

Full wwPDB X-ray Structure Validation Report (i)

Aug 23, 2023 – 12:23 AM EDT

PDB ID	:	3CXH
Title	:	Structure of yeast complex III with isoform-2 cytochrome c bound and defini-
		tion of a minimal core interface for electron transfer.
Authors	:	Solmaz, S.R.N.; Hunte, C.
Deposited on	:	2008-04-24
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
EDS	:	2.35
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)	:	2.35

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	٨	401	8%		
	A	431	68%	27%	5%
1	т	401	8%		_
	L	431	75%	21%	•
	Б	959	8%		_
2	В	352	69%	26%	•
		252	8%		
2	M	352	69%	26%	5%
	a		·%		
3	C	385	80%	18%	•



Mol	Chain	Length	Quality of chain	
		0	2%	
3	N	385	86%	13% •
4	D	248	85%	12% ••
4	О	248	83%	15% ••
5	Ε	185	77%	21% •
5	Р	185	10%	17% •
6	F	146	8% 41% 8% • 49	%
6	Q	146	8% 40% 10% • 49	%
7	G	126	3% 79 %	17% ••
7	R	126	3% 80%	17% ••
8	Н	93	80%	17% •
8	S	93	25%	20%
9	Ι	65	77%	6% • 15%
9	Т	65	71% 99	% 5% 15%
10	J	127	69%	28% •
10	U	127	66%	28% 6%
11	Κ	107	40% 56% 37%	6 7%
11	V	107	35% 71%	27% •
12	W	112	19% 79%	18% •
13	Х	2	50% 50%	%



2 Entry composition (i)

There are 23 unique types of molecules in this entry. The entry contains 36805 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

• Molecule 1 is a protein called Cytochrome b-c1 complex subunit 1, mitochondrial.

Mol	Chain	Residues		Ate	oms		ZeroOcc	AltConf	Trace	
1	Δ	421	Total	С	Ν	0	S	0	0	0
1		401	3344	2109	576	653	6	0	0	U
1	т	421	Total	С	Ν	0	S	0	0	0
	431	3344	2109	576	653	6	0	0	0	

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference	
А	153	ASP	GLU	conflict	UNP P07256	
L	153	ASP	GLU	conflict	UNP P07256	

• Molecule 2 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues		Ate	oms		ZeroOcc	AltConf	Trace	
2	В	352	Total	С	Ν	0	S	0	0	0
_		002	2735	1747	453	534	1	Ű	Ŭ	Ŭ
9	9 M	250	Total	С	Ν	0	\mathbf{S}	0	0	0
	- 552	2735	1747	453	534	1	0	U	0	

• Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues		At	oms		ZeroOcc	AltConf	Trace	
3	С	385	Total 3090	C 2082	N 484	O 503	S 21	0	0	0
3	Ν	385	Total 3090	C 2082	N 484	O 503	S 21	0	0	0

• Molecule 4 is a protein called Cytochrome c1, heme protein, mitochondrial.

Mol	Chain	Residues		Ate	oms		ZeroOcc	AltConf	Trace	
4	D	246	Total 1940	C 1237	N 334	0 360	S q	0	0	0
			1010	1201	1001	000	5			



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Mol	Chain	Residues		Ate	oms		ZeroOcc	AltConf	Trace	
4	0	246	Total 1940	C 1237	N 334	O 360	S 9	0	0	0

• Molecule 5 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues		\mathbf{A}	toms		ZeroOcc	AltConf	Trace	
5	Е	185	Total 1411	C 893	N 242	O 266	S 10	0	0	0
5	Р	185	Total 1411	C 893	N 242	O 266	S 10	0	0	0

• Molecule 6 is a protein called Cytochrome b-c1 complex subunit 6.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
6	Б	74	Total	С	Ν	0	S	0	0	0
0	Г	14	624	391	108	123	2	0	0	0
6	0	74	Total	С	Ν	0	S	0	0	0
0	Q	(4	624	391	108	123	2		0	U

• Molecule 7 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
7	C	195	Total	С	Ν	0	S	0	0	0
1	G	120	1012	648	172	190	2	0	0	0
7	D	195	Total	С	Ν	0	S	0	0	0
(n	120	1012	648	172	190	2	0	0	0

• Molecule 8 is a protein called Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
8	Н	93	Total 773	C 510	N 131	O 130	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0	0
8	S	93	Total 773	C 510	N 131	O 130	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0	0

• Molecule 9 is a protein called Cytochrome b-c1 complex subunit 9.

Mol	Chain	Residues		Aton	ns		ZeroOcc	AltConf	Trace
0	т	55	Total	С	Ν	0	0	0	0
9	1		448	298	75	75	0	0	0
0	т	55	Total	С	Ν	0	0	0	0
9	1		448	298	75	75	0	0	0



• Molecule 10 is a protein called HEAVY CHAIN (VH) OF FV-FRAGMENT.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
10	т	197	Total	С	Ν	0	S	0	0	0
10	J	127	1015	644	167	201	3	0	0	0
10	T	197	Total	С	Ν	0	S	0	0	0
10	U	121	1015	644	167	201	3	0		U

• Molecule 11 is a protein called LIGHT CHAIN (VL) OF FV-FRAGMENT.

Mol	Chain	Residues		Atoms				ZeroOcc	AltConf	Trace
11	K	107	Total	С	Ν	0	S	0	0	0
11	Γ	107	842	536	141	163	2	0	0	0
11	V	107	Total	С	Ν	0	S	0	0	0
	v	107	842	536	141	163	2	0	0	0

• Molecule 12 is a protein called Cytochrome c iso-2.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
12	W	112	Total 885	C 555	N 159	O 166	${ m S}{ m 5}$	0	1	0

• Molecule 13 is an oligosaccharide called beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose.



Mol	Chain	Residues	At	oms		ZeroOcc	AltConf	Trace
13	Х	2	Total 23	C 12	0 11	0	0	0

• Molecule 14 is UNDECYL-MALTOSIDE (three-letter code: UMQ) (formula: $C_{23}H_{44}O_{11}$).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	А	1	Total C O 34 23 11	0	0
14	L	1	Total C O 34 23 11	0	0

• Molecule 15 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).



Mol	Chain	Residues		Ate	\mathbf{oms}		ZeroOcc	AltConf	
15	С	1	Total 43	С 34	Fe 1	N 4	0 4	0	0



Mol	Chain	Residues		Ate	\mathbf{oms}			ZeroOcc	AltConf
15	C	1	Total	С	Fe	Ν	0	0	0
10	U	1	43	34	1	4	4	0	0
15	Л	1	Total	С	Fe	Ν	0	0	0
10	D	1	43	34	1	4	4	0	0
15	N	1	Total	С	Fe	Ν	0	0	0
10	11	1	43	34	1	4	4	0	0
15	N	1	Total	С	Fe	Ν	0	0	0
10	11	1	43	34	1	4	4	0	0
15	0	1	Total	С	Fe	Ν	0	0	0
10	0	1	43	34	1	4	4	0	0
15	W	1	Total	С	Fe	Ν	Ο	0	0
10	vv		43	34	1	4	4		U

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• Molecule 16 is STIGMATELLIN A (three-letter code: SMA) (formula: $C_{30}H_{42}O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	С	1	Total C O 37 30 7	0	0
16	Ν	1	Total C O 37 30 7	0	0

• Molecule 17 is (2R)-3-{[(S)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-2-(tetradecanoyloxy)propyl octadecanoate (three-letter code: 8PE) (formula: $C_{37}H_{74}NO_8P$).





Mol	Chain	Residues		Ato	oms			ZeroOcc	AltConf
17	С	1	Total	С	Ν	0	Р	0	0
11		I	47	37	1	8	1	0	0
17	N	1	Total	С	Ν	Ο	Р	0	0
11	IN	L	47	37	1	8	1	0	0

• Molecule 18 is (2R,5R,11S,14R)-2-(butanoyloxy)-5,8,11-trihydroxy-5,11-dioxido-16-oxo-14 -[(propanoyloxy)methyl]-4,6,10,12,15-pentaoxa-5,11-diphosphanonadec-1-yl undecanoate (three-letter code: CN6) (formula: $C_{31}H_{58}O_{17}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	С	1	Total	С	Ο	Р	0	0
18 U	T	50	31	17	2	0	0	



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Mol	Chain	Residues	A	Aton	ns		ZeroOcc	AltConf
18	Ν	1	Total	С	0	Р	0	0
		_	50	31	17	2		

• Molecule 19 is (1R)-2-{[(S)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-1-[(heptanoyloxy)m ethyl]ethyl octadecanoate (three-letter code: 9PE) (formula: $C_{30}H_{60}NO_8P$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf		
10	С	1	Total	С	Ν	0	Р	0	0
	I	40	30	1	8	1	0	0	
10	N	1	Total	С	Ν	Ο	Р	0	0
19	IN	N I		30	1	8	1	0	U

• Molecule 20 is (1R)-2-(dodecanoyloxy)-1-[(phosphonooxy)methyl]ethyl tetradecanoate (three-letter code: 7PH) (formula: C₂₉H₅₇O₈P).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	Л	1	Total	С	0	Р	0	0
20 D	T	38	29	8	1	0	0	
20	0	1	Total	С	0	Р	0	0
20	U	T	38	29	8	1	0	0

• Molecule 21 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	Е	1	TotalFeS422	0	0
21	Р	1	TotalFeS422	0	0



• Molecule 22 is (1R)-2-(phosphonooxy)-1-[(tridecanoyloxy)methyl]ethyl pentadecanoate (three-letter code: 6PH) (formula: $C_{31}H_{61}O_8P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	Е	1	Total C O P 40 31 8 1	0	0
22	L	1	Total C O P 40 31 8 1	0	0

• Molecule 23 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	А	42	$\begin{array}{cc} \text{Total} & \text{O} \\ 42 & 42 \end{array}$	0	0
23	В	17	Total O 17 17	0	0
23	С	75	Total O 75 75	0	0
23	D	50	$\begin{array}{cc} \text{Total} & \text{O} \\ 50 & 50 \end{array}$	0	0
23	Е	19	Total O 19 19	0	0
23	F	3	Total O 3 3	0	0
23	G	21	Total O 21 21	0	0
23	Н	10	Total O 10 10	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	Ι	4	Total O 4 4	0	0
23	J	2	Total O 2 2	0	0
23	K	1	Total O 1 1	0	0
23	L	54	$\begin{array}{cc} \text{Total} & \text{O} \\ 54 & 54 \end{array}$	0	0
23	М	15	Total O 15 15	0	0
23	Ν	88	Total O 88 88	0	0
23	О	74	Total O 74 74	0	0
23	Р	18	Total O 18 18	0	0
23	Q	3	Total O 3 3	0	0
23	R	22	TotalO2222	0	0
23	S	13	Total O 13 13	0	0
23	Т	5	Total O 5 5	0	0
23	U	2	Total O 2 2	0	0
23	W	10	Total O 10 10	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.





Ka97 G398 S399 S399 S399 S399 S399 S399 S399 L440 L440 L443 L443 L443 L443 T448 T448 K457



















4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	145.54Å 162.97Å 194.23Å	Depositor
a, b, c, α , β , γ	90.00° 104.39° 90.00°	Depositor
Bosolution (Å)	19.97 - 2.50	Depositor
Resolution (A)	19.97 - 2.50	EDS
% Data completeness	95.9 (19.97-2.50)	Depositor
(in resolution range)	96.0(19.97-2.50)	EDS
R_{merge}	(Not available)	Depositor
R _{sym}	0.66	Depositor
$< I/\sigma(I) > 1$	$2.01 (at 2.50 \text{\AA})$	Xtriage
Refinement program	CNS 1.1	Depositor
B B.	0.225 , 0.256	Depositor
II, II, <i>free</i>	0.226 , 0.256	DCC
R_{free} test set	14494 reflections (5.00%)	wwPDB-VP
Wilson B-factor $(Å^2)$	45.8	Xtriage
Anisotropy	0.430	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.34, 56.9	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	0.93	EDS
Total number of atoms	36805	wwPDB-VP
Average B, all atoms $(Å^2)$	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 9.27% 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: 9PE, FES, 8PE, HEM, 6PH, SMA, CN6, 7PH, GLC, FRU, M3L, UMQ

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	Mol Chain		lengths	Bo	ond angles
MIOI	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.36	0/3405	0.61	1/4614~(0.0%)
1	L	0.37	0/3405	0.63	0/4614
2	В	0.36	0/2781	0.66	2/3764~(0.1%)
2	М	0.37	0/2781	0.65	1/3764~(0.0%)
3	С	0.43	0/3192	0.64	1/4354~(0.0%)
3	N	0.44	0/3192	0.66	0/4354
4	D	0.37	0/2001	0.61	0/2726
4	0	0.40	0/2001	0.63	0/2726
5	Е	0.36	0/1444	0.60	0/1957
5	Р	0.35	0/1444	0.61	1/1957~(0.1%)
6	F	0.36	0/638	0.53	0/858
6	Q	0.37	0/638	0.58	0/858
7	G	0.37	0/1032	0.62	0/1397
7	R	0.40	0/1032	0.63	0/1397
8	Н	0.41	0/804	0.55	0/1088
8	S	0.44	0/804	0.56	0/1088
9	Ι	0.39	0/461	0.52	0/622
9	Т	0.42	0/461	0.51	0/622
10	J	0.35	0/1043	0.60	0/1422
10	U	0.34	0/1043	0.62	0/1422
11	Κ	0.33	0/863	0.54	0/1172
11	V	0.33	0/863	0.53	0/1172
12	W	0.34	0/891	0.60	0/1191
All	All	0.38	0/36219	0.62	6/49139~(0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.



Mol	Chain	#Chirality outliers	#Planarity outliers
3	С	0	1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
5	Р	65	LEU	CA-CB-CG	6.40	130.03	115.30
2	В	87	ILE	N-CA-C	-6.16	94.38	111.00
2	В	152	ARG	N-CA-C	5.45	125.71	111.00
2	М	87	ILE	N-CA-C	-5.44	96.31	111.00
1	А	251	LEU	CA-CB-CG	5.32	127.54	115.30
3	С	185	LEU	CA-CB-CG	5.15	127.15	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	С	279	TYR	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	3344	0	3321	99	0
1	L	3344	0	3321	80	0
2	В	2735	0	2774	74	0
2	М	2735	0	2774	77	0
3	С	3090	0	3129	52	0
3	N	3090	0	3129	30	0
4	D	1940	0	1862	30	0
4	0	1940	0	1862	30	0
5	Е	1411	0	1386	36	0
5	Р	1411	0	1386	25	0
6	F	624	0	581	10	0
6	Q	624	0	581	9	0
7	G	1012	0	1026	22	0
7	R	1012	0	1026	16	0



26	IVU	Г
\mathcal{I}	$\Lambda \Pi$	L

	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	Н	773		736	1/	
8	S	773	0	736	14	0
9	I	448	0	445	5	0
9	T	448	0	445	7	0
10	J	1015	0	959	29	0
10	U	1015	0	959	35	0
11	K	842	0	820	33	0
11	V	842	0	820	23	0
12	W	885	0	890	15	0
13	X	23	0	21	2	0
14	А	34	0	44	4	0
14	L	34	0	44	2	0
15	С	86	0	60	3	0
15	D	43	0	30	0	0
15	N	86	0	60	1	0
15	0	43	0	30	1	0
15	W	43	0	30	2	0
16	С	37	0	42	1	0
16	Ν	37	0	42	1	0
17	С	47	0	73	2	0
17	Ν	47	0	73	2	0
18	С	50	0	56	7	0
18	N	50	0	56	5	0
19	С	40	0	59	0	0
19	N	40	0	59	0	0
20	D	38	0	55	3	0
20	0	38	0	55	2	0
21	Ε	4	0	0	0	0
21	Р	4	0	0	1	0
22	E	40	0	59	1	0
22	L	40	0	59	0	0
23	A	42	0	0	0	0
23	В	17	0	0	1	0
23	С	75	0	0	4	0
23	D	50	0	0	0	0
23	E	19	0	0	0	0
23	F	3	0	0	0	0
23	G	21	0	0	1	0
23	H	10	0	0	0	0
23	I	4	0	0	0	0
23	J	2	0	0	1	0
23	K	1	0	0	0	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	L	54	0	0	2	0
23	М	15	0	0	0	0
23	Ν	88	0	0	3	0
23	0	74	0	0	2	0
23	Р	18	0	0	0	0
23	Q	3	0	0	0	0
23	R	22	0	0	1	0
23	S	13	0	0	0	0
23	Т	5	0	0	0	0
23	U	2	0	0	0	0
23	W	10	0	0	1	0
All	All	36805	0	35975	721	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (721) 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)
2:M:347:LYS:HD3	2:M:347:LYS:H	1.19	1.01
1:A:63:ASN:H	1:A:66:ASN:HD21	1.06	1.00
1:A:382:ASN:HD21	1:A:384:VAL:HG22	1.22	0.99
1:L:63:ASN:H	1:L:66:ASN:ND2	1.60	0.99
6:Q:77:GLN:H	6:Q:77:GLN:HE21	1.08	0.98
6:F:77:GLN:H	6:F:77:GLN:HE21	0.96	0.93
11:V:75:ILE:HG22	11:V:76:SER:H	1.35	0.90
1:L:63:ASN:H	1:L:66:ASN:HD21	0.94	0.90
6:F:77:GLN:H	6:F:77:GLN:NE2	1.69	0.90
6:F:78:LEU:HD13	6:F:142:LEU:HD22	1.52	0.89
6:Q:77:GLN:H	6:Q:77:GLN:NE2	1.73	0.86
1:A:58:GLY:H	1:A:61:ASN:HD22	1.24	0.86
2:M:49:HIS:HD2	2:M:161:TYR:H	1.24	0.85
1:L:317:HIS:HE1	1:L:351:TRP:HE1	1.23	0.84
2:M:62:ARG:HG2	2:M:62:ARG:HH21	1.43	0.84
10:U:29:ILE:H	10:U:77:ASN:HD21	1.25	0.84
5:E:134:MET:HG3	10:J:31:SER:HB3	1.61	0.81
11:V:93:LYS:HZ3	11:V:94:PHE:H	1.29	0.81
2:M:150:THR:HG22	2:M:352:ASN:HD22	1.45	0.81
11:K:21:ILE:HG22	11:K:22:SER:H	1.47	0.78
2:B:181:THR:HB	2:B:212:GLY:H	1.47	0.78
6:F:77:GLN:HE21	6:F:77:GLN:N	1.78	0.78



