG2	2.23	0.68
1:C:554:GLN:O	1:D:517:LYS:NZ	2.16	0.68
1:B:78:ILE:O	1:B:82:ILE:HG13	1.93	0.67
1:D:443:LEU:HD11	1:D:538:LEU:HD23	1.76	0.67
1:B:442:ARG:HA	1:B:444:GLN:HE22	1.58	0.67
1:E:441:ASN:ND2	1:E:499:SER:HB2	2.10	0.67
1:C:140:PRO:HA	1:D:740:THR:HG22	1.76	0.66
1:C:620:GLU:OE1	1:C:673:ASN:ND2	2.28	0.66
1:B:273:GLU:HG2	1:B:292:PRO:HG3	1.78	0.65
1:G:740:THR:CG2	1:H:140:PRO:HA	2.27	0.65



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	$ ext{overlap}( ext{\AA})$
2:D:903:TPP:H2	2:D:903:TPP:N4'	2.11	0.65
1:E:300:LYS:HE2	1:E:320:HIS:HA	1.80	0.64
1:G:60:ARG:NH2	1:H:547:ASP:OD2	2.31	0.64
1:H:356:VAL:HG21	1:H:361:LEU:HD11	1.80	0.63
1:H:766:ASP:HB3	1:H:769:LYS:HB3	1.80	0.63
1:H:435:PRO:HA	1:H:476:GLN:O	1.99	0.63
1:A:549:ASN:HD21	4:B:902:LMR:H3A	1.64	0.63
1:C:442:ARG:HA	1:C:444:GLN:NE2	2.11	0.63
1:D:144:ALA:HB1	1:D:145:PRO:HD2	1.80	0.63
1:A:144:ALA:HB1	1:A:145:PRO:HD2	1.82	0.62
1:E:541:SER:O	1:E:546:GLN:NE2	2.31	0.62
1:G:197:ASN:OD1	1:G:198:LYS:HE3	2.00	0.62
1:E:547:ASP:OD2	1:F:60:ARG:NH2	2.33	0.62
1:G:198:LYS:HG3	1:H:224:ILE:HG23	1.81	0.62
1:A:760:GLU:O	1:A:764:MET:HG3	1.99	0.61
1:A:799:THR:HG22	1:A:800:ASP:OD1	1.98	0.61
1:E:454:TRP:CE2	1:E:456:ALA:HB3	2.35	0.61
1:E:555:ASP:OD2	1:F:565:LYS:NZ	2.27	0.61
1:E:197:ASN:OD1	1:E:198:LYS:HE3	2.01	0.61
1:E:740:THR:OG1	1:F:140:PRO:HA	1.99	0.61
1:H:144:ALA:HB1	1:H:145:PRO:HD2	1.82	0.61
2:D:903:TPP:HN42	2:D:903:TPP:C2	2.11	0.60
1:G:612:LEU:HD21	1:G:628:TRP:CE2	2.35	0.60
1:G:543:VAL:HG21	1:G:734:TYR:CD1	2.36	0.60
2:A:900:TPP:H2	2:A:900:TPP:HN42	1.67	0.60
5:D:902:MLA:O1A	5:D:902:MLA:O3B	2.06	0.60
7:G:1012:HOH:O	2:H:902:TPP:H2	2.00	0.60
1:B:454:TRP:CE2	1:B:456:ALA:HB3	2.36	0.60
1:C:204:THR:HB	1:C:428:ARG:HH22	1.67	0.60
7:G:1149:HOH:O	1:H:548:HIS:HB3	2.01	0.60
1:A:576:TYR:HB3	1:A:587:ILE:HD13	1.83	0.59
1:G:441:ASN:HD22	1:G:499:SER:HB2	1.66	0.59
1:H:807:ASN:HD22	1:H:807:ASN:N	2.01	0.59
1:G:753:ASP:OD2	1:G:755:TYR:HB2	2.04	0.58
1:C:547:ASP:HB2	1:C:741:THR:O	2.04	0.58
1:C:756:GLU:HB2	1:C:781:ARG:HE	1.67	0.58
1:G:182:ASP:OD1	1:G:223:THR:HG21	2.04	0.58
1:G:505:VAL:HG11	1:G:558:VAL:HG21	1.85	0.58
1:H:701:ALA:HA	1:H:725:ASN:HB2	1.84	0.58
1:B:97:HIS:NE2	2:B:903:TPP:O3B	2.26	0.58
1:B:162:SER:OG	1:B:484:GLY:HA3	2.03	0.58



	is as pagen	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:F:219:ILE:HD11	2:F:900:TPP:C4	2.34	0.58
1:F:444:GLN:HE21	1:F:444:GLN:N	1.97	0.58
2:C:900:TPP:C2	5:D:901:MLA:C1	2.81	0.58
1:F:444:GLN:H	1:F:444:GLN:NE2	1.99	0.58
1:G:612:LEU:HD21	1:G:628:TRP:CZ2	2.39	0.58
1:E:498:TRP:CE2	1:E:537:LEU:HD13	2.39	0.57
1:E:313:THR:CG2	1:E:323:PRO:HB3	2.34	0.57
1:H:185:ALA:HA	1:H:190:LEU:HD12	1.85	0.57
1:C:612:LEU:HD11	1:C:628:TRP:HZ2	1.69	0.57
1:F:799:THR:HG22	1:F:800:ASP:OD1	2.05	0.57
1:F:660:ASP:OD1	1:F:804:SER:OG	2.23	0.57
1:G:788:ALA:HA	1:G:793:TYR:O	2.05	0.57
1:H:444:GLN:NE2	1:H:444:GLN:H	2.02	0.57
1:C:547:ASP:O	1:C:740:THR:HA	2.05	0.57
1:B:620:GLU:OE1	1:B:673:ASN:ND2	2.33	0.56
1:C:568:HIS:CD2	1:C:568:HIS:O	2.58	0.56
1:H:444:GLN:H	1:H:444:GLN:HE21	1.52	0.56
1:F:435:PRO:HA	1:F:476:GLN:O	2.05	0.56
2:C:900:TPP:H2	5:D:901:MLA:O1B	2.06	0.56
1:D:722:ASP:CG	1:D:722:ASP:O	2.45	0.56
1:D:379:GLY:HA3	1:D:491:LEU:O	2.05	0.55
1:D:286:VAL:HG13	1:E:459:ILE:O	2.07	0.55
1:E:200:VAL:O	7:E:1001:HOH:O	2.18	0.55
2:G:901:TPP:C2	2:G:901:TPP:HN42	2.20	0.55
1:E:215:ASN:HA	1:E:298:THR:O	2.07	0.55
1:G:766:ASP:HB3	1:G:769:LYS:HB3	1.89	0.55
1:G:803:TYR:O	1:G:806:VAL:HG23	2.07	0.55
2:E:902:TPP:HM41	1:F:477:LEU:HD22	1.90	0.54
1:C:300:LYS:HE2	1:C:320:HIS:HA	1.89	0.54
1:E:35:LEU:O	1:E:39:GLN:HG3	2.07	0.54
1:E:195:GLN:OE1	1:E:198:LYS:NZ	2.40	0.54
1:C:198:LYS:N	1:C:198:LYS:HD3	2.21	0.54
1:E:442:ARG:CA	1:E:444:GLN:NE2	2.69	0.54
1:C:214:LEU:HD11	1:C:226:SER:HA	1.90	0.54
1:F:637:ASN:HD22	1:F:700:THR:HA	1.72	0.54
1:C:134:SER:HA	1:D:740:THR:HG23	1.90	0.54
1:D:273:GLU:HG2	1:D:292:PRO:HG3	1.89	0.54
1:H:704:PRO:HA	1:H:728:ASN:HB3	1.89	0.54
1:G:215:ASN:HA	1:G:298:THR:O	2.08	0.54
1:A:737:GLU:HB3	1:A:749:VAL:HG13	1.90	0.54
1:E:804:SER:O	1:E:806:VAL:N	2.41	0.54



