

Full wwPDB X-ray Structure Validation Report (i)

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PDB ID	:	4D6T
Title	:	Cytochrome bc1 bound to the $4(1H)$ -pyridone GW844520
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Deposited on	:	2014-11-14
Resolution	:	3.57 Å(reported)

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

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

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

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

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.57 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.



Motria	Whole archive	Similar resolution			
Metric	$(\# {\rm Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA})$			
R _{free}	130704	1094 (3.66-3.50)			
Clashscore	141614	1181 (3.66-3.50)			
Ramachandran outliers	138981	1143 (3.66-3.50)			
Sidechain outliers	138945	1143 (3.66-3.50)			
RSRZ outliers	127900	1012 (3.66-3.50)			

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

Mol	Chain	Length	Quality of chain		
1	А	480	^{2%} 75%	16%	• 8%
1	Ν	480	% • 76%	15%	•• 8%
2	В	453	<u>6%</u> 71%	19%	• 7%
3	С	379	75%	19%	• •
3	Р	379	77%	17%	



Mol	Chain	Length	Quality of chain			
4	D	265	76%		13%	• 9%
4	Q	265	77%		12%	• 9%
5	Е	274	22% 5% 73%			
5	Ι	274	92%			
5	R	274	[%] 56% 13%	•	28%	
6	F	111	2% 66%	19	9% •	12%
6	S	111	68%		20% •	11%
7	G	82	% 		12%	5% ••
7	Т	82	^{2%} 72%		16% •	10%
8	Н	91	44% 19% 5%		29%	
8	U	91	5% 48% 18%	••	27%	
9	J	64	77%		12%	• 9%
9	W	64	^{2%}		12%	• 8%
10	0	453	2% 68%		21%	• 8%
11	V	274	% • 5% • 94%			

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	PO4	F	501	-	-	-	Х
14	PO4	N	501	-	-	-	Х
14	PO4	S	501	-	-	-	Х
15	PEE	С	505	Х	-	-	-
15	PEE	D	506	Х	-	-	-
15	PEE	Р	505	Х	-	-	-
15	PEE	Q	506	Х	-	-	-
18	FES	R	501	-	-	Х	-
19	GOL	R	502	-	-	-	Х



2 Entry composition (i)

There are 19 unique types of molecules in this entry. The entry contains 31051 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, MITOCHON-DRIAL.

Mol	Chain	Residues		At	oms		ZeroOcc	AltConf	Trace	
1	А	444	Total 3439	C 2148	N 607	0 664	S 20	0	0	0
1	Ν	444	Total 3432	C 2142	N 607	O 663	S 20	0	0	0

• Molecule 2 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 2, MITOCHON-DRIAL.

Mol	Chain	Residues		Ate	oms			ZeroOcc	AltConf	Trace
2	В	422	Total 3164	C 1988	N 561	O 608	S 7	0	0	0

• Molecule 3 is a protein called CYTOCHROME B.

Mol	Chain	Residues		At	oms		ZeroOcc	AltConf	Trace	
3	С	374	Total	С	Ν	0	\mathbf{S}	0	0	0
3 0	574	2968	1993	463	494	18	0	0		
9	D	270	Total	С	Ν	0	S	0	0	0
3	Г	570	2936	1973	456	489	18	U	0	U

• Molecule 4 is a protein called CYTOCHROME C1, HEME PROTEIN, MITOCHONDRIAL.

Mol	Chain	Residues		At	oms		ZeroOcc	AltConf	Trace	
4	Л	240	Total	С	Ν	Ο	\mathbf{S}	0	0	0
4 D	240	1912	1222	329	346	15	0	0		
4	0	241	Total	С	Ν	Ο	\mathbf{S}	0	0	0
4	Q	241	1918	1225	330	348	15	0		

• Molecule 5 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MI-TOCHONDRIAL.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	Е	73	Total C N O S 549 341 92 114 2	0	0	0
5	Ι	21	Total C N O S 157 97 31 28 1	0	0	0
5	R	196	Total C N O S 1518 957 263 290 8	0	0	0

• Molecule 6 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 7.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
6	Б	08	Total	С	Ν	0	\mathbf{S}	0	0	0
0	0 Г	90	860	547	154	157	2	0	0	0
6	C	00	Total	С	Ν	0	S	0	0	0
0	G	99	869	553	156	158	2	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	56	ASP	ASN	conflict	UNP P00129
S	56	ASP	ASN	conflict	UNP P00129

• Molecule 7 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	80	Total 677	C 439	N 127	0 110	S 1	0	0	0
7	Т	74	Total 624	C 408	N 117	0 98	S 1	0	0	0