Atom-1	Atom_2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
10:J:29:ILE:HG12	10:J:77:ASN:ND2	1.99	0.77
2:M:246:ASN:HD22	2:M:246:ASN:H	1.32	0.77
1:A:429:GLN:HA	1:A:429:GLN:HE21	1.48	0.76
1:L:179:ARG:HG2	1:L:179:ARG:HH21	1.49	0.76
10:J:99:SER:HB3	10:J:109:MET:HG2	1.69	0.75
2:M:347:LYS:HD3	2:M:347:LYS:N	1.98	0.75
7:G:77:ARG:HD3	7:G:88:LEU:HD11	1.67	0.75
2:B:49:HIS:HD2	2:B:161:TYR:H	1.34	0.75
1:L:344:ILE:HG21	1:L:448:ILE:HD12	1.68	0.75
2:B:62:ARG:HG2	2:B:62:ARG:HH21	1.50	0.75
5:E:44:LYS:NZ	5:E:52:GLY:H	1.83	0.75
2:M:49:HIS:CD2	2:M:161:TYR:H	2.05	0.75
9:T:8:LYS:O	9:T:12:LYS:HG3	1.87	0.75
11:V:6:GLN:HG2	11:V:23:CYS:SG	2.27	0.74
2:M:150:THR:HG22	2:M:352:ASN:ND2	2.03	0.74
4:D:286:TRP:CE3	5:E:59:MET:HG3	2.23	0.74
7:R:77:ARG:HD3	7:R:88:LEU:HD11	1.69	0.74
1:L:63:ASN:N	1:L:66:ASN:HD21	1.79	0.74
2:M:238:VAL:HG13	2:M:356:VAL:HB	1.68	0.74
4:O:96:VAL:HB	4:O:251:VAL:HG13	1.69	0.73
1:A:73:TRP:CE3	1:A:76:ILE:HD11	2.24	0.73
1:L:58:GLY:H	1:L:61:ASN:HD22	1.37	0.73
3:N:208:ASN:HD22	3:N:210:LEU:H	1.36	0.73
2:B:336:ILE:HD12	2:B:336:ILE:H	1.54	0.73
2:B:238:VAL:HG13	2:B:356:VAL:HB	1.71	0.72
1:A:382:ASN:ND2	1:A:384:VAL:HG22	2.01	0.72
2:B:300:ASN:O	2:B:304:ILE:HG12	1.89	0.72
1:A:317:HIS:HE1	1:A:351:TRP:HE1	1.38	0.72
3:C:208:ASN:HD22	3:C:210:LEU:H	1.38	0.72
1:A:63:ASN:H	1:A:66:ASN:ND2	1.83	0.71
5:E:172:ASP:H	5:E:184:HIS:HD2	1.38	0.71
17:N:4110:8PE:H1A	8:S:51:ARG:HE	1.56	0.71
4:D:272:LYS:O	4:D:276:ILE:HG22	1.90	0.71
2:M:137:CYS:SG	2:M:139:VAL:HG22	2.31	0.71
2:M:324:LYS:O	2:M:327:VAL:HG22	1.90	0.71
1:L:317:HIS:CE1	1:L:351:TRP:HE1	2.06	0.70
2:M:347:LYS:HG2	2:M:348:LEU:H	1.55	0.70
1:A:228:LEU:HG	1:A:229:SER:H	1.56	0.70
18:C:4031:CN6:HAA	7:G:85:HIS:NE2	2.06	0.70
1:L:241:LYS:H	1:L:241:LYS:HD2	1.57	0.69
3:N:214:GLY:O	3:N:218:ARG:HD2	1.93	0.69



Atom_1	Atom_2	Interatomic	Clash
	Atom-2	distance (Å)	overlap (Å)
2:B:37:GLY:HA3	2:B:179:VAL:HG11	1.73	0.69
2:B:30:THR:HG23	2:B:190:GLU:HB3	1.74	0.69
3:C:214:GLY:O	3:C:218:ARG:HD2	1.92	0.69
1:A:66:ASN:HD22	1:A:66:ASN:H	1.41	0.69
11:K:29:ILE:HG22	11:K:92:ILE:HD12	1.74	0.69
11:K:47:LEU:HA	11:K:58:VAL:HG11	1.74	0.69
18:N:4131:CN6:HAA	7:R:85:HIS:NE2	2.08	0.68
18:N:4131:CN6:HC	23:N:6998:HOH:O	1.92	0.68
3:C:107:ARG:HH21	3:C:107:ARG:HG3	1.58	0.68
1:A:361:THR:HG21	7:R:123:ILE:O	1.94	0.68
10:J:114:GLN:H	10:J:114:GLN:NE2	1.92	0.68
5:P:44:LYS:NZ	5:P:52:GLY:H	1.91	0.68
11:K:36:TYR:HE2	11:K:89:GLN:HG2	1.59	0.67
1:A:127:GLN:HG2	1:A:130:ASN:HD22	1.60	0.67
1:A:217:GLU:HA	1:A:220:VAL:HG12	1.76	0.67
3:N:323:LYS:CE	8:S:55:GLN:HE22	2.08	0.67
1:L:130:ASN:N	1:L:130:ASN:HD22	1.92	0.66
10:J:61:ASN:HD22	10:J:63:SER:H	1.44	0.66
8:H:56:PHE:O	8:H:60:LEU:HB2	1.96	0.66
5:P:172:ASP:H	5:P:184:HIS:HD2	1.43	0.66
10:J:38:ILE:HD11	10:J:46:LEU:HD22	1.78	0.66
10:U:61:ASN:HD22	10:U:63:SER:H	1.42	0.66
2:M:300:ASN:O	2:M:304:ILE:HG12	1.96	0.65
23:O:6502:HOH:O	12:W:25:GLN:HG3	1.95	0.65
3:C:185:LEU:HG	3:N:48:ILE:HD13	1.79	0.65
5:P:132:VAL:HG21	5:P:192:ARG:NH1	2.11	0.65
1:A:66:ASN:HA	1:A:188:LEU:HD11	1.79	0.65
10:U:41:PHE:HB2	10:U:45:LYS:HG3	1.79	0.65
1:L:172:THR:HG23	1:L:242:ALA:HA	1.79	0.64
4:D:147:ARG:HH21	4:D:150:LYS:HE3	1.62	0.64
3:C:253:HIS:HD2	3:C:255:ASP:H	1.45	0.64
9:T:52:VAL:HA	9:T:55:ARG:HD3	1.77	0.64
2:B:152:ARG:HH12	2:M:366:ASP:HB2	1.62	0.63
1:L:156:HIS:HD2	1:L:159:ARG:HH21	1.45	0.63
1:L:228:LEU:HG	1:L:229:SER:H	1.63	0.63
1:L:270:VAL:O	1:L:271:ASN:HB2	1.97	0.63
6:Q:77:GLN:HE21	6:Q:77:GLN:N	1.88	0.63
4:O:227:ARG:HH11	4:O:244:THR:HG21	1.63	0.63
2:M:31:LEU:HD12	2:M:105:LEU:HD12	1.81	0.63
5:P:103:LEU:O	5:P:120:HIS:HB3	1.98	0.63
5:E:106:ASN:ND2	5:E:119:ARG:HB2	2.14	0.62



Atom-1	Atom-2	Interatomic	Clash
	Atom-2	distance (Å)	overlap (Å)
1:A:57:SER:O	1:A:102:GLN:HG3	1.99	0.62
3:N:323:LYS:NZ	8:S:55:GLN:HE22	1.98	0.62
1:A:99:ARG:HD3	1:A:174:LEU:HD12	1.80	0.62
2:B:152:ARG:O	2:B:153:LYS:HB2	2.00	0.62
3:C:27:ASN:HB2	18:C:4031:CN6:O2'	1.99	0.62
2:M:329:ASN:N	2:M:329:ASN:HD22	1.98	0.62
1:A:276:PHE:HZ	1:A:401:LEU:HD21	1.64	0.62
7:G:62:ARG:HD2	2:M:121:GLU:OE2	1.98	0.62
1:A:172:THR:HG23	1:A:242:ALA:HA	1.82	0.62
1:L:179:ARG:HG2	1:L:179:ARG:NH2	2.14	0.62
2:M:336:ILE:H	2:M:336:ILE:HD12	1.65	0.62
2:M:315:SER:N	2:M:316:PRO:HD3	2.15	0.62
10:U:38:ILE:HD11	10:U:46:LEU:HD22	1.80	0.62
2:M:83:ASP:HB2	2:M:86:TYR:H	1.65	0.61
4:D:96:VAL:HB	4:D:251:VAL:HG13	1.83	0.61
3:N:253:HIS:HD2	3:N:255:ASP:H	1.48	0.61
7:R:77:ARG:HD2	23:R:5803:HOH:O	1.99	0.61
5:E:172:ASP:H	5:E:184:HIS:CD2	2.18	0.61
11:K:21:ILE:HG22	11:K:22:SER:N	2.15	0.61
1:L:72:LEU:HD23	1:L:193:LEU:HD21	1.81	0.61
7:G:77:ARG:HD2	23:G:5303:HOH:O	2.00	0.61
4:O:213:ASN:OD1	13:X:2:FRU:H62	2.00	0.61
10:U:68:LEU:HA	10:U:82:LYS:O	2.01	0.61
1:L:207:VAL:HG11	1:L:394:VAL:HG21	1.81	0.61
6:Q:78:LEU:HD13	6:Q:142:LEU:HD22	1.83	0.61
10:U:14:PRO:O	10:U:15:SER:HB3	2.01	0.61
3:C:44:ILE:O	3:C:48:ILE:HG12	2.01	0.60
1:L:149:GLN:O	1:L:153:ASP:HB2	2.02	0.60
2:B:152:ARG:HD3	2:B:224:PHE:CE1	2.36	0.60
7:G:43:LEU:HD21	7:G:78:ALA:CB	2.32	0.60
11:V:2:ILE:HD12	11:V:2:ILE:H	1.66	0.60
10:J:30:THR:O	10:J:54:ASN:HB2	2.00	0.60
14:A:4021:UMQ:HK1	22:E:4013:6PH:H39	1.83	0.60
3:N:253:HIS:CD2	3:N:255:ASP:H	2.19	0.60
11:V:34:ASN:ND2	11:V:50:TYR:H	1.99	0.60
2:M:65:LEU:O	2:M:69:ARG:HG2	2.00	0.60
3:C:4:ARG:HE	3:C:14:ASN:HD21	1.50	0.60
3:C:4:ARG:HE	3:C:14:ASN:ND2	1.99	0.60
1:L:229:SER:HB3	1:L:232:THR:HG21	1.84	0.60
11:K:2:ILE:HD12	11:K:2:ILE:H	1.67	0.59
10:U:41:PHE:HB2	10:U:45:LYS:CG	2.32	0.59



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:169:PHE:O	1:A:172:THR:HB	2.01	0.59
2:M:68:VAL:O	2:M:72:GLU:HG3	2.01	0.59
4:O:109:ARG:HG3	4:O:178:SER:CB	2.32	0.59
8:H:12:TRP:CE2	8:S:3:PRO:HG3	2.38	0.59
3:N:27:ASN:HB2	18:N:4131:CN6:O2'	2.02	0.59
4:0:78:HIS:HD2	23:O:5586:HOH:O	1.85	0.59
10:U:29:ILE:H	10:U:77:ASN:ND2	1.98	0.59
1:A:38:VAL:HA	1:A:208:VAL:HG13	1.85	0.59
5:E:93:LYS:HG3	5:E:214:VAL:O	2.02	0.59
2:M:246:ASN:H	2:M:246:ASN:ND2	1.99	0.59
10:U:28:SER:HB3	10:U:31:SER:OG	2.02	0.59
7:G:26:VAL:HG12	7:G:30:ASN:HD21	1.68	0.59
12:W:58:THR:HG22	12:W:61:ASN:H	1.68	0.59
1:L:394:VAL:HG12	1:L:399:SER:HA	1.85	0.59
1:A:117:LEU:HD11	1:A:219:LEU:HD12	1.84	0.58
4:D:247:MET:O	4:D:251:VAL:HG22	2.03	0.58
1:A:127:GLN:HG2	1:A:130:ASN:ND2	2.18	0.58
1:A:172:THR:HG23	1:A:173:PRO:HD2	1.85	0.58
4:O:201:GLU:HG3	4:O:202:PRO:HD2	1.86	0.58
5:E:115:PRO:HD2	5:E:158:ILE:HD11	1.84	0.58
1:L:382:ASN:OD1	1:L:384:VAL:HG22	2.03	0.58
2:M:308:LEU:HB2	2:M:348:LEU:HD22	1.85	0.58
11:K:34:ASN:HD22	11:K:49:TYR:HA	1.67	0.58
11:V:2:ILE:HD12	11:V:2:ILE:N	2.19	0.58
11:V:75:ILE:HG22	11:V:76:SER:N	2.14	0.58
3:N:147:ILE:O	3:N:150:LEU:HB2	2.03	0.58
3:N:208:ASN:HB2	3:N:209:PRO:HD2	1.86	0.58
5:P:51:LYS:HE2	5:P:55:TYR:CE1	2.39	0.58
1:A:252:ARG:HD3	1:A:254:ASP:OD1	2.04	0.58
3:C:40:LEU:HD12	15:C:4001:HEM:HBB1	1.86	0.58
14:L:4121:UMQ:O2'	9:T:18:VAL:HG22	2.04	0.58
2:B:49:HIS:CD2	2:B:161:TYR:H	2.19	0.57
2:M:146:LEU:O	2:M:150:THR:HG23	2.03	0.57
2:M:313:ASP:HB3	2:M:344:LYS:O	2.04	0.57
8:S:61:ILE:HB	8:S:62:PRO:HD3	1.85	0.57
1:A:234:THR:HG22	1:A:235:LYS:H	1.70	0.57
10:U:107:TYR:H	11:V:91:HIS:CD2	2.22	0.57
1:A:160:VAL:CG2	1:A:436:THR:HG22	2.35	0.57
3:C:173:ASN:HB3	3:C:174:PRO:HD3	1.85	0.57
8:H:12:TRP:CZ2	8:S:3:PRO:HG3	2.40	0.57
7:R:19:PRO:O	7:R:23:LYS:HG3	2.05	0.56



Atom_1	Atom_2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
10:J:24:VAL:HG21	10:J:29:ILE:HD11	1.85	0.56
1:L:172:THR:CG2	1:L:242:ALA:HA	2.35	0.56
5:E:103:LEU:O	5:E:120:HIS:HB3	2.05	0.56
11:V:36:TYR:HE2	11:V:89:GLN:HG2	1.69	0.56
5:P:172:ASP:H	5:P:184:HIS:CD2	2.23	0.56
6:F:81:LEU:HB3	6:F:138:THR:HG22	1.88	0.56
8:H:80:LEU:HB3	8:H:89:LEU:HD23	1.87	0.56
2:B:366:ASP:CB	2:M:152:ARG:HH12	2.19	0.56
5:E:44:LYS:HZ2	5:E:52:GLY:H	1.53	0.56
2:B:155:LEU:H	2:B:155:LEU:HD12	1.71	0.55
11:K:4:LEU:HD23	11:K:23:CYS:HB3	1.87	0.55
5:E:106:ASN:HD22	5:E:119:ARG:HB2	1.71	0.55
9:I:8:LYS:O	9:I:12:LYS:HD2	2.06	0.55
2:M:347:LYS:HG2	2:M:348:LEU:N	2.20	0.55
1:A:202:LEU:HD13	1:A:234:THR:HB	1.88	0.55
2:B:197:LEU:O	2:B:201:VAL:HG23	2.06	0.55
3:C:147:ILE:O	3:C:150:LEU:HB2	2.06	0.55
10:U:54:ASN:H	10:U:54:ASN:HD22	1.53	0.55
11:V:93:LYS:NZ	11:V:94:PHE:H	2.01	0.55
2:B:238:VAL:CG1	2:B:356:VAL:HB	2.36	0.55
10:J:61:ASN:ND2	10:J:63:SER:H	2.04	0.55
5:E:103:LEU:HG	5:E:122:THR:HG22	1.89	0.55
1:L:74:LYS:HG3	1:L:95:SER:HB3	1.89	0.55
5:P:55:TYR:O	5:P:59:MET:HG2	2.07	0.55
12:W:96:LYS:HD3	12:W:98:LYS:NZ	2.22	0.55
14:A:4021:UMQ:O2'	9:I:18:VAL:HG22	2.07	0.55
3:C:253:HIS:CD2	3:C:255:ASP:H	2.24	0.55
8:H:83:LYS:O	8:H:86:ARG:HG2	2.06	0.55
1:A:46:ALA:O	1:A:47:HIS:HB2	2.07	0.54
11:K:6:GLN:HG2	11:K:23:CYS:SG	2.47	0.54
5:P:118:ILE:HG12	5:P:154:ILE:HG12	1.89	0.54
12:W:50:GLY:HA2	12:W:57:TYR:CE1	2.42	0.54
3:C:304:VAL:HG12	3:C:308:THR:HG23	1.89	0.54
20:D:4014:7PH:H35	5:E:70:GLY:HA3	1.88	0.54
11:V:11:LEU:HG	11:V:12:ALA:H	1.72	0.54
1:L:29:VAL:HG12	1:L:30:THR:N	2.22	0.54
1:L:313:ASP:OD1	1:L:335:ARG:HD3	2.07	0.54
2:B:152:ARG:HG2	2:M:364:TYR:CE1	2.43	0.54
10:J:40:LEU:O	10:J:92:ALA:HB1	2.07	0.54
1:L:46:ALA:O	1:L:47:HIS:HB2	2.08	0.54
1:L:156:HIS:HD2	1:L:159:ARG:NH2	2.04	0.54