	A i a	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:430:PHE:HA	1:C:495:HIS:O	2.08	0.53
1:G:502:GLU:HG3	1:G:539:VAL:CG1	2.38	0.53
1:B:576:TYR:HA	1:B:675:ALA:O	2.07	0.53
1:D:611:TRP:CZ3	1:D:656:MET:HG3	2.44	0.53
1:F:182:ASP:CG	1:F:223:THR:HG21	2.28	0.53
1:F:534:SER:OG	1:F:597:LYS:HB2	2.07	0.53
1:F:591:CYS:O	1:F:594:SER:HB3	2.08	0.53
1:H:799:THR:HG21	7:H:1034:HOH:O	2.09	0.53
1:C:479:GLU:OE2	2:D:903:TPP:N1'	2.42	0.53
2:C:900:TPP:H2	2:C:900:TPP:HN42	1.74	0.53
1:D:151:ILE:HG23	1:D:377:ALA:HA	1.91	0.53
1:F:34:TYR:CE1	1:F:341:LEU:HD22	2.43	0.53
1:E:198:LYS:HG3	1:F:224:ILE:HG23	1.91	0.53
1:E:454:TRP:CZ2	1:E:456:ALA:HB3	2.44	0.53
1:C:199:LEU:O	1:C:453:GLN:NE2	2.43	0.52
1:H:46:PRO:HD3	1:H:127:GLN:HG3	1.91	0.52
1:B:547:ASP:O	1:B:740:THR:HA	2.09	0.52
2:B:903:TPP:HN42	2:B:903:TPP:C2	2.21	0.52
1:C:568:HIS:HB2	7:D:1068:HOH:O	2.08	0.52
1:G:235:GLU:OE2	1:H:238:HIS:ND1	2.34	0.52
1:H:96:GLY:HA3	1:H:153:GLU:O	2.10	0.52
1:C:620:GLU:CD	1:C:673:ASN:HD22	2.12	0.52
1:C:692:ASP:OD1	1:C:724:PRO:HD3	2.09	0.52
1:F:505:VAL:HG11	1:F:558:VAL:HG21	1.91	0.52
1:D:165:TYR:CD2	1:D:196:SER:HB2	2.44	0.52
1:B:50:GLU:OE2	1:B:50:GLU:HA	2.10	0.52
1:B:657:ALA:HA	1:B:801:TRP:CZ2	2.45	0.52
1:E:788:ALA:HA	1:E:793:TYR:O	2.10	0.52
1:G:286:VAL:HA	1:G:469:VAL:HG11	1.92	0.52
1:C:151:ILE:CG2	1:C:377:ALA:HA	2.40	0.52
1:F:399:VAL:HG21	1:F:610:THR:HG22	1.92	0.52
1:B:313:THR:CG2	1:B:323:PRO:HB3	2.40	0.52
1:B:459:ILE:O	1:H:284:ASP:HA	2.10	0.51
1:E:218:LYS:HB2	1:F:436:ASP:OD2	2.09	0.51
1:E:286:VAL:HA	1:E:469:VAL:HG11	1.93	0.51
1:F:379:GLY:HA3	1:F:491:LEU:O	2.10	0.51
2:A:900:TPP:N1'	1:B:479:GLU:OE2	2.43	0.51
1:C:214:LEU:HD11	1:C:226:SER:CA	2.40	0.51
1:F:766:ASP:HB3	1:F:769:LYS:HB3	1.93	0.51
1:A:90:VAL:O	1:A:176:VAL:HA	2.09	0.51
1:C:577:PHE:CE2	1:C:710:HIS:HB3	2.45	0.51



	lo us puge	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:766:ASP:HB3	1:C:769:LYS:HB3	1.91	0.51
1:D:442:ARG:HA	1:D:444:GLN:HE22	1.76	0.51
1:F:442:ARG:HA	1:F:444:GLN:NE2	2.15	0.51
1:H:637:ASN:ND2	1:H:700:THR:HA	2.25	0.51
1:G:620:GLU:OE1	1:G:673:ASN:ND2	2.44	0.51
1:D:28:TYR:O	1:D:31:VAL:HG12	2.11	0.51
1:G:281:ALA:HA	1:G:284:ASP:O	2.11	0.51
1:G:443:LEU:HD11	1:G:538:LEU:HD23	1.92	0.51
1:A:489:TYR:CE2	1:A:494:ARG:HB3	2.45	0.51
1:F:27:LYS:HB3	1:F:360:VAL:HG13	1.93	0.51
1:B:597:LYS:HD3	7:B:1049:HOH:O	2.10	0.51
1:C:383:ARG:NH1	1:C:385:ASP:OD1	2.43	0.51
1:H:505:VAL:HG11	1:H:558:VAL:HG21	1.93	0.51
1:A:398:GLU:HG2	1:A:406:TRP:CZ2	2.45	0.50
5:D:902:MLA:HC22	2:D:903:TPP:C2	2.42	0.50
1:G:144:ALA:HB1	1:G:145:PRO:HD2	1.94	0.50
1:D:734:TYR:CE2	1:D:736:GLU:HA	2.46	0.50
2:E:902:TPP:HN42	2:E:902:TPP:C2	2.25	0.50
1:H:646:ALA:HA	1:H:708:ALA:O	2.11	0.50
2:C:900:TPP:H2	5:D:901:MLA:C1	2.41	0.50
1:D:646:ALA:HA	1:D:708:ALA:O	2.12	0.50
1:H:700:THR:O	1:H:701:ALA:HB3	2.11	0.50
1:C:96:GLY:HA3	1:C:153:GLU:O	2.11	0.50
1:C:170:ASP:OD2	1:C:431:ARG:NE	2.40	0.50
1:F:163:HIS:HA	1:F:488:ALA:HB2	1.94	0.50
1:H:748:ARG:HA	1:H:753:ASP:OD2	2.12	0.50
1:B:286:VAL:HA	1:B:469:VAL:HG11	1.93	0.50
1:D:218:LYS:O	1:D:300:LYS:NZ	2.45	0.50
1:E:313:THR:HG21	1:E:323:PRO:CB	2.42	0.50
1:A:57:VAL:HG11	1:A:327:ALA:HB3	1.94	0.50
1:C:68:THR:N	1:C:69:PRO:HD2	2.26	0.50
1:C:736:GLU:OE1	1:D:520:GLU:OE2	2.29	0.50
1:F:144:ALA:HB1	1:F:145:PRO:HD2	1.93	0.50
1:E:486:LEU:O	1:E:490:LEU:HG	2.11	0.49
1:G:235:GLU:CD	1:H:238:HIS:HD1	2.15	0.49
1:H:219:ILE:HD11	2:H:902:TPP:C4	2.42	0.49
1:B:71:LEU:O	1:B:75:ILE:HG13	2.12	0.49
1:B:441:ASN:HD22	1:B:499:SER:HB2	1.77	0.49
1:B:288:ARG:HD3	1:B:455:ASP:O	2.11	0.49
1:D:21:ALA:O	1:D:25:VAL:HG23	2.13	0.49
1:E:54:ARG:HG2	7:E:1063:HOH:O	2.11	0.49



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:E:657:ALA:HA	1:E:801:TRP:CZ2	2.48	0.49
1:F:543:VAL:HG23	1:F:554:GLN:HB3	1.95	0.49
1:A:134:SER:CB	1:B:740:THR:HG21	2.42	0.49
1:D:583:MET:HA	1:D:617:ALA:HB1	1.94	0.49
1:G:552:SER:HG	1:G:553:HIS:CE1	2.24	0.49
1:G:441:ASN:ND2	1:G:499:SER:HB2	2.27	0.49
1:C:65:TRP:HE1	1:C:304:CYS:HB3	1.78	0.49
1:C:404:HIS:ND1	1:C:630:TRP:CE2	2.81	0.49
1:E:45:ASN:N	1:E:46:PRO:CD	2.76	0.49
1:F:28:TYR:CD1	1:F:28:TYR:C	2.86	0.49
1:H:807:ASN:HD22	1:H:807:ASN:H	1.61	0.49
1:A:657:ALA:HA	1:A:801:TRP:CZ2	2.48	0.48
1:E:135:TYR:HE2	1:F:789:VAL:O	1.95	0.48
1:G:151:ILE:CG2	1:G:377:ALA:HA	2.43	0.48
1:E:219:ILE:HD11	2:E:902:TPP:C4	2.43	0.48
1:D:274:ILE:HG13	1:D:292:PRO:HG2	1.95	0.48
1:H:195:GLN:OE1	1:H:198:LYS:NZ	2.46	0.48
1:H:342:GLU:HG2	7:H:1016:HOH:O	2.13	0.48
2:A:900:TPP:HN42	2:A:900:TPP:C2	2.25	0.48
1:G:97:HIS:NE2	2:G:901:TPP:O3B	2.28	0.48
1:D:708:ALA:HB1	1:D:752:ILE:HD11	1.95	0.48
1:D:30:ARG:NH1	7:D:1003:HOH:O	2.46	0.48
1:F:668:LYS:HE2	7:F:1093:HOH:O	2.13	0.48
1:D:612:LEU:HD21	1:D:628:TRP:CE2	2.49	0.48
1:E:182:ASP:CG	1:E:223:THR:HG21	2.34	0.48
1:C:623:LYS:HE3	1:C:623:LYS:HA	1.96	0.48
1:D:430:PHE:HA	1:D:495:HIS:O	2.14	0.48
1:C:134:SER:HA	1:D:740:THR:CG2	2.44	0.48
1:B:489:TYR:CE2	1:B:494:ARG:HB3	2.48	0.48
1:A:778:GLU:OE1	1:A:778:GLU:HA	2.14	0.47
1:B:215:ASN:HA	1:B:298:THR:O	2.14	0.47
1:B:383:ARG:NH1	1:B:385:ASP:OD1	2.46	0.47
2:B:903:TPP:HN42	2:B:903:TPP:H2	1.78	0.47
1:D:773:LYS:O	1:D:776:GLU:N	2.46	0.47
1:D:799:THR:HB	7:D:1028:HOH:O	2.14	0.47
1:A:479:GLU:OE2	2:B:903:TPP:N1'	2.47	0.47
1:G:47:LEU:HD11	1:G:354:GLY:HA2	1.95	0.47
1:G:591:CYS:O	1:G:594:SER:OG	2.27	0.47
1:C:9:PRO:HA	1:C:87:GLN:OE1	2.14	0.47
1:C:630:TRP:CZ3	1:C:631:ALA:HB2	2.50	0.47
1:F:110:GLY:O	1:F:114:GLU:HG3	2.15	0.47



	hi a	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:430:PHE:HA	1:A:495:HIS:O	2.15	0.47
1:D:54:ARG:HD2	1:D:328:ARG:O	2.15	0.47
1:C:62:VAL:CG1	1:C:134:SER:HB3	2.45	0.47
1:E:547:ASP:O	1:E:740:THR:HA	2.14	0.47
1:E:568[A]:HIS:O	1:E:568[A]:HIS:HD2	1.92	0.47
1:H:188:GLY:N	1:H:189:PRO:CD	2.78	0.47
1:B:68:THR:N	1:B:69:PRO:HD2	2.30	0.47
1:B:454:TRP:CZ2	1:B:456:ALA:HB3	2.50	0.47
1:C:140:PRO:HA	1:D:740:THR:HG21	1.95	0.47
1:D:230:ASP:OD1	1:D:246:GLU:OE2	2.32	0.47
1:F:644:LEU:HD11	1:F:662:LEU:HD12	1.96	0.47
1:H:168:ILE:HD13	1:H:208:VAL:HG23	1.97	0.47
1:A:171:ASN:ND2	1:A:174:LEU:HD22	2.30	0.47
1:H:182:ASP:CG	1:H:223:THR:HG21	2.34	0.47
1:F:498:TRP:CE2	1:F:537:LEU:HD13	2.50	0.47
1:G:740:THR:HG23	1:H:134:SER:HA	1.95	0.47
1:B:770:TYR:O	1:B:773:LYS:N	2.48	0.47
1:C:375:PRO:HB2	1:C:382:ILE:HD11	1.96	0.47
1:F:660:ASP:CG	1:F:804:SER:OG	2.53	0.47
1:B:444:GLN:H	1:B:444:GLN:NE2	2.13	0.46
1:D:185:ALA:HA	1:D:190:LEU:HD12	1.97	0.46
1:D:383:ARG:NH1	1:D:385:ASP:OD1	2.49	0.46
1:F:709:TYR:CE2	1:F:715:ASP:HB2	2.50	0.46
1:C:378:ASN:O	1:C:381:VAL:HG13	2.15	0.46
1:C:568:HIS:O	1:C:568:HIS:CG	2.69	0.46
1:G:630:TRP:CZ3	1:G:631:ALA:HB2	2.50	0.46
1:H:453:GLN:HB3	1:H:474:VAL:HG22	1.97	0.46
1:A:230:ASP:OD1	1:A:246:GLU:OE2	2.33	0.46
2:A:900:TPP:HM41	1:B:477:LEU:HD22	1.97	0.46
1:C:742:THR:HG23	1:D:136:PRO:HG3	1.96	0.46
1:E:313:THR:HG21	1:E:323:PRO:HB2	1.98	0.46
1:F:46:PRO:HB2	1:F:126:LEU:HD23	1.97	0.46
1:F:502:GLU:HA	1:F:539:VAL:HG13	1.97	0.46
1:C:163:HIS:HA	1:C:488:ALA:HB2	1.98	0.46
1:E:394:TYR:HB2	1:E:585:LEU:HD21	1.98	0.46
1:G:140:PRO:HA	1:H:740:THR:HG21	1.93	0.46
1:B:643:VAL:HB	1:B:705:VAL:HG22	1.98	0.46
1:F:464:ASP:HA	1:F:467:MET:CE	2.45	0.46
1:F:541:SER:HB3	1:F:546:GLN:NE2	2.30	0.46
1:F:676:ASP:C	1:F:676:ASP:OD1	2.53	0.46
1:B:435:PRO:HA	1:B:476:GLN:O	2.16	0.46



	h h	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:C:44:SER:OG	1:C:56:ASP:HA	2.16	0.46
1:C:502:GLU:HA	1:C:539:VAL:HG13	1.97	0.46
1:F:806:VAL:HG12	1:F:807:ASN:N	2.29	0.46
1:A:542:HIS:CG	1:A:710:HIS:HE1	2.33	0.46
1:C:612:LEU:HD11	1:C:628:TRP:CZ2	2.50	0.46
1:D:170:ASP:OD1	1:D:428:ARG:NH1	2.49	0.46
1:D:238:HIS:HA	1:D:242:TYR:O	2.16	0.46
1:D:612:LEU:HD21	1:D:628:TRP:CZ2	2.50	0.46
1:E:198:LYS:HE2	7:F:1067:HOH:O	2.16	0.46
1:C:690:LEU:O	1:C:723:ARG:NH2	2.40	0.46
1:D:454:TRP:CE2	1:D:456:ALA:HB3	2.50	0.46
1:E:142:HIS:HD2	1:E:155:GLY:HA2	1.81	0.46
1:G:763:ARG:NH2	1:G:778:GLU:OE2	2.42	0.46
1:H:747:VAL:HG23	1:H:753:ASP:HB3	1.98	0.46
1:E:726:HIS:NE2	1:F:727:ASP:OD1	2.41	0.46
1:C:767:ALA:O	1:C:771:ALA:HB2	2.16	0.45
1:G:218:LYS:HB2	1:H:436:ASP:OD2	2.16	0.45
1:H:61:LEU:HD12	1:H:325:ALA:O	2.16	0.45
1:G:540:SER:O	1:G:541:SER:C	2.54	0.45
1:C:90:VAL:O	1:C:176:VAL:HA	2.16	0.45
1:C:313:THR:O	1:C:319:SER:HB3	2.16	0.45
1:E:465:GLU:OE2	1:F:318:ARG:NH2	2.50	0.45
1:E:543:VAL:HG21	1:E:734:TYR:CD1	2.51	0.45
1:F:47:LEU:HD11	1:F:354:GLY:HA2	1.98	0.45
1:D:57:VAL:HG11	1:D:327:ALA:HB3	1.99	0.45
1:B:351:ASP:OD1	1:B:351:ASP:C	2.55	0.45
1:C:131:ARG:O	1:C:135:TYR:HB2	2.17	0.45
1:D:131:ARG:O	1:D:135:TYR:HB2	2.16	0.45
1:D:459:ILE:O	1:E:284:ASP:HA	2.16	0.45
1:H:300:LYS:HE2	1:H:320:HIS:HA	1.97	0.45
1:A:99:GLY:N	1:A:100:PRO:CD	2.79	0.45
1:A:435:PRO:HA	1:A:476:GLN:O	2.17	0.45
1:C:230:ASP:OD1	1:C:246:GLU:OE2	2.35	0.45
1:D:415:LEU:HD23	1:D:538:LEU:HD22	1.97	0.45
1:D:650:VAL:HB	1:D:651:PRO:HD3	1.99	0.45
1:H:2:THR:N	1:H:429:ASP:OD2	2.49	0.45
1:A:134:SER:HB3	1:B:740:THR:HG21	1.99	0.45
1:A:300:LYS:HE2	1:A:320:HIS:HA	1.99	0.45
1:B:152:HIS:HB3	7:B:1143:HOH:O	2.15	0.45
1:C:144:ALA:HB1	1:C:145:PRO:HD2	1.99	0.45
1:C:214:LEU:O	1:C:297:ARG:HA	2.16	0.45



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:787:PHE:CE1	1:D:791:ASN:ND2	2.84	0.45
1:H:165:TYR:CD2	1:H:196:SER:HB2	2.52	0.45
1:B:96:GLY:HA3	1:B:153:GLU:O	2.16	0.45
2:C:900:TPP:N1'	1:D:479:GLU:OE2	2.50	0.45
1:D:286:VAL:HA	1:D:469:VAL:HG11	1.97	0.45
1:B:300:LYS:HE2	1:B:320:HIS:HA	1.98	0.45
1:C:736:GLU:O	1:D:524:ARG:NH2	2.42	0.45
1:F:756:GLU:OE1	1:F:778:GLU:OE2	2.34	0.45
1:G:552:SER:OG	1:G:553:HIS:CE1	2.69	0.45
2:H:902:TPP:C2	2:H:902:TPP:N4'	2.78	0.45
1:E:435:PRO:HA	1:E:476:GLN:O	2.16	0.45
1:A:778:GLU:OE1	1:A:781:ARG:HD3	2.16	0.44
1:C:452:LYS:HA	1:C:473:VAL:O	2.16	0.44
1:E:722:ASP:OD1	1:E:722:ASP:C	2.56	0.44
1:H:390:ASN:HD22	1:H:392:GLU:CG	2.25	0.44
1:B:722:ASP:OD1	1:B:722:ASP:C	2.55	0.44
1:E:313:THR:CG2	1:E:323:PRO:CB	2.95	0.44
1:A:216:GLY:HA2	1:A:226:SER:CB	2.48	0.44
1:C:2:THR:N	1:C:429:ASP:OD2	2.50	0.44
1:D:498:TRP:CE2	1:D:537:LEU:HD13	2.53	0.44
1:E:497:ILE:HA	1:E:536:ASN:O	2.17	0.44
1:G:791:ASN:HB3	1:G:793:TYR:CE1	2.52	0.44
1:A:246:GLU:HA	1:A:295:ILE:O	2.17	0.44
1:B:799:THR:HG22	1:B:800:ASP:OD1	2.17	0.44
1:C:165:TYR:CD2	1:C:196:SER:HB2	2.52	0.44
1:E:142:HIS:CD2	1:E:155:GLY:HA2	2.52	0.44
1:G:143:PHE:O	1:G:153:GLU:HA	2.17	0.44
1:G:408:GLN:NE2	1:G:408:GLN:HA	2.33	0.44
1:G:520:GLU:OE2	1:H:736:GLU:OE1	2.34	0.44
2:C:900:TPP:C2	2:C:900:TPP:HN42	2.30	0.44
1:E:296:PHE:CZ	1:E:298:THR:HG21	2.52	0.44
1:E:803:TYR:O	1:E:806:VAL:HG23	2.17	0.44
1:G:759:ALA:O	1:G:763:ARG:HG3	2.17	0.44
1:H:230:ASP:OD1	1:H:246:GLU:OE2	2.35	0.44
1:C:454:TRP:CE2	1:C:456:ALA:HB3	2.52	0.44
1:C:542:HIS:O	1:C:546:GLN:HG2	2.18	0.44
1:D:620:GLU:OE1	1:D:673:ASN:ND2	2.44	0.44
1:F:85:HIS:NE2	1:F:268:GLU:OE2	2.51	0.44
1:G:555:ASP:OD2	1:H:565:LYS:NZ	2.27	0.44
1:G:645:ALA:HA	1:G:672:VAL:O	2.17	0.44
1:B:144:ALA:HB1	1:B:145:PRO:CD	2.43	0.44