Atom-1	Atom-2	Interatomic	Clash
1100111-1	Atom-2	distance (Å)	overlap (Å)
4:O:227:ARG:NH1	4:O:244:THR:HG21	2.22	0.54
11:V:38:GLN:O	11:V:84:ALA:HB1	2.07	0.54
2:B:151:PHE:O	2:B:153:LYS:N	2.37	0.54
2:M:152:ARG:HD3	2:M:224:PHE:CE1	2.43	0.54
7:G:43:LEU:HD21	7:G:78:ALA:HB2	1.90	0.54
1:L:241:LYS:H	1:L:241:LYS:CD	2.15	0.54
4:D:109:ARG:HG3	4:D:178:SER:CB	2.38	0.54
4:D:276:ILE:HD13	20:D:4014:7PH:O32	2.07	0.54
1:A:289:ASN:C	1:A:289:ASN:HD22	2.11	0.53
1:L:227:ASN:HD22	1:L:228:LEU:H	1.56	0.53
4:0:286:TRP:CE3	5:P:59:MET:HG3	2.43	0.53
1:A:207:VAL:HG11	1:A:394:VAL:HG21	1.90	0.53
10:J:61:ASN:HD22	10:J:62:PRO:N	2.05	0.53
1:L:258:LYS:HG2	1:L:335:ARG:HG3	1.91	0.53
2:M:115:LYS:HB2	2:M:118:GLU:HG3	1.89	0.53
3:C:14:ASN:ND2	3:C:18:ILE:HB	2.24	0.53
11:V:21:ILE:HG22	11:V:22:SER:N	2.24	0.53
2:M:197:LEU:O	2:M:201:VAL:HG23	2.09	0.53
1:A:67:ASN:ND2	1:A:181:THR:HG23	2.22	0.53
1:A:317:HIS:CE1	1:A:351:TRP:HE1	2.24	0.53
18:N:4131:CN6:HAA	7:R:85:HIS:CE1	2.43	0.53
4:0:247:MET:0	4:O:251:VAL:HG22	2.09	0.53
2:B:65:LEU:O	2:B:69:ARG:HG2	2.09	0.53
3:C:15:SER:O	3:C:202:HIS:HE1	1.92	0.53
4:0:72:PRO:HB2	6:Q:139:ALA:HB2	1.90	0.53
10:U:18:LEU:O	10:U:82:LYS:HA	2.08	0.52
1:A:373:GLN:HG3	1:A:374:LEU:N	2.24	0.52
1:A:86:ALA:HB2	1:A:119:PHE:CZ	2.44	0.52
2:B:49:HIS:HE1	2:B:130:ASP:OD1	1.93	0.52
2:B:83:ASP:HB2	2:B:86:TYR:H	1.74	0.52
3:N:301:VAL:O	3:N:304:VAL:HG12	2.09	0.52
10:U:38:ILE:HD13	10:U:112:TRP:HH2	1.73	0.52
5:E:134:MET:HG3	10:J:31:SER:CB	2.35	0.52
6:F:91:GLY:O	6:F:95:VAL:HG13	2.10	0.52
3:N:4:ARG:HE	3:N:14:ASN:ND2	2.07	0.52
5:P:115:PRO:HD2	5:P:158:ILE:HD11	1.91	0.52
1:L:252:ARG:HD3	1:L:254:ASP:OD1	2.10	0.52
2:M:260:LEU:O	2:M:271:ILE:HD11	2.10	0.52
1:A:179:ARG:HH21	1:A:179:ARG:HG2	1.74	0.52
1:A:181:THR:O	1:A:185:LEU:HB2	2.10	0.52
2:B:35:VAL:CG1	2:B:179:VAL:HG12	2.40	0.52



Atom-1	Atom-2	Interatomic	Clash
	1100111-2	distance (Å)	overlap (Å)
15:C:4002:HEM:HMB1	15:C:4002:HEM:HBB2	1.92	0.52
4:D:69:LEU:HD23	6:F:128:PHE:CD1	2.45	0.52
1:L:241:LYS:HD2	1:L:241:LYS:N	2.24	0.52
3:C:25:SER:OG	7:G:79:HIS:HD2	1.93	0.51
3:C:184:TYR:CD1	15:C:4001:HEM:HBC1	2.45	0.51
3:N:4:ARG:HE	3:N:14:ASN:HD21	1.56	0.51
3:N:335:LEU:O	3:N:339:ILE:HG12	2.10	0.51
1:L:182:LEU:O	1:L:186:GLU:HG2	2.10	0.51
1:A:306:ILE:HA	1:A:311:LEU:HD22	1.92	0.51
4:O:92:ARG:HG2	4:O:236:TYR:CD2	2.46	0.51
4:0:231:ASP:OD1	4:O:244:THR:HG23	2.09	0.51
20:O:4114:7PH:H25	20:O:4114:7PH:H29	1.93	0.51
10:U:49:VAL:CG1	10:U:68:LEU:HD23	2.41	0.51
10:U:59:ASN:HD22	10:U:59:ASN:C	2.13	0.51
11:V:29:ILE:HG22	11:V:92:ILE:HD12	1.93	0.51
12:W:36:LYS:HB3	23:W:7422:HOH:O	2.10	0.51
2:B:115:LYS:HB2	2:B:118:GLU:HG3	1.92	0.51
2:B:264:LEU:HD12	2:B:317:ALA:HB2	1.92	0.51
18:C:4031:CN6:HC	23:C:6590:HOH:O	2.11	0.51
2:B:232:ARG:NH1	2:M:164:VAL:HG21	2.26	0.51
3:C:58:ILE:H	3:C:173:ASN:HD22	1.58	0.51
2:M:62:ARG:HH21	2:M:62:ARG:CG	2.17	0.51
2:M:315:SER:HB3	2:M:344:LYS:HA	1.93	0.51
12:W:28:THR:HG23	12:W:36:LYS:HE2	1.93	0.51
2:M:247:LYS:O	2:M:250:LEU:HD22	2.10	0.51
2:B:183:GLU:HB2	2:B:213:LYS:O	2.10	0.51
10:J:107:TYR:H	11:K:91:HIS:CD2	2.29	0.51
11:K:17:ASP:HB2	11:K:18:ARG:HH21	1.75	0.51
2:M:298:SER:O	2:M:302:LYS:HB2	2.11	0.51
2:B:62:ARG:HH21	2:B:62:ARG:CG	2.24	0.50
4:D:92:ARG:HG2	4:D:236:TYR:CD2	2.45	0.50
4:O:135:ASP:OD2	4:O:146:LYS:HE2	2.11	0.50
1:A:350:GLN:O	1:A:353:ARG:HB2	2.12	0.50
2:B:255:VAL:HG12	2:B:321:THR:HG21	1.94	0.50
2:B:364:TYR:CZ	2:M:152:ARG:HG2	2.46	0.50
2:M:26:THR:HG21	2:M:191:ASN:HD21	1.77	0.50
1:A:67:ASN:HD22	1:A:181:THR:HG23	1.76	0.50
2:B:246:ASN:HB2	2:B:249:SER:HB3	1.93	0.50
8:H:61:ILE:HB	8:H:62:PRO:HD3	1.92	0.50
3:N:320:VAL:HG13	8:S:58:TYR:HE2	1.76	0.50
10:U:38:ILE:HD13	10:U:112:TRP:CH2	2.46	0.50



Atom-1	Atom-2	Interatomic	Clash
7 100III ⁻ 1	1100111-2	distance (Å)	overlap (Å)
10:U:87:THR:O	10:U:120:VAL:HG21	2.10	0.50
11:V:21:ILE:HG22	11:V:22:SER:H	1.75	0.50
1:L:179:ARG:H	1:L:179:ARG:HD2	1.76	0.50
2:M:308:LEU:CB	2:M:348:LEU:HD22	2.41	0.50
1:A:239:LYS:HD2	1:A:239:LYS:N	2.25	0.50
1:A:345:HIS:O	1:A:349:LYS:HB2	2.12	0.50
5:P:44:LYS:HB3	8:S:35:LYS:HG3	1.92	0.50
1:A:99:ARG:HD3	1:A:174:LEU:CD1	2.41	0.50
1:A:164:LEU:HD13	1:A:327:LEU:HD13	1.94	0.50
1:A:214:ILE:O	1:A:214:ILE:HD12	2.11	0.50
3:C:107:ARG:HG3	3:C:107:ARG:NH2	2.27	0.50
11:K:37:GLN:HB2	11:K:47:LEU:HD11	1.91	0.50
1:L:63:ASN:N	1:L:66:ASN:ND2	2.44	0.50
7:R:97:GLN:H	7:R:97:GLN:NE2	2.10	0.50
1:A:198:ASN:O	1:A:202:LEU:HD21	2.11	0.50
4:O:286:TRP:CD2	5:P:59:MET:HG3	2.46	0.50
5:P:38:ASN:HD21	5:P:40:ASP:CG	2.15	0.50
1:A:172:THR:HG21	1:A:243:ALA:H	1.77	0.50
3:C:313:VAL:HG22	3:C:319:LYS:HE3	1.94	0.50
8:H:35:LYS:O	8:H:37:LEU:N	2.34	0.50
3:C:229:ASP:O	3:C:233:VAL:HG23	2.12	0.49
3:C:313:VAL:HG22	3:C:319:LYS:CE	2.43	0.49
1:L:238:LEU:N	1:L:238:LEU:HD22	2.27	0.49
1:A:350:GLN:HE22	1:A:353:ARG:HH21	1.59	0.49
1:A:397:LYS:HG3	1:A:399:SER:O	2.13	0.49
1:L:375:GLY:HA3	2:M:28:ILE:HG13	1.93	0.49
4:O:163:GLN:H	4:O:163:GLN:NE2	2.11	0.49
4:O:301:VAL:CG2	8:S:25:THR:HB	2.42	0.49
3:C:222:HIS:O	3:C:223:SER:HB2	2.13	0.49
3:C:14:ASN:HD22	3:C:18:ILE:HB	1.76	0.49
3:C:326:PHE:CZ	17:C:4010:8PE:H34A	2.47	0.49
3:C:77:ILE:O	3:C:81:LEU:HB2	2.13	0.49
3:C:110:ARG:NH2	3:C:205:GLY:O	2.46	0.49
1:L:29:VAL:HG12	1:L:30:THR:H	1.75	0.49
1:A:265:VAL:HG21	1:A:426:LEU:HD13	1.94	0.49
1:A:275:TYR:CZ	1:A:279:LYS:HE2	2.46	0.49
11:K:103:LYS:HG2	11:K:104:LEU:H	1.78	0.49
1:L:57:SER:HA	1:L:61:ASN:ND2	2.28	0.49
2:M:310:LYS:HE3	2:M:312:LYS:HB3	1.94	0.49
3:C:104:GLY:HA2	3:C:106:TYR:CE2	2.48	0.49
3:C:326:PHE:HZ	17:C:4010:8PE:H34A	1.78	0.49



Atom-1	Atom-2	Interatomic	Clash
2100111 1	At0111-2	distance (Å)	overlap (Å)
10:U:7:SER:OG	10:U:21:THR:HG23	2.12	0.49
11:V:11:LEU:HG	11:V:12:ALA:N	2.27	0.49
1:A:235:LYS:HB2	1:A:235:LYS:NZ	2.26	0.49
11:K:12:ALA:HA	11:K:105:GLU:O	2.13	0.49
1:L:306:ILE:HA	1:L:311:LEU:HD22	1.94	0.49
3:N:76:TYR:CG	4:O:262:GLU:HG3	2.48	0.49
1:A:302:LEU:HB2	1:A:350:GLN:HG3	1.95	0.49
7:G:91:ASN:H	7:G:91:ASN:ND2	2.10	0.49
1:L:172:THR:HG23	1:L:173:PRO:HD2	1.95	0.49
2:M:62:ARG:NH2	2:M:67:LEU:HD13	2.28	0.49
3:N:320:VAL:HG23	23:N:6971:HOH:O	2.13	0.49
5:P:168:GLY:HA2	5:P:176:TRP:CD1	2.47	0.49
12:W:26:CYS:HB3	12:W:37:VAL:HB	1.94	0.49
1:A:122:GLN:HG3	1:A:126:GLN:NE2	2.28	0.48
2:M:44:LYS:O	2:M:47:VAL:HG23	2.13	0.48
1:A:247:SER:O	1:A:432:ALA:HA	2.13	0.48
18:C:4031:CN6:O14	4:D:288:LYS:NZ	2.46	0.48
5:E:93:LYS:HE3	5:E:213:ILE:HD11	1.94	0.48
12:W:20:LYS:HA	12:W:24:GLN:HG2	1.94	0.48
1:A:280:LEU:HD13	1:A:413:ILE:HG21	1.96	0.48
10:J:87:THR:HG22	10:J:88:THR:N	2.28	0.48
1:L:230:LEU:HD13	1:L:231:GLN:HG3	1.94	0.48
1:A:30:THR:HB	1:A:216:HIS:CD2	2.48	0.48
1:A:156:HIS:HD2	1:A:159:ARG:HH21	1.61	0.48
2:B:193:VAL:HG23	2:B:193:VAL:O	2.12	0.48
5:E:122:THR:O	5:E:126:ILE:HG13	2.13	0.48
2:M:347:LYS:O	2:M:348:LEU:HB2	2.12	0.48
1:A:172:THR:CG2	1:A:242:ALA:HA	2.43	0.48
2:B:52:ASN:ND2	2:B:80:SER:OG	2.45	0.48
1:L:73:TRP:CE3	1:L:76:ILE:HD11	2.47	0.48
1:L:429:GLN:HA	1:L:429:GLN:OE1	2.14	0.48
1:A:86:ALA:HB2	1:A:119:PHE:CE1	2.48	0.48
3:C:220:PRO:HB2	23:C:7439:HOH:O	2.13	0.48
3:C:234:PHE:CZ	4:D:280:LEU:HG	2.49	0.48
1:L:172:THR:HG21	1:L:243:ALA:H	1.78	0.48
1:A:36:ILE:HA	1:A:203:ASN:HD21	1.79	0.48
1:A:58:GLY:H	1:A:61:ASN:ND2	2.02	0.48
5:E:146:ARG:CZ	5:E:202:ILE:HD11	2.44	0.48
4:O:136:ASP:HB3	4:O:145:LYS:HG3	1.96	0.48
7:R:53:ASN:ND2	7:R:56:MET:H	2.11	0.48
1:A:121:ASN:O	1:A:125:ILE:HB	2.14	0.48



Atom 1	Atom 2	Interatomic	Clash
	Atom-2	distance (\AA)	overlap (Å)
2:B:35:VAL:HG12	2:B:179:VAL:HG12	1.96	0.48
2:B:104:ALA:O	2:B:108:VAL:HG23	2.14	0.48
2:M:305:VAL:O	2:M:309:LYS:HG2	2.14	0.48
11:V:50:TYR:O	11:V:51:THR:HG22	2.13	0.48
1:L:141:LYS:HE3	1:L:186:GLU:HA	1.94	0.48
6:Q:91:GLY:O	6:Q:95:VAL:HG13	2.14	0.48
2:B:315:SER:N	2:B:316:PRO:HD3	2.29	0.47
4:D:286:TRP:HZ3	5:E:56:ALA:HA	1.79	0.47
17:N:4110:8PE:H37A	17:N:4110:8PE:H3AA	1.66	0.47
5:E:65:LEU:HD21	9:I:24:GLY:C	2.35	0.47
4:O:109:ARG:HG3	4:O:178:SER:HB2	1.96	0.47
6:Q:90:GLU:HG2	6:Q:133:TYR:CE1	2.50	0.47
5:E:187:ILE:HG13	5:E:187:ILE:O	2.14	0.47
10:J:49:VAL:CG1	10:J:68:LEU:HD23	2.44	0.47
11:K:2:ILE:HD12	11:K:2:ILE:N	2.30	0.47
2:M:318:ILE:O	2:M:321:THR:HG22	2.14	0.47
3:N:222:HIS:O	3:N:223:SER:HB2	2.14	0.47
1:L:28:GLU:O	1:L:41:GLU:HG3	2.13	0.47
1:L:76:ILE:HG23	1:L:140:THR:HG21	1.95	0.47
5:P:43:LEU:HD21	8:S:29:VAL:HG11	1.96	0.47
10:J:18:LEU:O	10:J:82:LYS:HA	2.14	0.47
1:A:141:LYS:O	1:A:145:LEU:HB2	2.15	0.47
4:D:203:PRO:HG2	4:D:206:VAL:HG21	1.96	0.47
4:D:227:ARG:HH11	4:D:244:THR:HG21	1.80	0.47
5:E:154:ILE:HD12	5:E:205:TYR:CE2	2.50	0.47
1:L:67:ASN:ND2	1:L:180:GLY:HA2	2.29	0.47
14:A:4021:UMQ:HC1	9:I:18:VAL:CG1	2.45	0.47
5:E:51:LYS:HD2	8:H:36:PRO:HG3	1.96	0.47
1:L:66:ASN:H	1:L:66:ASN:HD22	1.63	0.47
1:L:67:ASN:HD21	1:L:177:PRO:HG2	1.80	0.47
1:L:169:PHE:HB3	1:L:172:THR:HG22	1.96	0.47
15:N:4022:HEM:HMC2	15:N:4022:HEM:HBC2	1.95	0.47
11:V:75:ILE:CG2	11:V:76:SER:H	2.18	0.47
2:B:317:ALA:O	2:B:321:THR:HG22	2.15	0.47
3:C:208:ASN:HD22	3:C:210:LEU:N	2.09	0.47
7:G:45:PHE:O	7:G:48:LEU:HB2	2.15	0.47
11:K:2:ILE:HG22	11:K:3:GLU:N	2.29	0.47
1:L:72:LEU:HD22	1:L:188:LEU:HD23	1.97	0.47
2:M:233:PHE:HB3	2:M:357:GLY:HA2	1.97	0.47
4:O:225:MET:HB2	15:O:4023:HEM:C1D	2.49	0.47
2:B:43:THR:HG22	2:B:178:LYS:HZ2	1.80	0.47



Atom_1	Atom_2	Interatomic	Clash
	Atom-2	distance (Å)	overlap (Å)
3:C:332:ASN:HD21	3:C:355:ALA:HA	1.79	0.47
4:D:69:LEU:HD12	4:D:217:TYR:CE2	2.49	0.47
4:D:92:ARG:O	4:D:96:VAL:HG23	2.15	0.47
3:N:17:ILE:HG23	3:N:226:ILE:HD11	1.97	0.47
2:B:271:ILE:HG22	2:B:289:VAL:HG22	1.97	0.47
3:C:323:LYS:NZ	8:H:55:GLN:HE22	2.13	0.47
2:M:152:ARG:O	2:M:153:LYS:HB2	2.14	0.47
10:U:99:SER:HB3	10:U:109:MET:HG2	1.97	0.46
1:A:156:HIS:HD2	1:A:159:ARG:NH2	2.13	0.46
5:P:106:ASN:ND2	5:P:119:ARG:HH21	2.14	0.46
10:U:21:THR:HB	10:U:80:PHE:HD2	1.79	0.46
1:A:261:ILE:HG13	1:A:262:SER:N	2.29	0.46
10:J:20:LEU:HD12	10:J:81:LEU:HD23	1.97	0.46
2:B:43:THR:HG22	2:B:178:LYS:NZ	2.31	0.46
3:C:208:ASN:HB2	3:C:209:PRO:HD2	1.96	0.46
5:E:114:LYS:H	5:E:114:LYS:HD3	1.81	0.46
2:M:347:LYS:H	2:M:347:LYS:CD	2.07	0.46
10:U:37:TRP:CE2	10:U:81:LEU:HB2	2.50	0.46
1:A:291:PHE:HZ	1:A:335:ARG:HH11	1.63	0.46
3:C:35:LEU:HD13	23:C:5040:HOH:O	2.15	0.46
5:E:146:ARG:NH2	5:E:202:ILE:HD11	2.31	0.46
8:H:3:PRO:HG3	8:S:12:TRP:CZ2	2.49	0.46
1:L:252:ARG:HD2	8:S:21:GLN:HB2	1.96	0.46
4:D:286:TRP:CZ3	5:E:56:ALA:HA	2.51	0.46
1:L:109:LEU:HB3	1:L:110:PRO:HD2	1.97	0.46
1:A:37:VAL:HG13	1:A:207:VAL:HA	1.97	0.46
16:C:4005:SMA:H39	16:C:4005:SMA:H33	1.97	0.46
2:B:251:ALA:HB2	2:B:339:ASN:HB3	1.97	0.46
7:G:43:LEU:HD21	7:G:78:ALA:HB1	1.97	0.46
11:K:4:LEU:HD23	11:K:88:CYS:SG	2.55	0.46
1:A:270:VAL:HG21	1:A:396:ILE:HD13	1.98	0.46
2:B:315:SER:HB2	2:B:318:ILE:HD13	1.96	0.46
4:D:109:ARG:HG3	4:D:178:SER:HB2	1.98	0.46
6:Q:87:ASN:O	6:Q:92:LYS:HE2	2.15	0.46
1:A:102:GLN:HE22	1:A:196:PHE:HE1	1.63	0.46
2:B:146:LEU:O	2:B:150:THR:HG23	2.16	0.46
3:C:193:MET:HE2	3:C:196:MET:SD	2.56	0.46
4:D:223:ILE:HG12	4:D:225:MET:H	1.79	0.46
11:K:37:GLN:O	11:K:44:ILE:HA	2.16	0.46
4:O:286:TRP:CZ3	5:P:56:ALA:HA	2.50	0.46
3:C:263:LEU:HD22	5:P:115:PRO:HB3	1.98	0.45