	i i i i i i i i i i i i i i i i i i i	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:696:ALA:O	1:C:700:THR:CA	2.65	0.44
1:E:230:ASP:OD1	1:E:246:GLU:OE2	2.36	0.44
1:E:505:VAL:HG11	1:E:558:VAL:HG21	2.00	0.44
1:F:57:VAL:HG12	1:F:58:LYS:N	2.33	0.44
1:F:107:TYR:OH	1:F:126:LEU:HD12	2.18	0.44
1:B:316:SER:OG	1:B:317:TRP:N	2.49	0.44
1:B:614:LEU:HD12	1:B:614:LEU:HA	1.85	0.44
1:D:398:GLU:HG2	1:D:406:TRP:CH2	2.53	0.44
1:E:436:ASP:OD2	1:F:218:LYS:HB2	2.17	0.44
1:A:180:VAL:HG11	1:A:190:LEU:HD11	1.99	0.43
1:A:444:GLN:H	1:A:444:GLN:NE2	2.16	0.43
1:C:547:ASP:OD2	1:D:60:ARG:NH2	2.51	0.43
1:D:478:SER:O	1:D:482:MET:HG2	2.18	0.43
1:F:657:ALA:HA	1:F:801:TRP:CZ2	2.53	0.43
1:H:541:SER:OG	1:H:605:LYS:HD3	2.18	0.43
1:C:518:TRP:O	1:C:522:THR:OG1	2.31	0.43
1:C:651:PRO:HB3	1:C:708:ALA:HB1	2.00	0.43
1:D:68:THR:N	1:D:69:PRO:HD2	2.33	0.43
1:D:501:TYR:HE2	5:D:901:MLA:C2	2.31	0.43
2:E:902:TPP:N1'	1:F:479:GLU:OE2	2.50	0.43
1:F:583:MET:HG3	1:F:587:ILE:HD11	2.00	0.43
1:B:90:VAL:O	1:B:176:VAL:HA	2.18	0.43
1:B:201:ASN:HB2	1:B:469:VAL:O	2.19	0.43
1:C:630:TRP:CE3	1:C:631:ALA:HB2	2.54	0.43
1:C:723:ARG:O	1:C:726:HIS:ND1	2.43	0.43
1:E:723:ARG:O	1:E:726:HIS:ND1	2.51	0.43
1:A:623:LYS:NZ	1:A:694:GLU:OE2	2.35	0.43
1:C:432:ILE:O	1:C:473:VAL:HA	2.19	0.43
1:D:157:LEU:HB3	1:D:184:GLU:HG3	2.01	0.43
1:G:19:GLU:OE2	1:G:261:ARG:NH1	2.51	0.43
1:H:548:HIS:H	1:H:548:HIS:CD2	2.37	0.43
5:E:901:MLA:O3A	2:E:902:TPP:H2	2.19	0.43
1:G:50:GLU:HB3	7:G:1154:HOH:O	2.18	0.43
1:G:195:GLN:OE1	1:G:198:LYS:NZ	2.52	0.43
1:H:288:ARG:HD3	1:H:455:ASP:O	2.19	0.43
1:D:151:ILE:CG2	1:D:377:ALA:HA	2.49	0.43
1:D:744:TYR:HB3	1:D:794:ASP:OD1	2.19	0.43
1:F:96:GLY:HA3	1:F:153:GLU:O	2.18	0.43
1:F:404:HIS:CD2	1:F:630:TRP:CD2	3.05	0.43
1:G:454:TRP:CZ2	1:G:456:ALA:HB3	2.54	0.43
1:A:9:PRO:HB2	1:A:10:TRP:CD1	2.53	0.43



	in the page.	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:34:TYR:CE2	1:A:346:PRO:HG3	2.54	0.43
1:A:568:HIS:O	1:A:568:HIS:CD2	2.71	0.43
1:A:576:TYR:HA	1:A:675:ALA:O	2.19	0.43
1:F:614:LEU:O	1:F:617:ALA:HB3	2.19	0.43
1:H:46:PRO:HD3	1:H:127:GLN:CG	2.47	0.43
1:D:163:HIS:HA	1:D:488:ALA:HB2	2.00	0.43
1:F:430:PHE:HA	1:F:495:HIS:O	2.19	0.43
1:F:556:PRO:HD2	1:F:712:TYR:CE2	2.54	0.43
1:A:41:TYR:O	1:A:57:VAL:HA	2.19	0.43
1:C:644:LEU:O	1:C:671:VAL:HA	2.18	0.43
1:H:583:MET:HA	1:H:617:ALA:HB1	2.00	0.43
1:B:652:THR:O	1:B:656:MET:HG2	2.19	0.43
1:C:33:ASN:ND2	7:C:1017:HOH:O	2.52	0.43
1:D:454:TRP:O	1:D:469:VAL:HA	2.19	0.43
1:H:444:GLN:HE21	1:H:444:GLN:N	2.17	0.43
1:H:807:ASN:N	1:H:807:ASN:ND2	2.66	0.43
1:B:748:ARG:O	1:B:781:ARG:NH2	2.51	0.42
1:C:633:THR:OG1	1:C:668:LYS:HA	2.19	0.42
2:D:903:TPP:N4'	2:D:903:TPP:C2	2.77	0.42
1:C:709:TYR:CE2	1:C:711:SER:HB3	2.54	0.42
1:H:645:ALA:HA	1:H:672:VAL:O	2.19	0.42
1:B:313:THR:CG2	1:B:323:PRO:CB	2.98	0.42
1:B:543:VAL:HG21	1:B:734:TYR:CD1	2.53	0.42
1:C:47:LEU:HD11	1:C:354:GLY:HA2	2.01	0.42
1:F:699:PHE:CD1	1:F:729:PHE:CZ	3.07	0.42
1:G:156:GLU:HG3	1:H:504:PHE:CD1	2.55	0.42
1:H:197:ASN:OD1	1:H:198:LYS:HE3	2.19	0.42
1:A:434:GLY:O	1:A:475:GLU:HA	2.19	0.42
1:A:583:MET:HA	1:A:617:ALA:HB1	2.01	0.42
1:C:435:PRO:HA	1:C:476:GLN:O	2.19	0.42
1:D:340:TRP:O	1:D:343:SER:OG	2.27	0.42
1:D:408:GLN:NE2	1:D:408:GLN:HA	2.35	0.42
1:D:646:ALA:HB2	1:D:655:ILE:HG13	2.01	0.42
1:G:479:GLU:OE2	2:H:902:TPP:N1'	2.53	0.42
1:G:726:HIS:NE2	1:H:727:ASP:OD1	2.52	0.42
1:H:421:ASP:O	1:H:425:ASN:ND2	2.51	0.42
1:C:47:LEU:HD11	1:C:354:GLY:CA	2.50	0.42
1:E:47:LEU:HD11	1:E:354:GLY:HA2	2.02	0.42
1:F:65:TRP:HE1	1:F:304:CYS:HB3	1.84	0.42
1:G:655:ILE:HD13	1:G:655:ILE:HA	1.93	0.42
1:G:742:THR:HG23	1:H:136:PRO:HG3	2.01	0.42



	A A A	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:H:787:PHE:CD1	1:H:787:PHE:C	2.92	0.42
1:A:54:ARG:NH1	1:A:331:GLU:HG2	2.34	0.42
1:E:161:LEU:HD23	1:E:161:LEU:HA	1.91	0.42
1:F:170:ASP:OD2	1:F:489:TYR:OH	2.35	0.42
1:G:181:GLY:HA3	2:G:901:TPP:O1A	2.20	0.42
1:G:433:PHE:HB2	1:G:498:TRP:HB3	2.02	0.42
1:G:737:GLU:OE2	1:H:568[B]:HIS:CD2	2.72	0.42
1:H:655:ILE:HD13	1:H:757:LEU:HD13	2.02	0.42
1:C:75:ILE:HG21	1:C:105:GLN:HG3	2.00	0.42
1:E:44:SER:O	1:E:56:ASP:HB3	2.19	0.42
1:E:109:ASP:O	1:E:370:ARG:HD2	2.20	0.42
1:E:434:GLY:O	1:E:475:GLU:HA	2.20	0.42
1:E:658:ALA:O	1:E:662:LEU:HG	2.20	0.42
1:G:140:PRO:HA	1:H:740:THR:HG23	1.94	0.42
1:H:49:LYS:HE3	1:H:123:GLU:OE2	2.20	0.42
1:E:152:HIS:HA	7:E:1112:HOH:O	2.19	0.42
1:E:777:LEU:HD12	1:E:777:LEU:HA	1.94	0.42
1:F:434:GLY:O	1:F:475:GLU:HA	2.18	0.42
1:H:38:GLY:HA3	1:H:130:PHE:CE2	2.55	0.42
1:H:369:LEU:HD12	1:H:369:LEU:HA	1.96	0.42
1:A:759:ALA:O	1:A:763:ARG:HG3	2.19	0.42
1:C:415:LEU:CD2	1:C:538:LEU:HD13	2.50	0.42
1:D:571:HIS:HE1	1:D:686:ASN:OD1	2.02	0.42
1:E:77:HIS:NE2	1:E:260:HIS:ND1	2.60	0.42
1:G:219:ILE:O	1:G:317:TRP:HB2	2.19	0.42
1:H:9:PRO:HB2	1:H:10:TRP:CD1	2.55	0.42
1:B:490:LEU:HD11	1:B:535:MET:HA	2.02	0.41
1:C:644:LEU:HD11	1:C:662:LEU:HD12	2.02	0.41
1:D:214:LEU:HD11	1:D:226:SER:HA	2.01	0.41
1:F:464:ASP:HA	1:F:467:MET:HE2	2.01	0.41
1:F:681:GLN:HG3	1:F:719:LEU:HD22	2.02	0.41
1:H:185:ALA:HA	1:H:190:LEU:CD1	2.49	0.41
1:B:427:PRO:C	1:B:428:ARG:HG2	2.41	0.41
1:D:375:PRO:HB2	1:D:382:ILE:HD11	2.02	0.41
1:D:704:PRO:HA	1:D:728:ASN:HB3	2.02	0.41
1:H:163:HIS:HA	1:H:488:ALA:HB2	2.01	0.41
1:A:568:HIS:HB2	7:B:1198:HOH:O	2.20	0.41
1:C:218:LYS:O	1:C:300:LYS:NZ	2.52	0.41
1:E:391:LEU:HD21	1:E:589:GLU:HB2	2.01	0.41
1:E:578:ALA:HB1	1:E:584:LEU:HB2	2.02	0.41
1:F:189:PRO:HG3	1:F:480:HIS:CD2	2.55	0.41



	h h	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:497:ILE:HA	1:C:536:ASN:O	2.20	0.41
1:H:190:LEU:C	1:H:190:LEU:HD13	2.40	0.41
1:A:452:LYS:HA	1:A:473:VAL:O	2.21	0.41
1:F:296:PHE:CZ	1:F:298:THR:HG21	2.55	0.41
1:H:637:ASN:HD22	1:H:700:THR:HA	1.86	0.41
1:B:65:TRP:NE1	1:B:304:CYS:HB3	2.36	0.41
1:E:669:PHE:O	1:E:669:PHE:CD1	2.72	0.41
1:F:433:PHE:CE2	1:F:485:PHE:HB3	2.55	0.41
1:F:502:GLU:OE1	1:F:543:VAL:N	2.53	0.41
1:H:313:THR:HG23	1:H:323:PRO:CB	2.50	0.41
1:B:41:TYR:CE2	1:B:61:LEU:HD13	2.55	0.41
1:B:391:LEU:HG	1:B:614:LEU:HD21	2.03	0.41
1:C:453:GLN:HG3	1:C:471:GLY:N	2.36	0.41
1:E:201:ASN:HB2	1:E:469:VAL:O	2.20	0.41
1:F:748:ARG:HA	1:F:753:ASP:OD2	2.20	0.41
7:A:1185:HOH:O	1:B:131:ARG:HD3	2.21	0.41
1:B:491:LEU:HD23	1:B:532:ILE:HD13	2.02	0.41
1:C:477:LEU:HD13	2:D:903:TPP:HM42	2.02	0.41
1:C:543:VAL:HG23	1:C:554:GLN:HB3	2.03	0.41
1:E:182:ASP:OD1	1:E:223:THR:HG21	2.20	0.41
1:E:396:VAL:HB	1:E:582:ASN:HD21	1.86	0.41
1:E:556:PRO:HD2	1:E:712:TYR:CE2	2.56	0.41
1:G:170:ASP:OD1	1:G:428:ARG:NH1	2.54	0.41
2:G:901:TPP:HN42	2:G:901:TPP:H2	1.85	0.41
1:H:161:LEU:HD23	1:H:161:LEU:HA	1.92	0.41
1:H:569:ASN:OD1	1:H:687:ASP:CG	2.59	0.41
1:A:719:LEU:HD23	1:A:719:LEU:HA	1.91	0.41
1:C:238:HIS:HA	1:C:242:TYR:O	2.20	0.41
1:D:256:HIS:O	1:D:260:HIS:CD2	2.73	0.41
1:D:502:GLU:HA	1:D:539:VAL:HG13	2.03	0.41
1:E:78:ILE:O	1:E:82:ILE:HG13	2.20	0.41
1:E:134:SER:OG	1:E:141:SER:HB3	2.21	0.41
1:E:417:ALA:O	1:E:420:ARG:HB3	2.21	0.41
1:E:737:GLU:OE2	1:F:568:HIS:ND1	2.54	0.41
1:F:806:VAL:CG1	1:F:807:ASN:N	2.83	0.41
1:G:219:ILE:HG13	2:G:901:TPP:H62	2.02	0.41
1:G:717:ARG:HD3	1:H:721:TYR:CG	2.55	0.41
1:H:439:ALA:HA	1:H:444:GLN:NE2	2.36	0.41
1:A:709:TYR:CE2	1:A:711:SER:HB3	2.55	0.41
1:B:198:LYS:NZ	1:B:240:MET:O	2.53	0.41
1:B:503:SER:HB3	1:B:553:HIS:O	2.21	0.41



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:281:ALA:C	1:C:283:THR:H	2.24	0.41
1:C:531:PRO:HA	1:C:596:ASN:OD1	2.21	0.41
1:C:540:SER:O	1:C:541:SER:C	2.59	0.41
1:C:737:GLU:HB2	1:C:750:ASN:OD1	2.21	0.41
1:F:31:VAL:O	1:F:35:LEU:HG	2.21	0.41
1:G:96:GLY:HA3	1:G:153:GLU:O	2.21	0.41
1:G:802:VAL:CG1	1:G:806:VAL:HG21	2.51	0.41
1:H:409:LEU:HD23	1:H:409:LEU:HA	1.94	0.41
1:H:702:ASP:O	1:H:728:ASN:ND2	2.54	0.41
1:H:709:TYR:O	1:H:733:GLY:HA2	2.20	0.41
1:A:198:LYS:HE2	7:A:1126:HOH:O	2.21	0.40
1:D:313:THR:CG2	1:D:323:PRO:CB	2.99	0.40
1:F:127:GLN:HE21	1:F:127:GLN:HB3	1.62	0.40
1:G:543:VAL:CG2	1:G:734:TYR:CD1	3.04	0.40
1:G:709:TYR:CE2	1:G:715:ASP:HB2	2.56	0.40
1:A:169:MET:HA	1:A:205:ASP:OD1	2.20	0.40
1:B:91:ILE:HG22	1:B:177:PRO:HG2	2.02	0.40
1:C:109:ASP:O	1:C:370:ARG:HD2	2.21	0.40
1:D:546:GLN:OE1	1:D:549:ASN:HB2	2.21	0.40
1:G:406:TRP:CG	1:G:407:GLY:N	2.89	0.40
1:G:502:GLU:HA	1:G:539:VAL:HG13	2.04	0.40
1:B:313:THR:HG21	1:B:323:PRO:CB	2.52	0.40
1:B:796:PRO:HA	1:B:799:THR:HB	2.02	0.40
1:C:633:THR:O	1:C:635:LYS:HE2	2.22	0.40
1:D:35:LEU:O	1:D:39:GLN:HG3	2.22	0.40
1:E:740:THR:HG21	1:F:141:SER:HB2	2.04	0.40
1:F:324:LEU:HD21	1:F:336:VAL:HB	2.03	0.40
1:F:410:GLU:OE1	1:F:442:ARG:HD2	2.21	0.40
1:H:709:TYR:CE2	1:H:711:SER:HB3	2.56	0.40
1:A:737:GLU:CB	1:A:749:VAL:HG13	2.51	0.40
2:A:900:TPP:CM4	1:B:477:LEU:HD22	2.51	0.40
1:B:399:VAL:HG21	1:B:610:THR:HG22	2.02	0.40
1:C:115:THR:HG22	1:C:116:PHE:CD1	2.57	0.40
1:C:182:ASP:CG	1:C:223:THR:HG21	2.41	0.40
1:D:216:GLY:HA2	1:D:226:SER:CB	2.52	0.40
1:F:284:ASP:CG	1:F:287:HIS:HD1	2.24	0.40
1:H:198:LYS:HE2	7:H:1087:HOH:O	2.21	0.40
1:A:669:PHE:O	1:A:669:PHE:CD1	2.74	0.40
1:A:709:TYR:CE2	1:A:715:ASP:HB2	2.56	0.40
1:C:679:SER:HA	1:C:689:ALA:HA	2.04	0.40
1:H:799:THR:HG22	1:H:800:ASP:N	2.36	0.40



There are no symmetry-related clashes.