Atom 1	Atom 9	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
4:D:277:LEU:HD21	20:D:4014:7PH:H33A	1.99	0.45
5:E:55:TYR:O	5:E:59:MET:HG2	2.16	0.45
5:E:213:ILE:O	5:E:213:ILE:HG12	2.16	0.45
6:F:117:LEU:C	6:F:119:HIS:H	2.19	0.45
2:M:30:THR:HG21	2:M:90:LYS:HE2	1.98	0.45
4:O:268:ARG:NH1	9:T:33:ASP:OD1	2.49	0.45
5:P:51:LYS:HE2	5:P:55:TYR:HE1	1.81	0.45
10:U:36:ASN:OD1	10:U:51:TYR:HB3	2.16	0.45
2:B:53:ARG:HB3	2:B:123:VAL:HG13	1.98	0.45
1:L:130:ASN:N	1:L:130:ASN:ND2	2.64	0.45
1:L:230:LEU:O	1:L:231:GLN:HB2	2.16	0.45
1:A:57:SER:HA	1:A:61:ASN:ND2	2.30	0.45
2:B:152:ARG:HD3	2:B:224:PHE:CD1	2.52	0.45
7:G:53:ASN:ND2	7:G:56:MET:H	2.13	0.45
10:J:99:SER:HA	10:J:109:MET:HA	1.97	0.45
1:L:130:ASN:HD22	1:L:130:ASN:H	1.63	0.45
1:L:181:THR:O	1:L:185:LEU:HB2	2.17	0.45
2:M:313:ASP:C	2:M:315:SER:H	2.20	0.45
5:P:146:ARG:CZ	5:P:202:ILE:HD11	2.46	0.45
2:B:141:SER:O	2:B:145:GLN:HG2	2.16	0.45
2:B:313:ASP:HB3	2:B:344:LYS:O	2.16	0.45
4:D:113:ARG:HG2	4:D:151:LEU:O	2.17	0.45
11:K:93:LYS:NZ	11:K:93:LYS:HB3	2.31	0.45
10:U:87:THR:HG22	10:U:88:THR:N	2.30	0.45
14:A:4021:UMQ:HC1	9:I:18:VAL:HG12	1.97	0.45
7:G:41:LEU:HB2	7:G:43:LEU:HD23	1.99	0.45
1:L:88:LYS:HG3	2:M:264:LEU:HD21	1.99	0.45
5:E:100:ALA:O	5:E:102:PRO:HD3	2.17	0.45
6:F:94:LEU:HB3	6:F:130:LEU:HD23	1.98	0.45
11:K:13:ALA:O	11:K:106:ILE:HG22	2.16	0.45
3:N:313:VAL:HG22	3:N:319:LYS:HE3	1.99	0.45
11:V:93:LYS:HZ3	11:V:94:PHE:N	2.08	0.45
1:A:74:LYS:HG3	1:A:95:SER:HB3	1.98	0.45
2:M:251:ALA:HB2	2:M:339:ASN:HB3	1.99	0.45
4:O:134:TYR:OH	4:O:156:PRO:HD3	2.17	0.45
2:M:289:VAL:HG12	2:M:297:VAL:HG13	1.99	0.45
1:A:239:LYS:HB2	1:A:240:LYS:H	1.54	0.45
7:G:26:VAL:HG12	7:G:30:ASN:ND2	2.31	0.45
10:J:91:THR:HG23	10:J:119:THR:HA	1.98	0.45
2:M:251:ALA:O	2:M:255:VAL:HG13	2.16	0.45
10:U:21:THR:HB	10:U:80:PHE:CD2	2.52	0.45


Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:382:ASN:HA	1:A:383:PRO:HD3	1.78	0.45
4:D:147:ARG:NH2	4:D:150:LYS:HE3	2.32	0.45
5:E:120:HIS:ND1	5:E:152:TRP:CH2	2.85	0.45
10:J:37:TRP:CE2	10:J:81:LEU:HB2	2.53	0.45
2:M:205:LEU:HD12	2:M:205:LEU:H	1.82	0.45
7:R:5:PHE:CD1	7:R:107:ILE:HG21	2.52	0.45
11:V:32:PHE:N	11:V:32:PHE:CD2	2.84	0.45
1:A:66:ASN:HD22	1:A:66:ASN:N	2.06	0.44
2:M:246:ASN:ND2	2:M:246:ASN:N	2.63	0.44
2:M:262:SER:HB3	2:M:320:TYR:CE1	2.52	0.44
10:U:82:LYS:HE2	10:U:84:ASN:OD1	2.16	0.44
11:K:29:ILE:HA	11:K:92:ILE:HG21	1.99	0.44
1:L:97:ILE:HD13	1:L:102:GLN:HG3	1.98	0.44
12:W:57:TYR:CD1	12:W:61:ASN:ND2	2.85	0.44
1:A:73:TRP:CZ3	1:A:76:ILE:HD11	2.53	0.44
1:A:234:THR:HG22	1:A:235:LYS:N	2.32	0.44
6:F:104:ARG:HG2	6:F:108:GLN:HE21	1.82	0.44
11:K:39:LYS:NZ	11:K:81:GLU:HG2	2.32	0.44
1:A:76:ILE:CG2	1:A:140:THR:HG21	2.47	0.44
2:B:215:LEU:HB2	23:B:7003:HOH:O	2.16	0.44
3:C:104:GLY:O	3:C:107:ARG:HG2	2.18	0.44
4:D:227:ARG:NH1	4:D:244:THR:HG21	2.33	0.44
7:G:97:GLN:H	7:G:97:GLN:NE2	2.15	0.44
1:L:302:LEU:HB2	1:L:350:GLN:HG3	2.00	0.44
1:A:62:GLU:OE1	1:A:67:ASN:HA	2.18	0.44
2:B:145:GLN:OE1	2:B:229:ASN:ND2	2.49	0.44
10:J:12:VAL:O	10:J:120:VAL:HA	2.18	0.44
2:M:205:LEU:HD12	2:M:205:LEU:N	2.33	0.44
10:U:34:TYR:HB2	10:U:99:SER:OG	2.18	0.44
5:E:134:MET:HG2	23:J:7001:HOH:O	2.16	0.44
7:G:18:SER:OG	7:G:21:LEU:HD23	2.18	0.44
4:O:111:ALA:HA	4:O:154:TYR:HA	2.00	0.44
1:A:88:LYS:HE3	2:B:264:LEU:HD22	2.00	0.44
1:A:109:LEU:HB3	1:A:110:PRO:HD2	2.00	0.44
1:A:127:GLN:HA	1:A:130:ASN:HD22	1.82	0.44
1:A:141:LYS:HE3	1:A:186:GLU:HA	2.00	0.44
7:G:120:LEU:O	7:G:123:ILE:HG12	2.18	0.44
1:A:160:VAL:HG21	1:A:436:THR:HG22	1.99	0.43
2:B:232:ARG:NH1	2:M:164:VAL:CG2	2.81	0.43
2:B:326:ALA:C	2:B:328:GLN:H	2.20	0.43
1:L:429:GLN:HE22	9:T:13:ARG:NH2	2.16	0.43



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:C:157:VAL:O	3:C:161:ILE:HG12	2.18	0.43
11:V:32:PHE:N	11:V:32:PHE:HD2	2.15	0.43
1:A:248:GLU:HA	1:A:433:ILE:O	2.19	0.43
10:J:51:TYR:C	10:J:51:TYR:CD2	2.91	0.43
2:M:220:GLU:HA	2:M:221:PRO:HD3	1.83	0.43
4:0:76:TRP:CZ2	4:O:188:CYS:HB3	2.53	0.43
3:C:80:TYR:CE1	3:C:248:PRO:HB2	2.53	0.43
3:C:193:MET:HE2	3:C:193:MET:HA	1.99	0.43
2:M:56:PHE:CZ	2:M:78:PHE:HB3	2.53	0.43
3:N:125:ILE:HG22	16:N:4025:SMA:H37	2.00	0.43
5:P:107:VAL:CG1	5:P:118:ILE:HB	2.48	0.43
2:B:220:GLU:HA	2:B:221:PRO:HD3	1.84	0.43
2:B:250:LEU:HD21	2:B:336:ILE:HD13	2.00	0.43
1:L:311:LEU:HB3	1:L:343:LEU:HG	2.00	0.43
8:S:3:PRO:HA	8:S:4:PRO:HD3	1.86	0.43
10:U:65:LYS:HA	10:U:68:LEU:HD11	2.00	0.43
5:E:132:VAL:HG21	5:E:192:ARG:NH1	2.34	0.43
5:P:93:LYS:HG2	5:P:213:ILE:HD11	2.00	0.43
10:U:49:VAL:HG12	10:U:68:LEU:HD23	2.01	0.43
3:C:315:GLY:HA3	23:C:6558:HOH:O	2.17	0.43
8:H:48:SER:C	8:H:50:ARG:H	2.21	0.43
11:K:8:PRO:O	11:K:102:THR:HG23	2.19	0.43
2:M:204:SER:OG	2:M:206:LEU:HB2	2.18	0.43
3:N:253:HIS:HE1	3:N:268:SER:O	2.01	0.43
7:R:63:LEU:HD12	7:R:64:PRO:HD2	2.00	0.43
10:U:61:ASN:ND2	10:U:63:SER:H	2.12	0.43
1:A:366:ALA:O	1:A:370:LEU:HB2	2.18	0.43
1:A:430:ASP:OD2	1:A:449:ARG:NH2	2.51	0.43
18:C:4031:CN6:H3A	18:C:4031:CN6:H57	1.65	0.43
10:U:51:TYR:C	10:U:51:TYR:CD2	2.91	0.43
1:A:43:ASN:HA	1:A:44:PRO:HD2	1.85	0.43
4:D:187:GLY:O	4:D:191:ILE:HG12	2.19	0.43
10:J:41:PHE:HB3	10:J:42:PRO:HD2	2.00	0.43
1:L:169:PHE:O	1:L:172:THR:HB	2.18	0.43
5:P:181:HIS:HB2	21:P:4024:FES:S1	2.58	0.43
7:G:39:LYS:HG2	7:G:94:ILE:HB	2.00	0.43
11:K:103:LYS:HG2	11:K:104:LEU:N	2.34	0.43
2:B:42:ALA:HB1	2:B:47:VAL:HG12	2.01	0.42
2:B:121:GLU:OE2	7:R:62:ARG:HD2	2.19	0.42
3:C:216:LEU:HD12	3:C:216:LEU:N	2.33	0.42
1:L:74:LYS:HG3	1:L:95:SER:CB	2.49	0.42



Atom 1	Atom 2	Interatomic Clash		
Atom-1	Atom-2	distance (Å)	overlap (Å)	
2:M:49:HIS:HE1	2:M:130:ASP:OD1	2.02	0.42	
4:O:86:ASP:HA	9:T:47:LYS:HG2	2.00	0.42	
2:B:30:THR:CG2	2:B:190:GLU:HB3	2.46	0.42	
1:L:207:VAL:HG21	1:L:394:VAL:HG23	2.00	0.42	
10:J:98:ARG:O	10:J:109:MET:HA	2.19	0.42	
11:K:7:THR:HG23	11:K:22:SER:OG	2.19	0.42	
11:K:17:ASP:HB2	11:K:18:ARG:NH2	2.34	0.42	
1:L:401:LEU:HB3	23:L:7297:HOH:O	2.18	0.42	
2:M:251:ALA:CB	2:M:339:ASN:HB3	2.49	0.42	
3:N:138:GLN:HA	3:N:138:GLN:OE1	2.20	0.42	
5:P:93:LYS:HG3	5:P:214:VAL:O	2.18	0.42	
10:U:12:VAL:O	10:U:120:VAL:HA	2.19	0.42	
1:A:76:ILE:HG23	1:A:140:THR:HG21	2.01	0.42	
1:L:42:HIS:HB2	23:L:7033:HOH:O	2.18	0.42	
2:M:254:GLU:CG	2:M:278:LYS:HE3	2.50	0.42	
2:B:52:ASN:HD21	2:B:80:SER:C	2.23	0.42	
2:B:117:HIS:HB3	7:R:62:ARG:HG2	2.02	0.42	
2:B:270:LEU:HB3	2:B:304:ILE:HD11	2.01	0.42	
11:K:79:GLU:HA	11:K:80:PRO:HA	1.74	0.42	
4:D:111:ALA:HA	4:D:154:TYR:HA	2.01	0.42	
7:G:62:ARG:HG2	2:M:117:HIS:HB3	2.01	0.42	
10:J:38:ILE:HA	10:J:49:VAL:HG23	2.01	0.42	
10:J:61:ASN:HD22	10:J:61:ASN:C	2.23	0.42	
1:L:386:ASP:O	1:L:390:LEU:HB2	2.20	0.42	
2:M:347:LYS:CG	2:M:348:LEU:H	2.23	0.42	
4:D:147:ARG:HG2	4:D:148:PRO:O	2.20	0.42	
8:H:61:ILE:O	8:H:65:ILE:HG13	2.20	0.42	
11:K:4:LEU:CD2	11:K:88:CYS:SG	3.08	0.42	
1:L:58:GLY:H	1:L:61:ASN:ND2	2.10	0.42	
1:L:169:PHE:CD1	1:L:174:LEU:HB3	2.55	0.42	
3:N:216:LEU:N	3:N:216:LEU:HD12	2.35	0.42	
12:W:18:LEU:HD23	12:W:103:LEU:HB2	2.02	0.42	
1:A:386:ASP:O	1:A:390:LEU:HB2	2.19	0.42	
1:L:447:ARG:NH1	3:N:18:ILE:HG22	2.34	0.42	
4:0:123:GLU:CD	4:0:123:GLU:H	2.23	0.42	
6:Q:81:LEU:HB3	6:Q:138:THR:HG22	2.02	0.42	
1:A:344:ILE:HG21	1:A:448:ILE:HD12	2.02	0.42	
2:B:332:VAL:O	2:B:332:VAL:HG12	2.20	0.42	
5:P:120:HIS:ND1	5:P:152:TRP:CH2	2.87	0.42	
7:R:115:LYS:HE3	7:R:119:GLU:OE2	2.20	0.42	
10:U:6:GLU:HG2	10:U:96:CYS:SG	2.60	0.42	



Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:292:GLU:CD	2:B:53:ARG:HH12	2.23	0.41
2:B:39:SER:OG	2:B:84:ARG:HA	2.20	0.41
2:M:338:LEU:H	2:M:338:LEU:HD22	1.84	0.41
3:N:77:ILE:O	3:N:81:LEU:HB2	2.19	0.41
12:W:70:GLU:CD	12:W:70:GLU:H	2.22	0.41
2:B:66:LYS:HE3	2:B:70:GLU:OE2	2.20	0.41
18:C:4031:CN6:HAA	7:G:85:HIS:CE1	2.55	0.41
4:D:76:TRP:CZ2	4:D:188:CYS:HB3	2.55	0.41
4:D:256:ASN:C	4:D:256:ASN:HD22	2.23	0.41
5:E:125:GLU:HB3	5:E:187:ILE:HG12	2.02	0.41
11:K:19:VAL:HG12	11:K:75:ILE:HB	2.02	0.41
2:M:44:LYS:HB2	2:M:47:VAL:CG2	2.50	0.41
18:N:4131:CN6:H3A	18:N:4131:CN6:H57	1.81	0.41
10:U:36:ASN:HD21	10:U:99:SER:CB	2.33	0.41
2:B:53:ARG:HD3	2:B:130:ASP:OD1	2.19	0.41
3:C:99:LYS:HD2	3:C:99:LYS:C	2.40	0.41
5:E:165:VAL:HG23	3:N:142:TRP:CH2	2.55	0.41
11:K:46:LEU:HD23	11:K:55:HIS:CD2	2.54	0.41
2:B:98:LEU:O	2:B:102:VAL:HG23	2.20	0.41
3:C:313:VAL:CG2	3:C:319:LYS:HE3	2.50	0.41
1:A:447:ARG:NH1	3:C:18:ILE:HG22	2.36	0.41
7:G:91:ASN:H	7:G:91:ASN:HD22	1.69	0.41
11:K:48:ILE:HD13	11:K:54:LEU:HA	2.02	0.41
1:L:102:GLN:HE21	1:L:102:GLN:HB2	1.68	0.41
14:L:4121:UMQ:HC1	9:T:18:VAL:HG13	2.02	0.41
7:R:46:ASP:HB2	7:R:102:TYR:CE2	2.55	0.41
11:V:4:LEU:HD23	11:V:88:CYS:SG	2.61	0.41
2:B:183:GLU:HG2	2:B:211:ALA:HB1	2.03	0.41
7:G:127:LYS:HD3	7:G:127:LYS:N	2.36	0.41
1:L:379:GLU:OE1	2:M:26:THR:HB	2.21	0.41
1:A:220:VAL:O	1:A:224:GLU:HB2	2.21	0.41
5:E:38:ASN:HD21	5:E:40:ASP:CG	2.24	0.41
10:J:29:ILE:H	10:J:77:ASN:HD21	1.69	0.41
11:K:58:VAL:HA	11:K:59:PRO:HD3	1.86	0.41
2:M:230:ARG:HH21	2:M:230:ARG:HG2	1.86	0.41
3:N:58:ILE:HD11	3:N:136:TYR:CZ	2.55	0.41
3:N:107:ARG:NH1	3:N:311:SER:O	2.54	0.41
1:A:252:ARG:HG3	1:A:439:ILE:HG13	2.02	0.41
1:A:364:GLU:HG3	7:R:125:VAL:HG21	2.03	0.41
3:C:178:ARG:HE	3:C:178:ARG:HB3	1.72	0.41
3:C:193:MET:CE	3:C:196:MET:SD	3.09	0.41