### 5.3 Torsion angles (i)

#### 5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
1	А	805/831~(97%)	761 (94%)	43~(5%)	1 (0%)	51	73
1	В	805/831~(97%)	764 (95%)	39~(5%)	2~(0%)	47	68
1	С	805/831~(97%)	735 (91%)	61 (8%)	9(1%)	14	26
1	D	807/831~(97%)	736 (91%)	65 (8%)	6 (1%)	22	39
1	Ε	807/831~(97%)	740 (92%)	62~(8%)	5 (1%)	25	43
1	F	805/831~(97%)	752 (93%)	49 (6%)	4 (0%)	29	48
1	G	806/831~(97%)	748 (93%)	53~(7%)	5 (1%)	25	43
1	Н	806/831~(97%)	763 (95%)	39~(5%)	4 (0%)	29	48
All	All	6446/6648~(97%)	5999 (93%)	411 (6%)	36 (1%)	29	43

All (36) Ramachandran outliers are listed below:

Mol	Chain	$\operatorname{Res}$	Type
1	С	714	HIS
1	G	54	ARG
1	С	302	TRP
1	D	774	ILE
1	Е	805	GLY
1	Е	808	THR
1	В	578	ALA
1	С	520	GLU
1	С	697	ASP
1	С	739	SER
1	С	804	SER
1	D	725	ASN
1	F	771	ALA
1	F	807	ASN



Mol	Chain	Res	Type
1	Н	88	ASN
1	Н	700	THR
1	Н	701	ALA
1	С	88	ASN
1	С	630	TRP
1	D	302	TRP
1	D	568[A]	HIS
1	D	568[B]	HIS
1	F	302	TRP
1	F	357	LYS
1	А	15	ALA
1	С	652	THR
1	В	15	ALA
1	D	533	ALA
1	Е	442	ARG
1	Е	771	ALA
1	G	552	SER
1	G	568[A]	HIS
1	G	568[B]	HIS
1	G	739	SER
1	Н	739	SER
1	Е	752	ILE

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#### 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	А	676/693~(98%)	657~(97%)	19 (3%)	43	70
1	В	676/693~(98%)	658~(97%)	18 (3%)	44	71
1	С	676/693~(98%)	644 (95%)	32~(5%)	26	49
1	D	678/693~(98%)	650~(96%)	28 (4%)	30	55
1	Е	678/693~(98%)	649~(96%)	29 (4%)	29	53
1	F	676/693~(98%)	648~(96%)	28 (4%)	30	55
1	G	677/693~(98%)	655~(97%)	22 (3%)	39	65



Mol	Chain	Analysed	Rotameric	Outliers	Percentile	es
1	Н	677/693~(98%)	649~(96%)	28 (4%)	30 55	
All	All	5414/5544 (98%)	5210 (96%)	204 (4%)	33 58	

All (204) residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
1	А	11	LYS
1	А	20	GLU
1	А	49	LYS
1	А	60	ARG
1	А	105	GLN
1	А	198	LYS
1	А	321	GLN
1	А	353	ASN
1	А	369	LEU
1	А	444	GLN
1	А	477	LEU
1	А	638	ASP
1	А	668	LYS
1	А	700	THR
1	А	740	THR
1	А	749	VAL
1	А	775	ASP
1	А	777	LEU
1	А	779	LYS
1	В	2	THR
1	В	49	LYS
1	В	55	GLU
1	В	105	GLN
1	В	147	THR
1	В	190	LEU
1	В	198	LYS
1	В	255	ASP
1	В	273	GLU
1	В	353	ASN
1	В	444	GLN
1	В	477	LEU
1	В	661	LYS
1	В	707	PHE
1	В	752	ILE
1	В	775	ASP
1	В	777	LEU



Mol	Chain	Res	Type
1	В	807	ASN
1	С	60	ARG
1	С	105	GLN
1	С	128	LYS
1	С	198	LYS
1	С	231	GLU
1	С	273	GLU
1	С	286	VAL
1	С	313	THR
1	С	369	LEU
1	С	381	VAL
1	С	390	ASN
1	С	392	GLU
1	С	397	LYS
1	С	399	VAL
1	C	429	ASP
1	С	440	SER
1	С	444	GLN
1	С	446	SER
1	С	453	GLN
1	С	548	HIS
1	С	579	THR
1	С	623	LYS
1	С	635	LYS
1	С	661	LYS
1	С	668	LYS
1	С	684	LYS
1	С	702	ASP
1	C	722	ASP
1	C	727	ASP
1	С	777	LEU
1	C	779	LYS
1	C	807	ASN
1	D	11	LYS
1	D	23	GLU
1	D	105	GLN
1	D	126	LEU
1	D	147	THR
1	D	192	THR
1	D	255	ASP
1	D	321	GLN
1	D	348	GLU



Mol	Chain	Res	Type
1	D	353	ASN
1	D	369	LEU
1	D	383	ARG
1	D	384	ASN
1	D	414	THR
1	D	429	ASP
1	D	442	ARG
1	D	444	GLN
1	D	477	LEU
1	D	525	GLU
1	D	579	THR
1	D	655	ILE
1	D	668	LYS
1	D	684	LYS
1	D	702	ASP
1	D	768	ASP
1	D	776	GLU
1	D	777	LEU
1	D	790	ASP
1	Е	198	LYS
1	Е	255	ASP
1	Е	322	VAL
1	Е	331	GLU
1	Е	335	GLU
1	Е	366	LYS
1	Е	369	LEU
1	Е	383	ARG
1	Е	402	TYR
1	Е	429	ASP
1	Е	443	LEU
1	Е	444	GLN
1	Е	477	LEU
1	Е	563	LEU
1	Е	585	LEU
1	Е	590	LYS
1	Е	635	LYS
1	E	638	ASP
1	Е	668	LYS
1	E	684	LYS
1	Е	693	GLU
1	Е	707	PHE
1	Е	719	LEU



Mol	Chain	Res	Type
1	Е	740	THR
1	Е	772	ASP
1	Е	777	LEU
1	Е	783	GLU
1	Е	794	ASP
1	Е	807	ASN
1	F	3	SER
1	F	11	LYS
1	F	14	ASN
1	F	105	GLN
1	F	127	GLN
1	F	134	SER
1	F	198	LYS
1	F	255	ASP
1	F	324	LEU
1	F	335	GLU
1	F	357	LYS
1	F	369	LEU
1	F	383	ARG
1	F	392	GLU
1	F	429	ASP
1	F	444	GLN
1	F	477	LEU
1	F	494	ARG
1	F	542	HIS
1	F	548	HIS
1	F	590	LYS
1	F	618	ARG
1	F	635	LYS
1	F	659	SER
1	F	722	ASP
1	F	752	ILE
1	F	768	ASP
1	F	777	LEU
1	G	20	GLU
1	G	105	GLN
1	G	147	THR
1	G	198	LYS
1	G	255	ASP
1	G	321	GLN
1	G	357	LYS
1	G	366	LYS



Mol	Chain	Res	Type
1	G	369	LEU
1	G	383	ARG
1	G	424	LYS
1	G	429	ASP
1	G	444	GLN
1	G	477	LEU
1	G	551	PHE
1	G	622	GLU
1	G	727	ASP
1	G	752	ILE
1	G	773	LYS
1	G	775	ASP
1	G	777	LEU
1	G	783	GLU
1	Н	2	THR
1	Н	105	GLN
1	Н	127	GLN
1	Н	198	LYS
1	Н	213	HIS
1	Н	306	LYS
1	Н	321	GLN
1	Н	357	LYS
1	Н	369	LEU
1	Н	383	ARG
1	Н	384	ASN
1	Н	397	LYS
1	Н	429	ASP
1	Н	444	GLN
1	Н	477	LEU
1	Н	494	ARG
1	H	569	ASN
1	H	618	ARG
1	H	622	GLU
1	H	740	THR
1	H	752	ILE
1	H	768	ASP
1	H	773	LYS
1	H	775	ASP
1	H	677	LEU
1	H	779	LYS
1	H	799	THR
1	H	807	ASN

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Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	14	ASN
1	А	353	ASN
1	А	444	GLN
1	А	549	ASN
1	А	568	HIS
1	В	14	ASN
1	В	444	GLN
1	В	786	GLN
1	С	390	ASN
1	С	444	GLN
1	С	453	GLN
1	С	472	GLN
1	С	568	HIS
1	С	673	ASN
1	С	807	ASN
1	D	127	GLN
1	D	353	ASN
1	D	441	ASN
1	D	444	GLN
1	D	571	HIS
1	D	596	ASN
1	Е	14	ASN
1	Е	132	GLN
1	Е	384	ASN
1	Е	404	HIS
1	Е	408	GLN
1	Е	444	GLN
1	Ε	548	HIS
1	E	786	GLN
1	F	321	GLN
1	F	384	ASN
1	F	444	GLN
1	F	548	HIS
1	G	384	ASN
1	G	548	HIS
1	G	807	ASN
1	Н	59	HIS
1	Н	127	GLN
1	Н	384	ASN
1	Н	390	ASN
1	Н	444	GLN



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Mol	Chain	Res	Type
1	Н	548	HIS
1	Н	807	ASN

#### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

#### 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry (i)

Of 24 ligands modelled in this entry, 8 are monoatomic - leaving 16 for Mogul analysis.