Atom_1	Atom_2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
4:O:256:ASN:HD22	4:O:256:ASN:C	2.24	0.41
12:W:58:THR:HB	15:W:4026:HEM:O2D	2.20	0.41
1:A:179:ARG:HG2	1:A:179:ARG:NH2	2.35	0.41
1:A:266:GLU:O	1:A:425:ARG:HG3	2.21	0.41
2:B:31:LEU:HD21	2:B:197:LEU:HD11	2.03	0.41
2:B:41:TYR:HD2	2:B:215:LEU:HD13	1.86	0.41
2:B:46:GLY:HA3	2:B:161:TYR:HA	2.03	0.41
18:C:4031:CN6:H52A	18:C:4031:CN6:H2'	1.68	0.41
4:D:92:ARG:HG2	4:D:236:TYR:CE2	2.56	0.41
10:J:87:THR:HG22	10:J:89:GLU:H	1.85	0.41
1:L:43:ASN:HA	1:L:44:PRO:HD2	1.89	0.41
1:L:72:LEU:HD13	1:L:144:VAL:HG21	2.03	0.41
2:M:39:SER:OG	2:M:84:ARG:HA	2.20	0.41
2:M:193:VAL:HG23	2:M:196:ASP:HB2	2.02	0.41
1:A:74:LYS:HE3	1:A:95:SER:O	2.21	0.41
3:C:234:PHE:CE2	4:D:280:LEU:HG	2.55	0.41
8:H:48:SER:O	8:H:49:PHE:HB2	2.21	0.41
1:L:318:PHE:HB2	1:L:320:LEU:HD13	2.03	0.41
3:N:314:ARG:HD3	23:N:5535:HOH:O	2.20	0.41
11:V:34:ASN:ND2	11:V:49:TYR:HA	2.36	0.41
12:W:43:GLY:N	12:W:111:ALA:O	2.53	0.41
1:L:74:LYS:HB2	1:L:97:ILE:HD11	2.04	0.40
2:B:336:ILE:HD12	2:B:336:ILE:N	2.30	0.40
5:E:114:LYS:HD3	5:E:114:LYS:N	2.36	0.40
5:E:164:CYS:HB2	5:E:178:CYS:SG	2.62	0.40
8:H:3:PRO:HG3	8:S:12:TRP:CE2	2.56	0.40
12:W:37:VAL:O	15:W:4026:HEM:HMD3	2.22	0.40
2:B:146:LEU:HD13	2:B:146:LEU:HA	1.93	0.40
1:L:46:ALA:HB3	1:L:213:ASN:HB3	2.03	0.40
4:0:212:SER:0	13:X:2:FRU:H4	2.22	0.40
4:0:273:THR:OG1	20:O:4114:7PH:H2	2.22	0.40
7:R:43:LEU:HD21	7:R:78:ALA:CB	2.51	0.40
2:B:364:TYR:CE1	2:M:152:ARG:HG2	2.56	0.40
10:J:10:GLY:HA2	10:J:118:VAL:HG12	2.02	0.40
11:K:4:LEU:HD21	11:K:33:LEU:HD11	2.04	0.40
8:S:88:GLU:O	8:S:92:VAL:HG22	2.20	0.40
10:U:29:ILE:N	10:U:77:ASN:HD21	2.06	0.40
12:W:96:LYS:HD3	12:W:98:LYS:HZ3	1.85	0.40
1:A:271:ASN:HD21	1:A:397:LYS:NZ	2.20	0.40
2:B:30:THR:OG1	2:B:90:LYS:HE3	2.22	0.40
2:B:145:GLN:HB3	2:B:354:VAL:HG11	2.03	0.40



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:20:SER:HA	3:C:21:PRO:HD3	1.91	0.40
10:U:54:ASN:H	10:U:54:ASN:ND2	2.18	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	429/431~(100%)	395~(92%)	33 (8%)	1 (0%)	47	68
1	L	429/431~(100%)	393 (92%)	32 (8%)	4 (1%)	17	31
2	В	350/352~(99%)	310 (89%)	31 (9%)	9 (3%)	5	8
2	М	350/352~(99%)	320 (91%)	19 (5%)	11 (3%)	4	5
3	С	383/385~(100%)	364 (95%)	17 (4%)	2 (0%)	29	48
3	Ν	383/385~(100%)	367~(96%)	14 (4%)	2(0%)	29	48
4	D	244/248~(98%)	231 (95%)	12 (5%)	1 (0%)	34	54
4	Ο	244/248~(98%)	234 (96%)	10 (4%)	0	100	100
5	Е	183/185~(99%)	171 (93%)	9 (5%)	3 (2%)	9	17
5	Р	183/185~(99%)	171 (93%)	10 (6%)	2 (1%)	14	26
6	F	72/146~(49%)	68 (94%)	4 (6%)	0	100	100
6	Q	72/146~(49%)	67 (93%)	4 (6%)	1 (1%)	11	20
7	G	123/126~(98%)	121 (98%)	2 (2%)	0	100	100
7	R	123/126~(98%)	119 (97%)	4 (3%)	0	100	100
8	Н	91/93~(98%)	78~(86%)	10 (11%)	3 (3%)	4	5
8	S	91/93~(98%)	82 (90%)	6 (7%)	3 (3%)	4	5
9	Ι	53/65~(82%)	48 (91%)	4 (8%)	1 (2%)	8	13
9	Т	53/65~(82%)	50 (94%)	1 (2%)	2 (4%)	3	4



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
10	J	125/127~(98%)	110 (88%)	14 (11%)	1 (1%)	19 35
10	U	125/127~(98%)	110 (88%)	12 (10%)	3~(2%)	6 9
11	Κ	105/107~(98%)	80~(76%)	21 (20%)	4 (4%)	3 4
11	V	105/107~(98%)	82~(78%)	20 (19%)	3~(3%)	4 6
12	W	110/112~(98%)	98~(89%)	11 (10%)	1 (1%)	17 31
All	All	4426/4642 (95%)	4069 (92%)	300 (7%)	57 (1%)	12 21

Continued from previous page...

All (57) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	В	152	ARG
2	В	153	LYS
2	В	335	PRO
2	В	343	VAL
3	С	346	VAL
8	Н	37	LEU
8	Н	93	ASN
11	K	80	PRO
2	М	153	LYS
2	М	335	PRO
2	М	343	VAL
2	М	348	LEU
5	Р	103	LEU
2	В	214	SER
2	В	311	GLY
2	В	327	VAL
3	С	223	SER
5	Е	102	PRO
5	Е	103	LEU
8	Н	36	PRO
10	J	65	LYS
1	L	126	GLN
2	М	311	GLY
2	М	338	LEU
3	N	223	SER
6	Q	118	GLU
8	S	37	LEU
2	В	338	LEU
5	Е	46	ASN
9	Ι	55	ARG



	J	1	1 5
Mol	Chain	Res	Type
11	K	51	THR
1	L	227	ASN
2	М	313	ASP
5	Р	102	PRO
9	Т	12	LYS
9	Т	13	ARG
10	U	44	ASN
11	V	30	ASN
1	L	228	LEU
2	М	95	LYS
8	S	93	ASN
10	U	32	GLY
12	W	6	GLY
1	А	127	GLN
4	D	263	HIS
11	K	10	SER
2	М	315	SER
2	М	327	VAL
8	S	36	PRO
10	U	15	SER
11	K	16	GLY
1	L	231	GLN
2	М	314	LEU
3	N	346	VAL
11	V	68	GLY
2	В	332	VAL
11	V	80	PRO

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	Percentiles
1	А	370/370~(100%)	338 (91%)	32 (9%)	10 20
1	L	370/370~(100%)	334 (90%)	36 (10%)	8 16
2	В	301/301~(100%)	273 (91%)	28 (9%)	9 17

Continued on next page...



Mol	Chain	Analysed	Rotameric	Outliers	Perce	entiles
2	М	301/301~(100%)	274 (91%)	27 (9%)	9	19
3	С	338/338~(100%)	317 (94%)	21 (6%)	18	35
3	Ν	338/338~(100%)	320 (95%)	18 (5%)	22	43
4	D	204/206~(99%)	197~(97%)	7(3%)	37	63
4	Ο	204/206~(99%)	197~(97%)	7(3%)	37	63
5	Ε	151/151~(100%)	147 (97%)	4 (3%)	46	72
5	Р	151/151~(100%)	147 (97%)	4 (3%)	46	72
6	F	67/130~(52%)	64 (96%)	3 (4%)	27	51
6	Q	67/130~(52%)	64 (96%)	3 (4%)	27	51
7	G	109/110~(99%)	104 (95%)	5 (5%)	27	50
7	R	109/110 (99%)	104 (95%)	5 (5%)	27	50
8	Н	77/77~(100%)	76~(99%)	1 (1%)	69	87
8	S	77/77~(100%)	75~(97%)	2(3%)	46	72
9	Ι	45/53~(85%)	44 (98%)	1 (2%)	52	77
9	Т	45/53~(85%)	43 (96%)	2(4%)	28	52
10	J	112/112~(100%)	105 (94%)	7~(6%)	18	34
10	U	112/112~(100%)	102 (91%)	10 (9%)	9	19
11	Κ	93/93~(100%)	86 (92%)	7 (8%)	13	26
11	V	93/93~(100%)	88 (95%)	5 (5%)	22	42
12	W	92/91~(101%)	86 (94%)	6 (6%)	17	33
All	All	3826/3973~(96%)	3585 (94%)	241 (6%)	18	34

All (241) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	66	ASN
1	А	113	THR
1	А	115	LYS
1	А	126	GLN
1	А	164	LEU
1	А	172	THR
1	А	179	ARG
1	А	185	LEU
1	А	188	LEU
1	А	193	LEU



Mol	Chain	Res	Type
1	А	203	ASN
1	А	239	LYS
1	А	252	ARG
1	А	261	ILE
1	А	271	ASN
1	А	272	SER
1	А	289	ASN
1	А	311	LEU
1	А	320	LEU
1	А	330	PHE
1	А	336	ASN
1	А	343	LEU
1	А	361	THR
1	А	370	LEU
1	А	377	LEU
1	А	384	VAL
1	А	390	LEU
1	А	425	ARG
1	А	426	LEU
1	А	429	GLN
1	А	443	LEU
1	А	456	ARG
2	В	30	THR
2	В	31	LEU
2	В	53	ARG
2	В	54	PHE
2	В	62	ARG
2	В	73	LEU
2	В	128	ARG
2	В	136	GLN
2	В	144	ASP
2	В	146	LEU
2	В	150	THR
2	В	155	LEU
2	В	166	ARG
2	В	169	LEU
2	В	206	LEU
2	В	215	LEU
2	В	250	LEU
2	В	252	GLN
2	В	254	GLU
2	В	255	VAL



Mol	Chain	Res	Type
2	В	270	LEU
2	В	312	LYS
2	В	323	LEU
2	В	330	GLU
2	В	339	ASN
2	В	343	VAL
2	В	347	LYS
2	В	362	LEU
3	С	38	LEU
3	С	79	ARG
3	С	89	PHE
3	С	99	LYS
3	С	107	ARG
3	С	111	VAL
3	С	150	LEU
3	С	175	THR
3	С	182	LEU
3	С	184	TYR
3	С	185	LEU
3	С	238	LEU
3	С	247	SER
3	С	292	VAL
3	С	302	LEU
3	С	312	VAL
3	С	313	VAL
3	С	336	LEU
3	С	350	LEU
3	С	377	LEU
3	C	382	ARG
4	D	113	ARG
4	D	141	GLN
4	D	147	ARG
4	D	251	VAL
4	D	256	ASN
4	D	280	LEU
4	D	288	LYS
5	E	114	LYS
5	E	208	ASP
5	E	211	LYS
5	E	213	ILE
6	F	77	GLN
6	F	94	LEU



Mol	Chain	Res	Type
6	F	130	LEU
7	G	16	LEU
7	G	58	THR
7	G	97	GLN
7	G	123	ILE
7	G	127	LYS
8	Н	60	LEU
9	Ι	18	VAL
10	J	38	ILE
10	J	39	ARG
10	J	44	ASN
10	J	51	TYR
10	J	61	ASN
10	J	68	LEU
10	J	114	GLN
11	Κ	7	THR
11	K	18	ARG
11	Κ	33	LEU
11	Κ	77	ASN
11	K	81	GLU
11	Κ	92	ILE
11	K	93	LYS
1	L	30	THR
1	L	66	ASN
1	L	89	GLU
1	L	117	LEU
1	L	120	LEU
1	L	126	GLN
1	L	130	ASN
1	L	153	ASP
1	L	164	LEU
1	L	172	THR
1	L	174	LEU
1	L	176	LEU
1	L	179	ARG
1	L	185	LEU
1	L	188	LEU
1	L	218	ASP
1	L	237	VAL
1	L	238	LEU
1	L	239	LYS
1	L	241	LYS



Mol	Chain	Res	Type
1	L	261	ILE
1	L	289	ASN
1	L	293	PRO
1	L	311	LEU
1	L	320	LEU
1	L	330	PHE
1	L	336	ASN
1	L	343	LEU
1	L	370	LEU
1	L	374	LEU
1	L	377	LEU
1	L	390	LEU
1	L	424	LYS
1	L	425	ARG
1	L	426	LEU
1	L	443	LEU
2	М	17	LEU
2	М	30	THR
2	М	31	LEU
2	М	40	ARG
2	М	53	ARG
2	М	54	PHE
2	М	62	ARG
2	М	73	LEU
2	М	111	LYS
2	М	136	GLN
2	М	144	ASP
2	М	146	LEU
2	М	166	ARG
2	М	169	LEU
2	М	186	GLU
2	М	206	LEU
2	М	238	VAL
2	М	246	ASN
2	М	250	LEU
2	М	255	VAL
2	М	310	LYS
2	М	312	LYS
2	М	329	ASN
2	М	330	GLU
2	М	345	ASP
2	М	347	LYS



Mol	Chain	Res	Type
2	М	362	LEU
3	Ν	35	LEU
3	Ν	38	LEU
3	N	79	ARG
3	Ν	87	SER
3	N	89	PHE
3	N	99	LYS
3	N	150	LEU
3	Ν	182	LEU
3	Ν	184	TYR
3	Ν	185	LEU
3	Ν	208	ASN
3	Ν	218	ARG
3	Ν	302	LEU
3	Ν	312	VAL
3	Ν	336	LEU
3	Ν	350	LEU
3	Ν	377	LEU
3	Ν	382	ARG
4	0	69	LEU
4	0	163	GLN
4	0	179	LEU
4	0	251	VAL
4	0	256	ASN
4	0	280	LEU
4	0	283	LEU
5	Р	51	LYS
5	Р	65	LEU
5	Р	80	SER
5	Р	211	LYS
6	Q	77	GLN
6	Q	94	LEU
6	Q	130	LEU
7	R	16	LEU
7	R	41	LEU
7	R	97	GLN
7	R	125	VAL
7	R	127	LYS
8	S	50	ARG
8	S	68	TYR
9	Т	14	ASN
9	Т	18	VAL



Mol	Chain	Res	Type
10	U	3	LYS
10	U	21	THR
10	U	38	ILE
10	U	39	ARG
10	U	51	TYR
10	U	54	ASN
10	U	59	ASN
10	U	61	ASN
10	U	66	ASP
10	U	68	LEU
11	V	18	ARG
11	V	41	ASP
11	V	81	GLU
11	V	89	GLN
11	V	92	ILE
12	W	2	LYS
12	W	20	LYS
12	W	51	GLN
12	W	58	THR
12	W	82	LYS
12	W	98	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (136) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	61	ASN
1	А	66	ASN
1	А	67	ASN
1	А	96	ASN
1	А	102	GLN
1	А	130	ASN
1	А	156	HIS
1	А	199	ASN
1	А	231	GLN
1	А	271	ASN
1	А	274	ASN
1	А	289	ASN
1	А	317	HIS
1	А	336	ASN
1	А	350	GLN
1	А	382	ASN
1	А	385	ASN



Mol	Chain	Res	Type
1	А	388	ASN
1	А	429	GLN
2	В	49	HIS
2	В	52	ASN
2	В	55	ASN
2	В	57	GLN
2	В	103	ASN
2	В	191	ASN
2	В	246	ASN
2	В	252	GLN
2	В	258	ASN
2	В	339	ASN
3	С	14	ASN
3	С	22	GLN
3	С	74	ASN
3	С	173	ASN
3	С	202	HIS
3	С	208	ASN
3	С	253	HIS
3	С	332	ASN
4	D	78	HIS
4	D	79	ASN
4	D	127	ASN
4	D	141	GLN
4	D	256	ASN
5	Е	38	ASN
5	Е	47	ASN
5	Е	106	ASN
5	Е	184	HIS
6	F	77	GLN
6	F	84	HIS
6	F	108	GLN
6	F	109	GLN
6	F	111	GLN
6	F	129	HIS
7	G	30	ASN
7	G	53	ASN
7	G	79	HIS
7	G	91	ASN
7	G	97	GLN
8	Н	55	GLN
8	Н	74	ASN



Mol	Chain	Res	Type
9	Ι	14	ASN
9	Ι	29	GLN
10	J	44	ASN
10	J	54	ASN
10	J	61	ASN
10	J	77	ASN
10	J	78	GLN
11	K	34	ASN
11	K	89	GLN
11	K	91	HIS
1	L	61	ASN
1	L	66	ASN
1	L	67	ASN
1	L	102	GLN
1	L	127	GLN
1	L	130	ASN
1	L	156	HIS
1	L	170	GLN
1	L	199	ASN
1	L	227	ASN
1	L	274	ASN
1	L	283	GLN
1	L	289	ASN
1	L	317	HIS
1	L	336	ASN
1	L	350	GLN
1	L	385	ASN
1	L	388	ASN
1	L	438	GLN
2	М	49	HIS
2	М	52	ASN
2	М	55	ASN
2	М	246	ASN
2	М	252	GLN
2	М	329	ASN
2	М	339	ASN
3	Ν	14	ASN
3	Ν	22	GLN
3	Ν	43	GLN
3	Ν	74	ASN
3	Ν	208	ASN
3	Ν	253	HIS



Mol	Chain	Res	Type
3	Ν	332	ASN
4	0	78	HIS
4	0	79	ASN
4	0	127	ASN
4	0	163	GLN
4	0	256	ASN
5	Р	38	ASN
5	Р	97	ASN
5	Р	106	ASN
5	Р	112	GLN
5	Р	184	HIS
6	Q	77	GLN
7	R	30	ASN
7	R	31	GLN
7	R	53	ASN
7	R	57	GLN
7	R	79	HIS
7	R	91	ASN
7	R	97	GLN
8	S	38	GLN
8	S	55	GLN
9	Т	14	ASN
9	Т	29	GLN
10	U	54	ASN
10	U	58	ASN
10	U	59	ASN
10	U	61	ASN
10	U	77	ASN
10	U	78	GLN
11	V	34	ASN
11	V	90	HIS
11	V	91	HIS
12	W	25	GLN
12	W	61	ASN
12	W	101	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)

1 non-standard protein/DNA/RNA residue is 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).

Mol	Tuno	Chain	Res	es Link	Bond lengths			Bond angles		
	туре				Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
12	M3L	W	81	12	10,11,12	0.84	0	9,14,16	1.22	1 (11%)

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
12	M3L	W	81	12	-	0/9/10/12	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
12	W	81	M3L	CM3-NZ-CM1	-2.54	102.43	108.97

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

2 monosaccharides 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



13

13

length (or angle) is the number of standard deviations the observed value is removed from the

1 (6%)

0

(expecte	ed value.	A bond	length	(or ang	(gle) with $ Z > 2$ is considered	an outlier worth inspection.					
1	RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).											
	Mol	Tuno	Chain	Dog	Tink	Bond lengths	Bond angles					
	WIOI	Type	Unam	nes	LIIIK	Counts RMSZ $\# Z > 2$	Counts RMSZ $\# Z > 2$					

0.79

0.76

0

1(9%)

15,15,17

10,18,18

0.94

0.53

11,11,12

11,12,12

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
13	GLC	Х	1	13	-	0/2/19/22	0/1/1/1
13	FRU	Х	2	13	-	0/5/24/24	0/1/1/1

13

13

All (1) bond length outliers are listed below:

Х

Х

1

2

 GLC

FRU

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
13	Х	2	FRU	O2-C2	2.05	1.44	1.40

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
13	Х	1	GLC	C2-C3-C4	-3.02	105.66	110.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	Х	2	FRU	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.





5.6 Ligand geometry (i)

23 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	Chain	Dec	Tink	B	ond leng	gths	E	Bond angles		
WIOI	туре	Unam	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2	
15	HEM	С	4001	3	41,50,50	1.49	7 (17%)	45,82,82	1.04	3 (6%)	
15	HEM	Ν	4021	3	41,50,50	1.50	5 (12%)	45,82,82	1.22	5 (11%)	
18	CN6	С	4031	-	49,49,49	1.59	10 (20%)	55,61,61	1.53	8 (14%)	
16	SMA	С	4005	-	38,38,38	1.03	3 (7%)	48,52,52	0.93	3 (6%)	
22	6PH	L	4113	-	39,39,39	0.97	2 (5%)	43,44,44	1.53	5 (11%)	
21	FES	Е	4004	5	0,4,4	-	-	-			
14	UMQ	А	4021	-	35,35,35	0.99	2 (5%)	46,46,46	1.72	5 (10%)	



Mal	Tuno	Chain	Dog	Tink	B	ond leng	gths	B	Bond ang	gles
	туре	Ullalli	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
15	HEM	D	4003	4	41,50,50	1.44	4 (9%)	45,82,82	1.25	6 (13%)
17	8PE	N	4110	-	46,46,46	0.91	2 (4%)	49,51,51	1.18	3 (6%)
17	8PE	C	4010	-	46,46,46	0.96	3 (6%)	49,51,51	1.02	1 (2%)
15	HEM	С	4002	3	41,50,50	1.37	6 (14%)	45,82,82	0.91	2 (4%)
15	HEM	W	4026	12	41,50,50	1.49	6 (14%)	45,82,82	1.09	5 (11%)
19	9PE	С	4111	-	39,39,39	0.77	0	42,44,44	0.95	1 (2%)
18	CN6	N	4131	-	49,49,49	1.63	10 (20%)	55,61,61	1.66	9 (16%)
20	7PH	D	4014	-	37,37,37	1.03	2 (5%)	41,42,42	1.53	10 (24%)
16	SMA	N	4025	-	38,38,38	1.00	3 (7%)	48,52,52	0.80	1 (2%)
20	7PH	0	4114	-	37,37,37	1.04	2 (5%)	41,42,42	1.59	10 (24%)
19	9PE	N	4011	-	39,39,39	0.73	0	42,44,44	0.92	1 (2%)
15	HEM	N	4022	3	41,50,50	1.39	6 (14%)	45,82,82	1.03	3 (6%)
21	FES	Р	4024	5	0,4,4	-	-	-		
22	6PH	E	4013	-	39,39,39	0.95	2 (5%)	43,44,44	1.50	5 (11%)
14	UMQ	L	4121	-	35,35,35	1.01	1 (2%)	46,46,46	1.78	5 (10%)
15	HEM	0	4023	4	41,50,50	1.49	4 (9%)	45,82,82	1.16	5 (11%)

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
15	HEM	С	4001	3	-	4/12/54/54	-
15	HEM	Ν	4021	3	-	4/12/54/54	-
18	CN6	С	4031	-	-	27/60/60/60	-
16	SMA	С	4005	-	-	2/34/34/34	0/2/2/2
22	6PH	L	4113	-	-	20/41/41/41	-
21	FES	Е	4004	5	-	-	0/1/1/1
14	UMQ	А	4021	-	-	4/20/60/60	0/2/2/2
15	HEM	D	4003	4	-	8/12/54/54	-
17	8PE	Ν	4110	-	-	19/50/50/50	-
17	8PE	С	4010	-	-	24/50/50/50	-
15	HEM	С	4002	3	-	4/12/54/54	-
15	HEM	W	4026	12	-	4/12/54/54	-
19	9PE	С	4111	-	-	19/43/43/43	-



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CN6	Ν	4131	-	-	29/60/60/60	-
20	7PH	D	4014	-	-	14/39/39/39	-
16	SMA	Ν	4025	-	-	1/34/34/34	0/2/2/2
20	7PH	Ο	4114	-	-	12/39/39/39	-
19	9PE	Ν	4011	-	-	21/43/43/43	-
15	HEM	Ν	4022	3	-	4/12/54/54	-
21	FES	Р	4024	5	-	-	0/1/1/1
22	6PH	Е	4013	-	-	17/41/41/41	-
14	UMQ	L	4121	-	-	4/20/60/60	0/2/2/2
15	HEM	0	4023	4	-	8/12/54/54	-

All (80) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}(\operatorname{\AA})$
15	0	4023	HEM	CBB-CAB	4.86	1.54	1.30
15	Ν	4021	HEM	C3C-CAC	-4.79	1.38	1.47
15	С	4001	HEM	C3C-CAC	-4.77	1.38	1.47
15	D	4003	HEM	CBB-CAB	4.61	1.53	1.30
15	W	4026	HEM	CBB-CAB	4.44	1.52	1.30
18	Ν	4131	CN6	O31-C3	-4.26	1.35	1.45
18	С	4031	CN6	O31-C3	-4.19	1.35	1.45
14	L	4121	UMQ	C3-C2	-4.06	1.42	1.52
15	D	4003	HEM	C3C-C2C	-3.75	1.35	1.40
15	0	4023	HEM	C3C-C2C	-3.73	1.35	1.40
15	D	4003	HEM	CBC-CAC	3.68	1.53	1.29
15	Ν	4021	HEM	C3C-C2C	-3.63	1.35	1.40
15	W	4026	HEM	CBC-CAC	3.62	1.53	1.29
20	D	4014	7PH	O31-C3	-3.60	1.36	1.45
20	0	4114	7PH	O31-C3	-3.60	1.36	1.45
18	Ν	4131	CN6	O21-C2	-3.59	1.37	1.46
14	А	4021	UMQ	C3-C2	-3.58	1.43	1.52
18	С	4031	CN6	O21-C2	-3.56	1.37	1.46
15	0	4023	HEM	CBC-CAC	3.50	1.52	1.29
15	С	4002	HEM	C3C-C2C	-3.48	1.35	1.40
18	С	4031	CN6	O3'-CA	-3.44	1.31	1.44
15	С	4001	HEM	CAB-C3B	-3.40	1.38	1.47
18	N	4131	CN6	03'-CA	-3.37	1.31	1.44
15	Ν	4022	HEM	C3C-C2C	-3.37	1.35	1.40
15	W	4026	HEM	C3C-CAC	3.33	1.54	1.47
16	С	4005	SMA	O1-C2	3.30	1.40	1.36



3CXH

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\mathbf{Mol}	Chain	Res	Type	Atoms	\mathbf{Z}	Observed(Å)	Ideal(Å)	
15	С	4001	HEM	C3C-C2C	-3.29	1.35	1.40	
15	N	4022	HEM	CMA-C3A	3.20	1.58	1.51	
15	Ν	4021	HEM	CAB-C3B	-3.18	1.38	1.47	
16	Ν	4025	SMA	O1-C2	3.16	1.40	1.36	
15	W	4026	HEM	C3C-C2C	-3.13	1.36	1.40	
15	С	4002	HEM	CBB-CAB	3.10	1.45	1.30	
15	С	4002	HEM	C3C-CAC	-3.09	1.41	1.47	
15	Ν	4022	HEM	C3C-CAC	-3.09	1.41	1.47	
18	Ν	4131	CN6	O32-C31	-3.02	1.13	1.22	
17	С	4010	8PE	O21-C21	3.00	1.42	1.34	
16	С	4005	SMA	C20-C19	2.99	1.36	1.33	
18	Ν	4131	CN6	CA-CB	2.98	1.61	1.51	
15	Ν	4022	HEM	CAB-C3B	-2.96	1.39	1.47	
15	N	4022	HEM	CBC-CAC	2.92	1.48	1.29	
18	С	4031	CN6	CC-CB	2.88	1.61	1.51	
15	Ν	4021	HEM	CBB-CAB	2.86	1.44	1.30	
18	С	4031	CN6	O32-C31	-2.85	1.14	1.22	
16	Ν	4025	SMA	C8-C8A	2.77	1.44	1.39	
15	С	4002	HEM	CBC-CAC	2.70	1.47	1.29	
15	С	4002	HEM	CAB-C3B	-2.65	1.40	1.47	
18	Ν	4131	CN6	CC-CB	2.63	1.60	1.51	
17	Ν	4110	8PE	O21-C21	2.58	1.41	1.34	
15	Ν	4022	HEM	CBB-CAB	2.55	1.42	1.30	
18	Ν	4131	CN6	O11-C1	-2.54	1.35	1.44	
18	С	4031	CN6	CA-CB	2.52	1.60	1.51	
17	С	4010	8PE	O32-C31	-2.51	1.15	1.22	
18	С	4031	CN6	O11-C1	-2.49	1.35	1.44	
17	Ν	4110	8PE	O32-C31	-2.47	1.15	1.22	
18	Ν	4131	CN6	OA-CB	2.41	1.50	1.43	
15	С	4001	HEM	CMC-C2C	2.34	1.57	1.51	
22	L	4113	6PH	C1-C2	2.33	1.57	1.50	
20	0	4114	7PH	O22-C21	-2.32	1.15	1.22	
18	С	4031	CN6	OA-CB	2.30	1.50	1.43	
15	0	4023	HEM	C3C-CAC	2.27	1.52	1.47	
18	Ν	4131	CN6	O21-C21	2.22	1.40	1.34	
15	С	4001	HEM	CBB-CAB	2.21	1.41	1.30	
15	D	4003	HEM	C3C-CAC	2.20	1.52	1.47	
15	N	4021	HEM	CMB-C2B	2.18	1.55	1.50	
22	L	4113	6PH	C3-C2	2.18	1.57	1.50	
18	N	4131	CN6	O41-C3'	-2.16	1.40	1.45	
18	С	4031	CN6	O21-C21	2.15	1.40	1.34	
16	N	4025	SMA	C20-C19	2.13	1.35	1.33	
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2CVU	
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Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
20	D	4014	7PH	O22-C21	-2.11	1.16	1.22
17	С	4010	8PE	C3-C2	2.11	1.57	1.50
22	Е	4013	6PH	C3-C2	2.11	1.57	1.50
15	С	4001	HEM	CBC-CAC	2.10	1.43	1.29
22	Е	4013	6PH	C1-C2	2.10	1.57	1.50
14	А	4021	UMQ	O1'-C1'	2.08	1.43	1.40
15	W	4026	HEM	CHB-C1B	2.04	1.40	1.35
16	С	4005	SMA	C7-C8	2.04	1.43	1.40
18	С	4031	CN6	O41-C3'	-2.04	1.40	1.45
15	С	4001	HEM	CAA-C2A	-2.00	1.49	1.52
15	W	4026	HEM	CAB-C3B	2.00	1.52	1.47
15	С	4002	HEM	O2D-CGD	-2.00	1.24	1.30

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All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
14	L	4121	UMQ	CA-O1'-C1'	-8.75	99.33	113.84
14	А	4021	UMQ	CA-O1'-C1'	-8.10	100.40	113.84
18	N	4131	CN6	C2'-O51-C51	-5.50	104.25	117.79
22	L	4113	6PH	P-011-C1	4.66	131.14	118.30
22	Е	4013	6PH	P-011-C1	4.61	130.99	118.30
22	L	4113	6PH	C3-C2-C1	-4.38	101.42	111.79
22	Е	4013	6PH	C3-C2-C1	-4.21	101.83	111.79
18	С	4031	CN6	C2'-O51-C51	-4.20	107.45	117.79
20	0	4114	7PH	P-011-C1	4.06	129.47	118.30
18	N	4131	CN6	C2-O21-C21	-3.96	108.04	117.79
15	Ν	4021	HEM	CAD-C3D-C4D	3.90	131.47	124.66
18	С	4031	CN6	C2-O21-C21	-3.89	108.20	117.79
14	А	4021	UMQ	O1'-CA-CB	3.76	122.74	109.56
20	D	4014	7PH	P-011-C1	3.76	128.64	118.30
20	0	4114	7PH	O12-P-O11	3.75	116.70	106.73
18	Ν	4131	CN6	C3'-C2'-C1'	-3.74	102.93	111.79
22	Е	4013	6PH	O11-P-O12	3.66	116.73	106.47
20	D	4014	7PH	C38-C37-C36	-3.63	96.01	114.42
18	С	4031	CN6	C3-C2-C1	-3.62	103.22	111.79
22	L	4113	6PH	O11-P-O12	3.61	116.61	106.47
19	С	4111	9PE	C2-O21-C21	-3.59	108.95	117.79
15	D	4003	HEM	CBB-CAB-C3B	-3.58	109.79	127.62
15	0	4023	HEM	CBB-CAB-C3B	-3.53	110.04	127.62
15	Ν	4021	HEM	CBA-CAA-C2A	-3.52	106.61	112.62
20	D	4014	7PH	O12-P-O11	3.51	116.08	106.73
18	N	4131	CN6	C3-C2-C1	-3.51	103.48	111.79



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	Ideal(°)
14	L	4121	IIMO	O1'-CA-CB	3 50	121.84	109.56
20	0	4114	7PH	C38-C37-C36	-3.45	96.92	103.00 114.42
17	N	4110	8PE	$C_{2}-O_{2}1-C_{2}1$	-3 41	109.39	117.79
17	N	4110	8PE	C3-C2-C1	3 40	119.83	111.79
15	N	4021	HEM	CAD-C3D-C2D	-3.34	121.65	127.88
18	N	4131	CN6	P-013-CC	3 24	140.67	121.68
$\frac{10}{22}$	L	4113	6PH	013-P-011	3.11	115.00	106 73
15	W	4026	HEM	CBB-CAB-C3B	-3 10	112.19	100.10 127.62
15	D	4003	HEM	CAD-C3D-C4D	3 10	130.07	121.02
17	C	4010	8PE	C2-O21-C21	-3.08	110.20	117.79
19	N	4011	9PE	C2-O21-C21	-3.05	110.29	117.79
18	C	4031	CN6	P-013-CC	3.03	139.46	121.68
15	D	4003	HEM	CMD-C2D-C1D	2.96	129.55	125.04
18	C	4031	CN6	P-011-C1	-2.96	104.34	121.68
15	N	4022	HEM	C4C-CHD-C1D	2.94	126.44	122.56
20	D	4014	7PH	C3-C2-C1	-2.91	104.90	111.79
22	Е	4013	6PH	013-P-011	2.90	114.44	106.73
15	С	4001	HEM	CAB-C3B-C2B	-2.89	119.07	128.60
15	С	4002	HEM	C4C-CHD-C1D	2.85	126.31	122.56
18	N	4131	CN6	P-011-C1	-2.76	105.48	121.68
18	N	4131	CN6	O3'-P'-O4'	2.76	119.86	109.07
15	D	4003	HEM	C4C-CHD-C1D	2.75	126.19	122.56
20	0	4114	7PH	O13-P-O11	2.75	114.06	106.73
22	L	4113	6PH	O14-P-O11	-2.74	99.44	106.73
20	0	4114	7PH	O31-C3-C2	-2.71	100.55	108.43
15	0	4023	HEM	CAD-C3D-C4D	2.69	129.36	124.66
18	С	4031	CN6	O3'-P'-O4'	2.69	119.57	109.07
15	D	4003	HEM	C4B-CHC-C1C	2.62	126.01	122.56
22	Е	4013	6PH	O14-P-O11	-2.61	99.78	106.73
15	Ν	4021	HEM	C4B-CHC-C1C	2.60	125.99	122.56
15	D	4003	HEM	CAD-C3D-C2D	-2.58	123.06	127.88
16	С	4005	SMA	C4A-C4-C3	-2.56	115.02	118.79
18	С	4031	CN6	C3'-C2'-C1'	-2.56	105.74	111.79
20	D	4014	7PH	O13-P-O11	2.49	113.37	106.73
20	0	4114	7PH	C3-C2-C1	-2.49	105.89	111.79
20	0	4114	7PH	O11-P-O14	-2.45	99.59	106.47
17	N	4110	8PE	O31-C3-C2	-2.45	101.31	108.43
15	0	4023	HEM	C4C-CHD-C1D	2.41	125.74	122.56
14	A	4021	UMQ	C3'-C4'-C5'	-2.41	105.41	110.93
14	А	4021	UMQ	CD-CC-CB	-2.40	102.25	114.42
20	0	4114	7PH	O31-C31-C32	-2.40	104.39	111.91
14	L	4121	UMQ	C3'-C4'-C5'	-2.38	105.46	110.93



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
16	С	4005	SMA	O8-C8-C7	2.37	124.38	119.24
15	Ν	4022	HEM	CMB-C2B-C1B	-2.36	121.44	125.04
18	Ν	4131	CN6	OA-CB-CA	2.36	117.82	109.56
14	L	4121	UMQ	CD-CC-CB	-2.33	102.58	114.42
16	Ν	4025	SMA	C4A-C4-C3	-2.32	115.37	118.79
15	W	4026	HEM	C4C-CHD-C1D	2.29	125.58	122.56
18	Ν	4131	CN6	P'-O3'-CA	2.28	135.04	121.68
15	0	4023	HEM	C4B-CHC-C1C	2.26	125.54	122.56
20	D	4014	7PH	O11-P-O14	-2.24	100.18	106.47
15	С	4001	HEM	C4C-CHD-C1D	2.23	125.50	122.56
20	D	4014	7PH	O31-C31-C32	-2.22	104.92	111.91
20	D	4014	7PH	O31-C31-O32	2.20	129.15	123.59
18	С	4031	CN6	P'-O3'-CA	2.20	134.56	121.68
15	W	4026	HEM	C4B-CHC-C1C	2.19	125.44	122.56
20	0	4114	7PH	O31-C31-O32	2.18	129.10	123.59
15	0	4023	HEM	CAD-C3D-C2D	-2.16	123.86	127.88
15	Ν	4022	HEM	CMA-C3A-C4A	-2.12	125.20	128.46
20	D	4014	7PH	O12-P-O14	-2.12	102.38	110.68
20	D	4014	7PH	O31-C3-C2	-2.09	102.34	108.43
15	W	4026	HEM	CBD-CAD-C3D	-2.08	106.86	112.63
15	С	4002	HEM	CMC-C2C-C3C	2.06	128.54	124.68
14	L	4121	UMQ	O1'-C1'-C2'	2.06	111.52	108.30
15	Ν	4021	HEM	C4C-CHD-C1D	2.05	125.27	122.56
16	С	4005	SMA	C9-C10-C11	-2.05	110.77	114.52
20	0	4114	7PH	O12-P-O14	-2.05	102.67	110.68
15	W	4026	HEM	CBA-CAA-C2A	-2.03	109.16	112.62
14	А	4021	UMQ	O1-C1-O5	-2.01	105.05	110.67
15	С	4001	HEM	C4B-CHC-C1C	2.00	125.20	122.56

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There are no chirality outliers.