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

Mal	Turne	Chain	Dec	Tiple	Bo	ond leng	$_{\rm sths}$	B	ond ang	les
	wor rype Char	Unain	nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	TPP	А	900	3	22,27,27	0.76	0	29,40,40	1.22	3 (10%)
4	LMR	В	902	-	8,8,8	1.16	0	10,10,10	1.57	2 (20%)
2	TPP	Н	902	3	22,27,27	0.60	0	29,40,40	1.09	1 (3%)
2	TPP	Е	902	3	22,27,27	0.72	0	29,40,40	0.96	2 (6%)
2	TPP	В	903	3	22,27,27	0.69	0	29,40,40	1.23	4 (13%)
4	LMR	В	901	-	8,8,8	1.45	0	10,10,10	1.49	1 (10%)
6	SIN	Е	904	-	7,7,7	1.16	0	8,8,8	1.17	0
6	SIN	G	903	-	7,7,7	1.20	0	8,8,8	0.92	0
5	MLA	E	901	-	6,6,6	1.25	0	7,7,7	1.13	1 (14%)
2	TPP	С	900	3	22,27,27	0.73	0	29,40,40	0.88	0



Mal	Mol Type Chain		Ros Ii	Tink	Bond lengths			Bond angles		
MIOI	Mol Type Cha	Chain	nes	Res Link	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
2	TPP	G	901	3	22,27,27	0.60	0	$29,\!40,\!40$	1.06	2 (6%)
5	MLA	D	901	-	6,6,6	1.06	0	7,7,7	0.93	0
2	TPP	F	900	3	22,27,27	0.75	0	$29,\!40,\!40$	0.93	1 (3%)
5	MLA	D	902	-	6,6,6	1.43	0	7,7,7	1.26	1 (14%)
6	SIN	Н	901	-	7,7,7	1.35	0	8,8,8	1.30	1 (12%)
2	TPP	D	903	3	22,27,27	0.55	0	29,40,40	1.04	2 (6%)

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	TPP	А	900	3	-	4/16/17/17	0/2/2/2
4	LMR	В	902	-	-	4/8/8/8	-
2	TPP	Н	902	3	-	3/16/17/17	0/2/2/2
2	TPP	Е	902	3	-	7/16/17/17	0/2/2/2
2	TPP	В	903	3	-	1/16/17/17	0/2/2/2
4	LMR	В	901	-	-	2/8/8/8	-
6	SIN	Е	904	-	-	1/5/5/5	-
6	SIN	G	903	-	-	3/5/5/5	-
5	MLA	Е	901	-	-	2/4/4/4	-
2	TPP	С	900	3	-	4/16/17/17	0/2/2/2
2	TPP	G	901	3	-	8/16/17/17	0/2/2/2
5	MLA	D	901	-	-	2/4/4/4	-
2	TPP	F	900	3	-	3/16/17/17	0/2/2/2
5	MLA	D	902	-	-	0/4/4/4	-
6	SIN	Н	901	-	-	2/5/5/5	-
2	TPP	D	903	3	-	6/16/17/17	0/2/2/2

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	В	901	LMR	C2-C3-C4	3.12	119.84	112.13
2	В	903	TPP	O3B-PB-O3A	-2.82	95.17	104.64
2	А	900	TPP	O2B-PB-O3A	2.75	113.87	104.64
4	В	902	LMR	O1A-C1-C2	-2.70	117.26	122.54



Mol	Chain	$\mathbf{Res}$	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	F	900	TPP	C7'-N3-C2	-2.58	120.69	125.35
2	В	903	TPP	C6-C5-C4	2.53	129.47	127.43
2	D	903	TPP	O2A-PA-O7	-2.52	96.06	107.75
2	D	903	TPP	O2A-PA-O1A	2.47	124.44	112.24
2	Н	902	TPP	PA-O3A-PB	2.41	141.11	132.83
2	А	900	TPP	O2A-PA-O7	2.37	118.77	107.75
2	В	903	TPP	C7'-N3-C2	-2.33	121.14	125.35
4	В	902	LMR	O1B-C1-C2	2.32	117.83	112.72
2	Ε	902	TPP	O2B-PB-O3A	2.32	112.42	104.64
2	В	903	TPP	O3B-PB-O2B	2.32	116.50	107.64
2	G	901	TPP	C5-C4-N3	2.19	111.95	107.57
5	D	902	MLA	C3-C2-C1	-2.15	105.33	112.87
2	Ε	902	TPP	C5-C4-N3	2.14	111.85	107.57
5	Ε	901	MLA	O1A-C1-C2	2.12	121.32	114.54
6	Н	901	SIN	C2-C3-C4	2.06	118.04	113.60
2	А	900	TPP	C5-C4-N3	2.03	111.63	107.57
2	G	901	TPP	O2A-PA-O7	-2.02	98.36	107.75

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	А	900	TPP	PA-O3A-PB-O2B
2	С	900	TPP	PA-O3A-PB-O3B
2	D	903	TPP	C4'-C5'-C7'-N3
2	D	903	TPP	C4-C5-C6-C7
2	Е	902	TPP	C4'-C5'-C7'-N3
2	Ε	902	TPP	C4-C5-C6-C7
2	Е	902	TPP	PA-O3A-PB-O2B
2	Е	902	TPP	PA-O3A-PB-O3B
2	F	900	TPP	PA-O3A-PB-O3B
2	G	901	TPP	C4-C5-C6-C7
2	G	901	TPP	PA-O3A-PB-O2B
2	G	901	TPP	PA-O3A-PB-O3B
2	Н	902	TPP	C4'-C5'-C7'-N3
2	Н	902	TPP	C4-C5-C6-C7
2	Н	902	TPP	PA-O3A-PB-O3B
4	В	902	LMR	O2-C2-C3-C4
6	G	903	SIN	C1-C2-C3-C4
6	Е	904	SIN	C1-C2-C3-C4
4	В	902	LMR	C1-C2-C3-C4
5	Е	901	MLA	C1-C2-C3-O3B



Mol	Chain	Res	Type	Atoms
2	G	901	TPP	C5-C6-C7-O7
5	Е	901	MLA	C1-C2-C3-O3A
2	А	900	TPP	PA-O3A-PB-O3B
2	Е	902	TPP	PB-O3A-PA-O2A
2	А	900	TPP	C4-C5-C6-C7
2	С	900	TPP	C4-C5-C6-C7
2	F	900	TPP	C4-C5-C6-C7
5	D	901	MLA	C1-C2-C3-O3A
4	В	901	LMR	C1-C2-C3-C4
2	D	903	TPP	PB-O3A-PA-O1A
2	D	903	TPP	PB-O3A-PA-O2A
4	В	902	LMR	C2-C3-C4-O4B
4	В	902	LMR	C2-C3-C4-O4A
2	D	903	TPP	PA-O3A-PB-O1B
6	Н	901	SIN	C2-C3-C4-O3
6	Н	901	SIN	C2-C3-C4-O4
4	В	901	LMR	O2-C2-C3-C4
5	D	901	MLA	C1-C2-C3-O3B
2	G	901	TPP	PB-O3A-PA-O1A
2	G	901	TPP	C4'-C5'-C7'-N3
2	А	900	TPP	PA-O3A-PB-O1B
2	F	900	TPP	PA-O3A-PB-O1B
2	В	903	TPP	PA-O3A-PB-O3B
2	С	900	TPP	PA-O3A-PB-O2B
2	D	903	TPP	PA-O3A-PB-O2B
2	С	900	TPP	PB-O3A-PA-O2A
2	G	901	TPP	PB-O3A-PA-O2A
2	Е	902	TPP	C6'-C5'-C7'-N3
2	Е	902	TPP	C7-O7-PA-O1A
2	G	901	TPP	C7-O7-PA-O1A
6	G	903	SIN	C2-C3-C4-O4
6	G	903	SIN	C2-C3-C4-O3

Continued from previous page...

There are no ring outliers.

12 monomers are involved in 42 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	А	900	TPP	5	0
4	В	902	LMR	1	0
2	Н	902	TPP	6	0
2	Е	902	TPP	5	0
2	В	903	TPP	4	0



Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	Е	901	MLA	1	0
2	С	900	TPP	6	0
2	G	901	TPP	5	0
5	D	901	MLA	4	0
2	F	900	TPP	1	0
5	D	902	MLA	2	0
2	D	903	TPP	7	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>	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	А	807/831~(97%)	-0.51	12 (1%) 73 75	33, 45, 69, 118	0
1	В	807/831~(97%)	-0.46	21 (2%) 56 59	32, 45, 68, 120	0
1	С	807/831~(97%)	-0.18	29 (3%) 42 46	44, 66, 96, 141	0
1	D	808/831~(97%)	-0.14	33 (4%) 37 40	42, 67, 98, 128	0
1	Е	808/831~(97%)	-0.22	44 (5%) 25 27	37, 57, 95, 129	0
1	F	807/831~(97%)	-0.21	34 (4%) 36 39	40, 60, 89, 121	0
1	G	806/831~(96%)	-0.47	11 (1%) 75 77	34, 50, 77, 104	0
1	Н	$80\overline{7/831}\ (97\%)$	-0.34	27 (3%) 46 50	37, 53, 77, 118	0
All	All	6457/6648~(97%)	-0.32	211 (3%) 46 50	32, 55, 89, 141	0

Mol	Chain	Res	Type	RSRZ
1	С	507	VAL	5.6
1	D	507	VAL	5.5
1	F	157	LEU	5.4
1	Е	666	GLY	5.2
1	D	808	THR	5.1
1	Е	507	VAL	5.1
1	Е	549	ASN	5.0
1	F	507	VAL	4.7
1	Е	774	ILE	4.7
1	С	807	ASN	4.6
1	D	561	VAL	4.5
1	С	157	LEU	4.4
1	В	507	VAL	4.3
1	D	505	VAL	4.2
1	Н	808	THR	4.2
1	Е	543	VAL	4.0