All (249) torsion	outliers	are	listed	below:
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Mol	Chain	Res	Type	Atoms
18	С	4031	CN6	CC-O13-P-O12
18	С	4031	CN6	CC-O13-P-O14
18	С	4031	CN6	O11-C1-C2-O21
18	С	4031	CN6	O32-C31-O31-C3
18	С	4031	CN6	C22-C21-O21-C2
18	С	4031	CN6	CA-O3'-P'-O2'
18	С	4031	CN6	CA-O3'-P'-O4'
18	C	4031	CN6	O1'-C1'-C2'-O51
18	С	4031	CN6	O52-C51-O51-C2'



Mol	Chain	Res	Type	Atoms
18	С	4031	CN6	C52-C51-O51-C2'
18	С	4031	CN6	O3'-CA-CB-CC
18	N	4131	CN6	CC-O13-P-O12
18	N	4131	CN6	CC-013-P-014
18	N	4131	CN6	O11-C1-C2-O21
18	N	4131	CN6	C22-C21-O21-C2
18	N	4131	CN6	CA-O3'-P'-O1'
18	N	4131	CN6	CA-O3'-P'-O2'
18	N	4131	CN6	CA-O3'-P'-O4'
18	N	4131	CN6	O1'-C1'-C2'-O51
18	N	4131	CN6	C52-C51-O51-C2'
19	С	4111	9PE	C1-O11-P-O12
19	С	4111	9PE	C1-O11-P-O13
19	С	4111	9PE	C1-O11-P-O14
19	С	4111	9PE	C11-O13-P-O11
19	С	4111	9PE	C11-O13-P-O12
19	N	4011	9PE	C1-O11-P-O12
19	Ν	4011	9PE	C1-O11-P-O13
19	N	4011	9PE	C1-O11-P-O14
19	N	4011	9PE	C11-O13-P-O12
19	N	4011	9PE	O13-C11-C12-N
18	N	4131	CN6	O32-C31-O31-C3
18	С	4031	CN6	O22-C21-O21-C2
18	N	4131	CN6	O22-C21-O21-C2
18	N	4131	CN6	O52-C51-O51-C2'
18	С	4031	CN6	C32-C31-O31-C3
18	N	4131	CN6	C32-C31-O31-C3
18	С	4031	CN6	O3'-CA-CB-OA
14	А	4021	UMQ	O1'-CA-CB-CC
14	L	4121	UMQ	O1'-CA-CB-CC
20	0	4114	7PH	C21-C22-C23-C24
22	L	4113	6PH	C2B-C2C-C2D-C2E
17	Ν	4110	8PE	C21-C22-C23-C24
19	N	4011	9PE	C31-C32-C33-C34
20	D	4014	7PH	C31-C32-C33-C34
20	0	4114	7PH	C31-C32-C33-C34
18	С	4031	CN6	C41-C42-C43-C44
18	Ν	4131	CN6	O3'-CA-CB-OA
19	Ν	4011	9PE	C2E-C2F-C2G-C2H
17	С	4010	8PE	C37-C38-C39-C3A
18	С	4031	CN6	CC-013-P-011
18	С	4031	CN6	CA-O3'-P'-O1'

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Mol	Chain	Res	Type	Atoms
18	N	4131	CN6	CC-013-P-011
19	N	4011	9PE	C11-O13-P-O11
17	N	4110	8PE	C37-C38-C39-C3A
18	N	4131	CN6	O3'-CA-CB-CC
22	L	4113	6PH	C37-C38-C39-C3A
20	D	4014	7PH	C27-C28-C29-C2A
17	С	4010	8PE	C38-C39-C3A-C3B
19	N	4011	9PE	C32-C33-C34-C35
19	N	4011	9PE	C28-C29-C2A-C2B
19	С	4111	9PE	C2E-C2F-C2G-C2H
20	0	4114	7PH	C2A-C2B-C2C-C2D
22	L	4113	6PH	C29-C2A-C2B-C2C
16	N	4025	SMA	C9-C10-C11-C22
19	С	4111	9PE	C26-C27-C28-C29
20	D	4014	7PH	C32-C33-C34-C35
22	Е	4013	6PH	C29-C2A-C2B-C2C
17	С	4010	8PE	C24-C25-C26-C27
22	Е	4013	6PH	C27-C28-C29-C2A
14	L	4121	UMQ	CF-CG-CH-CI
17	С	4010	8PE	C34-C35-C36-C37
22	L	4113	6PH	C38-C39-C3A-C3B
17	С	4010	8PE	C33-C34-C35-C36
18	N	4131	CN6	C46-C47-C48-C49
22	L	4113	6PH	O22-C21-O21-C2
22	L	4113	6PH	C22-C21-O21-C2
17	N	4110	8PE	C3E-C3F-C3G-C3H
17	N	4110	8PE	C28-C29-C2A-C2B
22	L	4113	6PH	C36-C37-C38-C39
17	N	4110	8PE	O11-C1-C2-C3
14	А	4021	UMQ	CF-CG-CH-CI
17	N	4110	8PE	C3B-C3C-C3D-C3E
18	С	4031	CN6	C43-C44-C45-C46
19	С	4111	9PE	C2D-C2E-C2F-C2G
22	Е	4013	6PH	C36-C37-C38-C39
19	С	4111	9PE	O13-C11-C12-N
17	N	4110	8PE	C33-C34-C35-C36
17	С	4010	8PE	C39-C3A-C3B-C3C
17	N	4110	8PE	C29-C2A-C2B-C2C
20	0	4114	7PH	C32-C33-C34-C35
22	Е	4013	6PH	C35-C36-C37-C38
17	С	4010	8PE	C26-C27-C28-C29
17	N	4110	8PE	C2A-C2B-C2C-C2D

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Mol	Chain	Res	Type	Atoms
20	D	4014	7PH	C34-C35-C36-C37
19	N	4011	9PE	C23-C24-C25-C26
20	0	4114	7PH	C22-C23-C24-C25
22	L	4113	6PH	C34-C35-C36-C37
17	N	4110	8PE	C39-C3A-C3B-C3C
17	N	4110	8PE	C3C-C3D-C3E-C3F
19	N	4011	9PE	C2B-C2C-C2D-C2E
18	С	4031	CN6	C42-C43-C44-C45
17	С	4010	8PE	C2A-C2B-C2C-C2D
20	D	4014	7PH	C37-C38-C39-C3A
22	Е	4013	6PH	C22-C21-O21-C2
17	С	4010	8PE	C3A-C3B-C3C-C3D
20	D	4014	7PH	C22-C23-C24-C25
22	L	4113	6PH	C35-C36-C37-C38
20	D	4014	7PH	O22-C21-O21-C2
17	С	4010	8PE	C36-C37-C38-C39
22	L	4113	6PH	C27-C28-C29-C2A
19	N	4011	9PE	C22-C23-C24-C25
19	N	4011	9PE	C2C-C2D-C2E-C2F
20	D	4014	7PH	C22-C21-O21-C2
15	D	4003	HEM	C4D-C3D-CAD-CBD
15	0	4023	HEM	C4D-C3D-CAD-CBD
22	Е	4013	6PH	O22-C21-O21-C2
17	Ν	4110	8PE	C36-C37-C38-C39
19	Ν	4011	9PE	C26-C27-C28-C29
17	С	4010	8PE	O11-C1-C2-C3
18	С	4031	CN6	O11-C1-C2-C3
18	С	4031	CN6	O1'-C1'-C2'-C3'
18	N	4131	CN6	O11-C1-C2-C3
18	N	4131	CN6	O1'-C1'-C2'-C3'
19	N	4011	9PE	O11-C1-C2-C3
22	E	4013	6PH	O11-C1-C2-C3
20	0	4114	7PH	C27-C28-C29-C2A
18	C	4031	CN6	C48-C49-C4A-C4B
20	0	4114	7PH	C37-C38-C39-C3A
22	E	4013	6PH	C28-C29-C2A-C2B
20	D	4014	7PH	C26-C27-C28-C29
22	L	4113	6PH	C25-C26-C27-C28
20	0	4114	7PH	C23-C24-C25-C26
18	С	4031	CN6	C47-C48-C49-C4A
18	N	4131	CN6	C42-C41-O41-C3'
22	L	4113	6PH	C3A-C3B-C3C-C3D



Mol	Chain	Res	Type	Atoms
22	Е	4013	6PH	C24-C25-C26-C27
18	N	4131	CN6	C41-C42-C43-C44
17	N	4110	8PE	C2B-C2C-C2D-C2E
19	С	4111	9PE	O11-C1-C2-C3
22	L	4113	6PH	O11-C1-C2-C3
17	С	4010	8PE	O13-C11-C12-N
19	С	4111	9PE	C24-C25-C26-C27
20	D	4014	7PH	C28-C29-C2A-C2B
17	С	4010	8PE	C29-C2A-C2B-C2C
14	L	4121	UMQ	CI-CJ-CK-CL
18	N	4131	CN6	O42-C41-O41-C3'
16	С	4005	SMA	C9-C10-C11-C22
17	С	4010	8PE	O11-C1-C2-O21
17	N	4110	8PE	O11-C1-C2-O21
19	С	4111	9PE	O11-C1-C2-O21
14	А	4021	UMQ	CI-CJ-CK-CL
22	L	4113	6PH	C39-C3A-C3B-C3C
17	С	4010	8PE	C3E-C3F-C3G-C3H
15	D	4003	HEM	C2D-C3D-CAD-CBD
19	С	4111	9PE	C23-C24-C25-C26
19	С	4111	9PE	C21-C22-C23-C24
19	N	4011	9PE	C2D-C2E-C2F-C2G
20	D	4014	7PH	C2B-C2C-C2D-C2E
22	L	4113	6PH	C28-C29-C2A-C2B
19	С	4111	9PE	C2A-C2B-C2C-C2D
19	N	4011	9PE	C2A-C2B-C2C-C2D
17	N	4110	8PE	C3A-C3B-C3C-C3D
20	D	4014	7PH	C23-C24-C25-C26
15	D	4003	HEM	C2B-C3B-CAB-CBB
15	0	4023	HEM	C2B-C3B-CAB-CBB
15	W	4026	HEM	C2B-C3B-CAB-CBB
18	С	4031	CN6	CB-CC-O13-P
19	N	4011	9PE	O11-C1-C2-O21
15	W	4026	HEM	C4B-C3B-CAB-CBB
22	L	4113	6PH	C33-C34-C35-C36
17	С	4010	8PE	C23-C24-C25-C26
18	N	4131	CN6	C1-O11-P-O14
19	N	4011	9PE	C12-C11-O13-P
22	Е	4013	6PH	O11-C1-C2-O21
22	L	4113	6PH	O11-C1-C2-O21
18	N	4131	CN6	O31-C31-C32-C33
16	С	4005	SMA	C15-C14-O14-C25

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\mathbf{Mol}	Chain	Res	Type	Atoms	
17	С	4010	8PE	C28-C29-C2A-C2B	
15	0	4023	HEM	C2D-C3D-CAD-CBD	
17	С	4010	8PE	C32-C33-C34-C35	
17	N	4110	8PE	C3D-C3E-C3F-C3G	
19	N	4011	9PE	C29-C2A-C2B-C2C	
19	С	4111	9PE	C2B-C2C-C2D-C2E	
22	Е	4013	6PH	C37-C38-C39-C3A	
17	Ν	4110	8PE	C31-C32-C33-C34	
18	С	4031	CN6	O32-C31-C32-C33	
22	L	4113	6PH	C24-C25-C26-C27	
17	С	4010	8PE	C11-O13-P-O11	
17	Ν	4110	8PE	C11-O13-P-O11	
18	С	4031	CN6	C1'-O1'-P'-O3'	
18	N	4131	CN6	C1'-O1'-P'-O3'	
17	N	4110	8PE	C24-C25-C26-C27	
18	С	4031	CN6	O31-C31-C32-C33	
22	Е	4013	6PH	C2B-C2C-C2D-C2E	
19	С	4111	9PE	C2C-C2D-C2E-C2F	
15	D	4003	HEM	C4B-C3B-CAB-CBB	
15	0	4023	HEM	C4B-C3B-CAB-CBB	
15	С	4001	HEM	CAA-CBA-CGA-O2A	
18	Ν	4131	CN6	O32-C31-C32-C33	
15	N	4022	HEM	CAA-CBA-CGA-O1A	
19	С	4111	9PE	O31-C31-C32-C33	
15	Ν	4022	HEM	CAA-CBA-CGA-O2A	
22	L	4113	6PH	C32-C33-C34-C35	
15	С	4001	HEM	CAD-CBD-CGD-O1D	
20	0	4114	7PH	C2B-C2C-C2D-C2E	
15	С	4002	HEM	CAA-CBA-CGA-O1A	
18	N	4131	CN6	CB-CC-O13-P	
18	N	4131	CN6	C51-C52-C53-C54	
17	С	4010	8PE	C31-C32-C33-C34	
15	С	4001	HEM	CAA-CBA-CGA-O1A	
15	С	4002	HEM	CAA-CBA-CGA-O2A	
15	N	4021	HEM	CAD-CBD-CGD-O2D	
15	С	4001	HEM	CAD-CBD-CGD-O2D	
14	А	4021	UMQ	CG-CH-CI-CJ	
15	N	4022	HEM	CAD-CBD-CGD-O2D	
15	0	4023	HEM	CAD-CBD-CGD-O2D	
22	Е	4013	6PH	C2C-C2D-C2E-C2F	
15	N	4021	HEM	CAD-CBD-CGD-O1D	
15	0	4023	HEM	CAA-CBA-CGA-O2A	

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Mol	Chain	Res	Type	Atoms
20	D	4014	7PH	C25-C26-C27-C28
22	Е	4013	6PH	O31-C31-C32-C33
15	0	4023	HEM	CAA-CBA-CGA-O1A
15	D	4003	HEM	CAD-CBD-CGD-O2D
18	Ν	4131	CN6	C1-O11-P-O13
22	Е	4013	6PH	C33-C34-C35-C36
17	С	4010	8PE	C21-C22-C23-C24
20	0	4114	7PH	C25-C26-C27-C28
15	D	4003	HEM	CAD-CBD-CGD-O1D
15	Ν	4021	HEM	CAA-CBA-CGA-O2A
15	N	4022	HEM	CAD-CBD-CGD-O1D
15	0	4023	HEM	CAD-CBD-CGD-O1D
17	С	4010	8PE	O21-C21-C22-C23
15	D	4003	HEM	CAA-CBA-CGA-O2A
15	N	4021	HEM	CAA-CBA-CGA-O1A
15	D	4003	HEM	CAA-CBA-CGA-O1A
15	С	4002	HEM	CAD-CBD-CGD-O2D
19	С	4111	9PE	C25-C26-C27-C28
20	0	4114	7PH	C28-C29-C2A-C2B
17	С	4010	8PE	C2B-C2C-C2D-C2E
15	С	4002	HEM	CAD-CBD-CGD-O1D
17	С	4010	8PE	O22-C21-C22-C23
22	Е	4013	6PH	O32-C31-C32-C33
22	Е	4013	6PH	C25-C26-C27-C28
20	0	4114	7PH	C35-C36-C37-C38
15	W	4026	HEM	CAA-CBA-CGA-O2A
20	D	4014	7PH	C2A-C2B-C2C-C2D
22	L	4113	6PH	C22-C23-C24-C25
15	W	4026	HEM	CAA-CBA-CGA-O1A
14	L	4121	UMQ	CD-CF-CG-CH

There are no ring outliers.

17 monomers are involved in 37 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	С	4001	HEM	2	0
18	С	4031	CN6	7	0
16	С	4005	SMA	1	0
14	А	4021	UMQ	4	0
17	Ν	4110	8PE	2	0
17	С	4010	8PE	2	0
15	С	4002	HEM	1	0



Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	W	4026	HEM	2	0
18	N	4131	CN6	5	0
20	D	4014	7PH	3	0
16	Ν	4025	SMA	1	0
20	0	4114	7PH	2	0
15	Ν	4022	HEM	1	0
21	Р	4024	FES	1	0
22	Е	4013	6PH	1	0
14	Ĺ	4121	UMQ	2	0
15	Ō	4023	HEM	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and sufficient 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	431/431~(100%)	0.34	33 (7%) 13 13	32, 57, 121, 146	0
1	L	431/431~(100%)	0.28	35 (8%) 12 12	29, 53, 114, 140	0
2	В	352/352~(100%)	0.48	28 (7%) 12 12	40, 61, 101, 148	0
2	М	352/352~(100%)	0.43	27 (7%) 13 13	40, 59, 93, 137	0
3	С	385/385~(100%)	-0.34	5 (1%) 77 79	26, 35, 49, 113	0
3	Ν	385/385~(100%)	-0.30	6 (1%) 72 74	25, 33, 46, 104	0
4	D	246/248~(99%)	-0.05	11 (4%) 33 36	32, 48, 70, 79	0
4	Ο	246/248~(99%)	-0.19	1 (0%) 92 93	25, 42, 64, 80	0
5	Е	185/185~(100%)	0.46	19 (10%) 6 6	32, 54, 90, 117	0
5	Р	185/185~(100%)	0.37	18 (9%) 7 7	34, 52, 92, 114	0
6	F	74/146~(50%)	0.78	12 (16%) 1 1	44, 62, 112, 114	0
6	Q	74/146~(50%)	0.41	12 (16%) 1 1	39, 57, 108, 110	0
7	G	125/126~(99%)	-0.04	4 (3%) 47 51	32, 45, 72, 92	0
7	R	125/126~(99%)	-0.05	4 (3%) 47 51	28, 42, 69, 88	0
8	Н	93/93~(100%)	1.08	20 (21%) 0 0	29, 57, 147, 154	0
8	S	93/93~(100%)	1.33	23 (24%) 0 0	26, 55, 154, 160	0
9	Ι	55/65~(84%)	0.58	8 (14%) 2 2	41, 56, 111, 124	0
9	Т	55/65~(84%)	0.51	8 (14%) 2 2	37, 49, 112, 124	0
10	J	127/127~(100%)	0.95	20 (15%) 2 1	50, 74, 93, 99	0
10	U	127/127~(100%)	0.90	20 (15%) 2 1	52, 74, 89, 97	0
11	K	107/107~(100%)	1.87	43 (40%) 0 0	70, 105, 135, 141	0
11	V	$1\overline{07/107}\ (100\%)$	1.88	37 (34%) 0 0	72, 104, 133, 136	0
12	W	$\overline{111/112} \ (99\%)$	1.13	21 (18%) 1 1	50, 70, 108, 136	0
All	All	4471/4642 (96%)	0.35	415 (9%) 8 8	25, 53, 111, 160	0



Mol	Chain	Res	Type	RSRZ
8	S	43	ASN	15.1
12	W	4	SER	12.4
8	S	42	HIS	11.4
9	Т	58	ALA	10.9
8	S	46	PHE	10.8
8	Н	43	ASN	10.4
8	S	40	ILE	10.1
1	А	27	ALA	9.7
1	L	27	ALA	9.4
12	W	5	THR	8.8
2	В	331	SER	8.7
8	Н	42	HIS	8.6
8	S	45	VAL	8.6
3	N	384	ASN	8.4
12	W	3	GLU	8.3
1	А	231	GLN	8.0
12	W	1	ALA	7.7
1	А	228	LEU	7.7
8	Н	41	PHE	7.6
5	Е	47	ASN	7.5
11	V	80	PRO	7.5
9	Ι	58	ALA	7.2
5	Е	46	ASN	7.0
5	Р	47	ASN	6.9
8	Н	46	PHE	6.9
2	В	333	SER	6.7
8	S	41	PHE	6.5
8	S	50	ARG	6.5
2	В	336	ILE	6.4
9	Т	57	ALA	6.4
12	W	2	LYS	6.4
3	С	385	LYS	6.4
2	В	332	VAL	6.3
2	В	338	LEU	6.2
2	М	338	LEU	6.2
8	Н	94	VAL	6.2
11	V	106	ILE	6.1
1	L	128	LYS	6.1
1	L	127	GLN	6.1
8	S	52	PHE	6.1
1	А	230	LEU	6.0
1	А	229	SER	5.9

All (415) RSRZ outliers are listed below:



Mol	Chain	Res	Type	RSRZ
9	Ι	57	ALA	5.9
1	А	29	VAL	5.9
2	М	311	GLY	5.8
2	В	330	GLU	5.8
8	Н	44	ALA	5.8
5	Е	100	ALA	5.7
2	М	330	GLU	5.7
6	F	112	PRO	5.6
3	N	385	LYS	5.6
1	L	129	ALA	5.5
1	L	228	LEU	5.5
3	С	384	ASN	5.5
6	Q	118	GLU	5.5
8	S	44	ALA	5.5
11	V	30	ASN	5.4
8	Н	49	PHE	5.4
6	Q	119	HIS	5.4
1	L	28 GLU		5.3
8	Н	47 ASN		5.3
1	А	28	GLU	5.3
10	J	65	LYS	5.2
1	L	230	LEU	5.1
8	Н	38	GLN	5.0
8	Н	39	GLY	5.0
6	F	113	GLY	5.0
8	Н	50	ARG	5.0
5	Р	46	ASN	4.9
1	А	234	THR	4.9
11	K	86	TYR	4.9
2	М	336	ILE	4.9
10	U	42	PRO	4.9
5	Е	153	LEU	4.8
7	R	127	LYS	4.8
8	S	49	PHE	4.8
8	S	2	GLY	4.7
8	S	94	VAL	4.7
11	Κ	15	LEU	4.7
1	L	234	THR	4.7
1	L	231	GLN	4.7
8	Н	5	SER	4.7
1	А	126	GLN	4.7
12	W	112	LYS	4.6



Mol	Chain	Res	Type	RSRZ
8	S	47	ASN	4.6
1	L	126	GLN	4.5
1	L	29	VAL	4.5
5	Р	209	GLY	4.5
11	Κ	75	ILE	4.5
5	Р	153	LEU	4.4
6	F	119	HIS	4.4
2	М	331	SER	4.4
11	V	18	ARG	4.4
11	V	29	ILE	4.4
11	V	79	GLU	4.4
11	Κ	8	PRO	4.4
1	А	457	TRP	4.3
1	А	233	GLY	4.3
9	Ι	56	ILE	4.3
8	S	48	SER	4.3
10	J	62	PRO	4.3
1	А	127	GLN	4.3
5	Е	210	ASP	4.3
11	Κ	107	LYS	4.3
4	D	239	GLY	4.2
11	Κ	16	GLY	4.2
8	S	68	TYR	4.2
11	V	24	ARG	4.2
3	Ν	383	VAL	4.2
1	А	238	LEU	4.2
1	L	42	HIS	4.2
1	L	217	GLU	4.2
1	L	229	SER	4.2
8	S	39	GLY	4.1
10	U	1	GLU	4.1
10	J	55	VAL	4.1
2	М	333	SER	4.1
6	F	116	ASP	4.1
8	Н	40	ILE	4.1
2	В	240	ALA	4.1
11	Κ	65	SER	4.0
2	В	343	VAL	4.0
11	V	88	CYS	4.0
1	L	31	GLN	4.0
1	L	213	ASN	4.0
5	Р	91	MET	3.9



Mol	Chain	Res	Type	RSRZ
10	J	15	SER	3.9
10	U	66	ASP	3.9
11	Κ	30	ASN	3.9
6	Q	113	GLY	3.9
5	Р	210	ASP	3.9
1	А	124	PHE	3.8
2	М	314	LEU	3.8
5	Р	124	HIS	3.8
11	Κ	79	GLU	3.8
11	Κ	76	SER	3.8
10	U	55	VAL	3.8
10	J	42	PRO	3.8
11	V	17	ASP	3.8
2	М	332	VAL	3.8
2	М	213	LYS	3.7
1	L	271	ASN	3.7
11	Κ	24	ARG	3.7
1	L	237	VAL	3.7
10	J	31	SER	3.7
11	V	10	SER	3.7
10	U	75	SER	3.7
7	G	127	LYS	3.7
8	Н	45	VAL	3.7
2	В	239	ALA	3.7
11	Κ	103	LYS	3.6
11	Κ	83	ILE	3.6
1	L	124	PHE	3.6
11	V	14	SER	3.6
11	V	65	SER	3.6
2	М	337	GLU	3.6
11	V	100	ALA	3.6
2	В	337	GLU	3.6
6	F	110	GLN	3.6
4	D	210	PRO	3.5
11	Κ	40	PRO	3.5
11	V	9	VAL	3.5
11	Κ	60	SER	3.5
11	V	40	PRO	3.5
11	V	86	TYR	3.5
1	А	398	GLY	3.5
2	М	344	LYS	3.5
9	Т	56	ILE	3.4



Mol	Chain	Res	Type	RSRZ
11	V	107	LYS	3.4
5	Р	99	ALA	3.4
10	U	43	GLY	3.4
6	Q	114	TYR	3.4
6	Q	117	LEU	3.4
1	А	225	SER	3.4
10	J	127	PRO	3.4
5	Ε	154	ILE	3.4
11	V	42	GLY	3.4
12	W	32	GLY	3.4
10	U	65	LYS	3.4
9	Т	55	ARG	3.4
11	Κ	10	SER	3.3
11	V	41	ASP	3.3
11	V	28	ASP	3.3
6	F	118	GLU	3.3
2	В	314	LEU	3.3
11	V	15	LEU	3.3
10	J	125	ARG	3.3
1	А	31	GLN	3.3
12	W	67	LYS	3.3
6	F	114	TYR	3.3
8	Н	68	TYR	3.3
4	D	67	HIS	3.2
11	V	60	SER	3.2
7	G	17	LYS	3.2
5	Р	48	ASP	3.2
10	J	44	ASN	3.2
8	S	38	GLN	3.2
1	L	457	TRP	3.2
1	А	81	GLU	3.2
11	K	29	ILE	3.2
2	М	211	ALA	3.1
5	Е	99	ALA	3.1
3	С	156	PHE	3.1
8	H	48	SER	3.1
11	K	35	TRP	3.1
11	K	89	GLN	3.1
12	W	53	LYS	3.1
4	D	307	PRO	3.1
12	W	34	PRO	3.1
3	С	383	VAL	3.1



Mol	Chain	Res	Type	RSRZ
10	J	1	GLU	3.1
11	V	3	GLU	3.1
9	Ι	5	SER	3.1
2	М	343	VAL	3.0
11	K	14	SER	3.0
11	K	106	ILE	3.0
6	F	115	ALA	3.0
7	G	20	VAL	3.0
5	Е	103	LEU	3.0
2	В	329	ASN	3.0
11	K	41	ASP	3.0
11	V	4	LEU	2.9
5	Р	45	GLU	2.9
2	М	334	SER	2.9
5	Е	91	MET	2.9
1	L	111	GLY	2.9
10	U	87	THR	2.9
11	V	77	ASN	2.9
10	U	127	PRO	2.9
9	Т	54	ALA	2.9
2	М	329	ASN	2.9
5	Р	100	ALA	2.9
6	Q	115	ALA	2.9
2	В	339	ASN	2.8
5	Е	97	ASN	2.8
11	K	61	ARG	2.8
10	U	114	GLN	2.8
10	U	15	SER	2.8
11	K	100	ALA	2.8
11	V	70	ASP	2.8
11	V	83	ILE	2.8
2	М	202	ASP	2.8
9	Ι	54	ALA	2.8
11	K	4	LEU	2.8
1	L	35	GLY	2.8
9	Т	5	SER	2.8
1	L	236	PRO	2.8
11	K	18	ARG	2.8
11	V	74	THR	2.8
1	А	401	LEU	2.8
5	Е	209	GLY	2.8
2	М	238	VAL	2.7



Mol	Mol Chain Res		Type	RSRZ
3	N	346	VAL	2.7
6	F	117	LEU	2.7
10	J	68	LEU	2.7
6	F	120	LYS	2.7
10	J	76	LYS	2.7
1	А	217	GLU	2.7
2	В	218	LYS	2.7
2	М	218	LYS	2.7
2	М	341	ASP	2.7
6	F	111	GLN	2.7
8	S	56	PHE	2.7
6	Q	112	PRO	2.7
5	Р	103	LEU	2.7
8	S	37	LEU	2.7
9	Т	10	PHE	2.7
1	А	76	ILE	2.6
10	U	44	ASN	2.6
1	L	240	LYS	2.6
4	D	70	HIS	2.6
5	Р	154	ILE	2.6
1	L	122	GLN	2.6
12	W	17	THR	2.6
10	U	76	LYS	2.6
7	G	90	ARG	2.6
11	V	89	GLN	2.6
12	W	54	GLY	2.6
11	К	87	PHE	2.6
12	W	12	ALA	2.5
3	N	307	PHE	2.5
2	В	215	LEU	2.5
1	А	210	GLY	2.5
2	В	312	LYS	2.5
12	W	13	LYS	2.5
1	А	129	ALA	2.5
2	В	241	ILE	2.5
10	J	30	THR	2.5
10	U	88	THR	2.5
1	L	44	PRO	2.5
10	J	57	ASP	2.5
5	Р	105	LYS	2.5
1	А	232	THR	2.5
2	М	239	ALA	2.5



Mol	Chain	Res	Type	RSRZ
4	D	207	ALA	2.5
5	Е	124	HIS	2.5
5	Е	40	ASP	2.5
2	В	238	VAL	2.4
10	U	45	LYS	2.4
8	S	6	GLY	2.4
12	W	98	LYS	2.4
2	В	51	LEU	2.4
9	Ι	6	LEU	2.4
1	L	235	LYS	2.4
8	S	84	ALA	2.4
3	С	346	VAL	2.4
12	W	9	PRO	2.4
5	Е	208	ASP	2.4
11	К	23	CYS	2.4
9	Т	9	THR	2.4
5	Е	188	SER	2.4
11	Κ	26	SER	2.4
4	D	211	GLY	2.4
9	Ι	12	LYS	2.4
11	K	39	LYS	2.4
10	U	35	TRP	2.4
8	Н	37	LEU	2.4
1	А	213	ASN	2.3
11	Κ	70	ASP	2.3
10	U	37	TRP	2.3
1	L	135	SER	2.3
11	K	64	GLY	2.3
10	U	125	ARG	2.3
5	Е	48	ASP	2.3
11	V	81	GLU	2.3
7	R	17	LYS	2.3
5	Р	97	ASN	2.3
1	А	226	LYS	2.3
4	D	138	PRO	2.3
2	В	219	SER	2.3
1	А	44	PRO	2.3
10	U	62	PRO	2.3
1	L	88	LYS	2.3
12	W	14	LYS	2.2
1	L	227	ASN	2.2
1	А	215	LYS	2.2



Mol	Chain	Res	Type	RSRZ
12	W	82	LYS	2.2
5	Р	102	PRO	2.2
12	W	30	GLU	2.2
1	L	241	LYS	2.2
10	J	9	ALA	2.2
7	R	24	LEU	2.2
2	В	25	PRO	2.2
11	V	23	CYS	2.2
2	В	166	ARG	2.2
10	J	18	LEU	2.2
10	J	49	VAL	2.2
2	М	61	THR	2.2
5	Р	213	ILE	2.2
3	N	156	PHE	2.2
1	L	238	LEU	2.2
8	Н	7	LYS	2.2
10	U	57	ASP	2.2
2	М	195	ALA	2.2
6	Q	103 GLU		2.2
11	Κ	81	GLU	2.2
5	Е	102	PRO	2.2
8	S	5	SER	2.2
11	V	35	TRP	2.2
2	В	293	ASP	2.2
2	В	321	THR	2.2
11	K	7	THR	2.2
11	K	21	ILE	2.2
11	V	82	ASP	2.2
2	М	335	PRO	2.2
6	Q	74	VAL	2.1
8	S	51	ARG	2.1
11	Κ	85	THR	2.1
1	А	224	GLU	2.1
1	А	405	GLU	2.1
1	L	397	LYS	2.1
6	Q	110	GLN	2.1
2	М	166	ARG	2.1
12	W	73	MET	2.1
6	F	74	VAL	2.1
11	K	80	PRO	2.1
11	K	90	HIS	2.1
1	L	150	ASP	2.1



Mol Chain Res		Type	RSRZ	
5	Р	208	ASP	2.1
11	K	77	ASN	2.1
2	М	240	ALA	2.1
1	А	271	ASN	2.1
2	В	335	PRO	2.1
4	D	140	GLU	2.1
5	Е	45	GLU	2.1
7	R	10	ARG	2.1
10	J	74	THR	2.1
1	А	408	LYS	2.1
2	М	339	ASN	2.1
11	V	66	GLY	2.1
6	Q	111	GLN	2.1
8	Н	51	ARG	2.1
4	0	307	PRO	2.1
11	K	74	THR	2.1
2	В	334	SER	2.1
1	L	34	ASN	2.1
11	V	61	ARG	2.1
8	Н	84	ALA	2.0
11	K	28	ASP	2.0
11	V	84	ALA	2.0
2	В	136	GLN	2.0
2	М	241	ILE	2.0
12	W	97	GLU	2.0
10	J	3	LYS	2.0
2	В	292	GLN	2.0
10	J	43	GLY	2.0
11	K	36	TYR	2.0
11	V	43	THR	2.0
1	А	72	LEU	2.0
5	Е	213	ILE	2.0
11	K	92	ILE	2.0
9	Ι	10	PHE	2.0
6	Q	116	ASP	2.0
4	D	62	MET	2.0
4	D	209	PRO	2.0

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

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



median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q < 0.9
12	M3L	W	81	12/13	0.89	0.30	60,63,64,66	0

6.3 Carbohydrates (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
13	FRU	Х	2	12/12	0.76	0.33	77,79,81,81	0
13	GLC	Х	1	11/12	0.82	0.27	72,75,77,78	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.





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
18	CN6	С	4031	50/50	0.87	0.23	50,70,78,80	0
18	CN6	N	4131	50/50	0.89	0.21	$53,\!67,\!77,\!79$	0
22	6PH	Е	4013	40/40	0.89	0.17	56,65,72,72	0
22	6PH	L	4113	40/40	0.90	0.17	49,60,69,69	0
17	8PE	С	4010	47/47	0.91	0.17	39,59,62,65	0
17	8PE	N	4110	47/47	0.91	0.19	28,65,74,75	0
19	9PE	С	4111	40/40	0.92	0.17	45,57,75,76	0
20	7PH	D	4014	38/38	0.93	0.21	48,53,61,62	0



Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(A^2)$	Q<0.9
20	7PH	0	4114	38/38	0.93	0.20	38,44,51,54	0
14	UMQ	А	4021	34/34	0.94	0.16	42,48,65,67	0
19	9PE	N	4011	40/40	0.94	0.19	50,54,63,64	0
14	UMQ	L	4121	34/34	0.94	0.15	39,44,59,60	0
15	HEM	W	4026	43/43	0.96	0.16	47,55,57,58	0
16	SMA	С	4005	37/37	0.96	0.14	29,33,37,37	0
16	SMA	N	4025	37/37	0.97	0.13	23,28,31,32	0
15	HEM	D	4003	43/43	0.98	0.13	35,39,43,44	0
15	HEM	N	4022	43/43	0.99	0.11	21,23,32,35	0
15	HEM	0	4023	43/43	0.99	0.10	32,37,41,42	0
15	HEM	С	4002	43/43	0.99	0.11	20,26,37,37	0
21	FES	Е	4004	4/4	0.99	0.13	30,32,32,37	0
21	FES	Р	4024	4/4	0.99	0.10	32,36,36,37	0
15	HEM	С	4001	43/43	0.99	0.12	21,26,32,35	0
15	HEM	N	4021	43/43	0.99	0.11	15,23,30,34	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.