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Mol	Chain	Res   Type		RSRZ
1	Н	508	ILE	4.0
1	Н	511	MET	3.9
1	Н	507	VAL	3.9
1	А	157	LEU	3.9
1	Е	504	PHE	3.9
1	А	808	THR	3.9
1	D	508	ILE	3.9
1	F	508	ILE	3.8
1	Е	548	HIS	3.8
1	Е	501	TYR	3.7
1	D	767	ALA	3.7
1	Е	772	ASP	3.7
1	Н	512	LEU	3.6
1	В	508	ILE	3.6
1	Е	552	SER	3.6
1	D	558	VAL	3.6
1	F	160	ALA	3.5
1	А	507	VAL	3.5
1	Н	504	PHE	3.5
1	Е	809	ASP	3.4
1	D	562	LEU	3.4
1	Е	157	LEU	3.4
1	G	157	LEU	3.4
1	D	511	MET	3.4
1	А	508	ILE	3.3
1	А	807	ASN	3.3
1	Ε	505	VAL	3.3
1	Е	477	LEU	3.3
1	Е	808	THR	3.3
1	В	157	LEU	3.2
1	Н	157	LEU	3.2
1	С	765	ILE	3.2
1	С	511	MET	3.2
1	F	159	TYR	3.2
1	D	157	LEU	3.2
1	H	505	VAL	3.1
1	F	808	THR	3.1
1	D	809	ASP	3.1
1	С	561	VAL	3.1
1	В	505	VAL	3.0
1	D	159	TYR	3.0
1	Е	503	SER	3.0



Mol	Chain	Res Type		RSRZ
1	С	510 SER		3.0
1	С	512	LEU	3.0
1	F	477	LEU	3.0
1	В	158	GLY	3.0
1	D	807	ASN	3.0
1	G	507	VAL	2.9
1	Е	768	ASP	2.9
1	F	480	HIS	2.9
1	F	158	GLY	2.9
1	Е	502	GLU	2.9
1	Н	537	LEU	2.9
1	С	401	GLU	2.9
1	А	158	GLY	2.9
1	C	614	LEU	2.9
1	F	155	GLY	2.9
1	D	512	LEU	2.9
1	F	512	LEU	2.8
1	Ε	766	ASP	2.8
1	G	508	ILE	2.8
1	F	771 ALA		2.8
1	Ε	807 ASN		2.8
1	Н	510 SER		2.8
1	Ε	546 GLN		2.8
1	С	508 ILE		2.8
1	Н	477	LEU	2.8
1	F	187	THR	2.8
1	С	156	GLU	2.8
1	C	506	HIS	2.8
1	F	352	ALA	2.8
1	В	808	THR	2.7
1	Е	775	ASP	2.7
1	Ε	506	HIS	2.7
1	В	511	MET	2.7
1	D	189	PRO	2.7
1	D	510	SER	2.7
1	C	185	ALA	2.7
1	G	187	THR	2.7
1	C	189	PRO	2.6
1	F	189	PRO	2.6
1	D	804	SER	2.6
1	Н	514	GLN	2.6
1	Е	402	TYR	2.6



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Mol	Chain	Res Type		RSRZ
1	Е	545 ARG		2.6
1	С	399	VAL	2.6
1	С	158	68 GLY 2	
1	С	768	ASP	2.6
1	С	480	HIS	2.6
1	G	511	MET	2.6
1	D	642	VAL	2.5
1	Е	508	ILE	2.5
1	F	156	GLU	2.5
1	Н	160	ALA	2.5
1	А	561	VAL	2.5
1	В	477	LEU	2.5
1	С	632	SER	2.5
1	Е	779	LYS	2.5
1	С	767	ALA	2.5
1	F	95	PRO	2.5
1	F	190	LEU	2.5
1	Н	506	HIS	2.5
1	В	504	PHE	2.5
1	F	666 GLY		2.5
1	D	506 HIS		2.5
1	Е	478 SER		2.5
1	G	512 LEU		2.4
1	С	478 SER		2.4
1	Н	159 TYR		2.4
1	Е	551	PHE	2.4
1	Н	552	SER	2.4
1	D	504	PHE	2.4
1	D	158	GLY	2.4
1	Е	553	HIS	2.4
1	F	331	GLU	2.4
1	В	552	SER	2.4
1	F	153	GLU	2.4
1	F	807	ASN	2.4
1	А	189	PRO	2.4
1	Е	558	VAL	2.3
1	Е	642	VAL	2.3
1	G	159	TYR	2.3
1	F	510	SER	2.3
1	В	189	PRO	2.3
1	Н	573	ILE	2.3
1	F	504	PHE	2.3



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Mol	Chain	Res Type		RSRZ
1	В	159 TYR		2.3
1	G	552	SER	2.3
1	D	563	LEU	2.3
1	F	97	HIS	2.3
1	А	159	TYR	2.3
1	С	770	TYR	2.3
1	В	190	LEU	2.3
1	F	505	VAL	2.3
1	Н	575	ILE	2.3
1	Е	635	LYS	2.2
1	Е	158	GLY	2.2
1	Е	767	ALA	2.2
1	F	506	HIS	2.2
1	D	557	GLY	2.2
1	Н	158	GLY	2.2
1	С	562	LEU	2.2
1	В	666	GLY	2.2
1	Н	154	GLY	2.2
1	В	92	ILE	2.2
1	Е	602	ILE	2.2
1	D	503 SER		2.2
1	Н	503	SER	2.2
1	С	619	ALA	2.2
1	Е	187 THR		2.2
1	F	517	LYS	2.2
1	Н	562	LEU	2.2
1	D	500	SER	2.2
1	D	539	VAL	2.2
1	Н	480	HIS	2.2
1	А	187	THR	2.2
1	D	390	ASN	2.2
1	В	501	TYR	2.2
1	G	510	SER	2.2
1	G	158	GLY	2.2
1	E	665	LEU	2.2
1	В	478	SER	2.2
1	C	406	TRP	2.1
1	С	808	THR	2.1
1	F	183	GLY	2.1
1	A	504	PHE	2.1
1	G	190	LEU	2.1
1	В	553	HIS	2.1



Mol	Chain	n Res Typ		RSRZ	
1	А	511	MET	2.1	
1	В	539	VAL	2.1	
1	Е	769	LYS	2.1	
1	Н	190	LEU	2.1	
1	D	766	ASP	2.1	
1	Е	550	GLY	2.1	
1	Н	435	PRO	2.1	
1	F	219	ILE	2.1	
1	F	484	GLY	2.1	
1	Н	558	VAL	2.1	
1	Е	770	TYR	2.1	
1	D	779	LYS	2.1	
1	Е	512	LEU	2.1	
1	F	162	SER	2.1	
1	D	400	ALA	2.1	
1	D	553	HIS	2.1	
1	D	162	SER	2.1	
1	Е	762	LEU	2.1	
1	С	188	GLY	2.1	
1	Е	401	GLU	2.0	
1	F	154	GLY	2.0	
1	В	558	VAL	2.0	
1	F	142	HIS	2.0	
1	Н	598	ILE	2.0	
1	D	156	GLU	2.0	
1	С	635	LYS	2.0	
1	В	179	ILE	2.0	

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

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

### 6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

### 6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,



Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(A^2)$	Q<0.9
6	SIN	G	903	8/8	0.67	1.64	59,67,70,71	8
5	MLA	D	902	7/7	0.72	0.97	42,42,51,53	7
6	SIN	Е	904	8/8	0.72	1.61	48,55,61,62	8
4	LMR	В	902	9/9	0.72	1.05	36,49,53,55	9
5	MLA	Е	901	7/7	0.74	1.20	38,43,53,57	7
6	SIN	Н	901	8/8	0.75	1.31	38,46,54,55	8
3	CA	D	904	1/1	0.81	0.04	71,71,71,71	0
3	CA	Н	903	1/1	0.82	0.04	69,69,69,69	0
4	LMR	В	901	9/9	0.86	1.45	39,42,48,53	9
3	CA	G	902	1/1	0.88	0.14	70,70,70,70	0
3	CA	А	901	1/1	0.89	0.04	60,60,60,60	0
3	CA	В	904	1/1	0.89	0.08	$55,\!55,\!55,\!55$	0
5	MLA	D	901	7/7	0.90	1.14	42,52,55,56	7
3	CA	F	901	1/1	0.91	0.04	$79,\!79,\!79,\!79$	0
3	CA	Е	903	1/1	0.92	0.04	62,62,62,62	0
3	CA	С	901	1/1	0.92	0.05	70,70,70,70	0
2	TPP	А	900	26/26	0.94	0.20	$37,\!44,\!48,\!58$	0
2	TPP	С	900	26/26	0.95	0.17	49,60,66,90	0
2	TPP	D	903	26/26	0.95	0.14	42,56,65,83	0
2	TPP	Е	902	26/26	0.95	0.16	$40,\!47,\!54,\!58$	0
2	TPP	F	900	26/26	0.95	0.22	48,60,69,74	0
2	TPP	В	903	26/26	0.95	0.18	37,42,46,52	0
2	TPP	G	901	26/26	0.96	0.18	38,46,52,54	0
2	TPP	Н	902	26/26	0.96	0.15	43,50,55,60	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.

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.