• Molecule 8 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 6, MITOCHON-DRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
0	п	65	Total	С	Ν	0	S	0	0	0
0	11	05	529	321	96	107	5	0	0	
0	T	66	Total	С	Ν	0	S	0	0	0
0	U	00	538	327	98	108	5	0	0	0

• Molecule 9 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 9.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace	
9	J	58	Total 482	C 317	N 83	O 82	0	0	0



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace	
9	W	59	Total 487	C 320	N 84	O 83	0	0	0

• Molecule 10 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 2, MITO-CHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	0	419	Total 3140	C 1972	N 555	O 606	S 7	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	305	GLU	GLN	conflict	UNP P23004

• Molecule 11 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	V	17	Total 127	C 81	N 24	0 22	0	0	0

• Molecule 12 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).





Mol	Chain	Residues		Ate	oms			ZeroOcc	AltConf
19	С	1	Total	С	Fe	Ν	Ο	0	0
	U	1	43	34	1	4	4	0	0
19	С	1	Total	С	Fe	Ν	Ο	0	0
	U	1	43	34	1	4	4	0	0
10	D	1	Total	С	Fe	Ν	0	0	0
12	1	1	43	34	1	4	4	0	0
19	D	1	Total	С	Fe	Ν	Ο	0	0
12	1	1	43	34	1	4	4		U

• Molecule 13 is 3-chloro-2,6-dimethyl-5-{4-[4-(trifluoromethoxy)phenoxy]phenyl}pyridin-4-ol (three-letter code: 4X9) (formula: $C_{20}H_{15}ClF_3NO_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
12	С	1	Total	С	Cl	F	Ν	Ο	0	0
	T	28	20	1	3	1	3	0	0	
12	D	1	Total	С	Cl	F	Ν	Ο	0	0
10	L	L	28	20	1	3	1	3	0	U

• Molecule 14 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	С	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0
14	D	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0
14	D	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0
14	D	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0
14	Е	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0
14	F	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0
14	Ν	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0
14	Ν	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0
14	Q	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0
14	Q	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0
14	S	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0

• Molecule 15 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula: $C_{41}H_{78}NO_8P$).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	С	1	Total	С	Ν	0	Р	0	0
10	U	I	49	39	1	8	1	0	0
15	Л	1	Total	С	Ν	0	Р	0	0
10	D	I	26	16	1	8	1	0	0
15	D	1	Total	С	Ν	0	Р	0	0
10	1	I	49	39	1	8	1	0	0
15	0	1	Total	С	Ν	0	Р	0	0
10	Q	L	51	41	1	8	1	0	0

• Molecule 16 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
16 D	Л	1	Total	С	Fe	Ν	Ο	0	0
	D		43	34	1	4	4	0	
16 G	Q	1	Total	С	Fe	Ν	Ο	0	0
		Q I	43	34	1	4	4	0	U

• Molecule 17 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
17	л	1	Total	С	Ο	Р	0	0	
11	D	T	39	24	13	2	0	0	
17	G	1	Total	С	Ο	Р	0	0	
11		1	44	25	17	2	0	0	
17	0	Q 1	Total	С	Ο	Р	0	0	
11	Q		39	24	13	2		0	
17	Т	T 1	Total	С	Ο	Р	0	0	
11			49	30	17	2		0	

• Molecule 18 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	R	1	Total 4	Fe 2	${ m S} { m 2}$	0	0

• Molecule 19 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	R	1	Total 6	${ m C} { m 3}$	O 3	0	0



3 Residue-property plots (i)

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

• Molecule 1: CYTOCHROME B-C1 COMPLEX SUBUNIT 1, MITOCHONDRIAL









L143 F149 F149 M179 M178 M178 M178 M181 V182 M204 M204 M204 M211 L218 L216 L218 L216 L218 L218 L218 L218 K231 K231 K231 K231 K231 K231

• Molecule 4: CYTOCHROME C1, HEME PROTEIN, MITOCHONDRIAL



4D6T

Chain Q:	77%		12% • 9%
LEU SER ALLA ALLA LEU CLY MET MET ALA ALA ALA CLY CLY CLY ALA ALA ALA LEU ALA	HES SER ALA ALA SI SI 13 13 13 14 14 17 11 17 17 17 17 17 17 17 17 17 17 17	K34 Q35 V36 C37 C40 C40 F48 Y48 Y48 Y48 A65	V68 N105 P110 P111 R118 K118 L131 P137
P133 1139 5142 6146 6146 6155 6155 6155 6155 7173 7173 7173 7173	V182 A194 A194 M204 M211 P216 P217 R224 S232	1237 1237 1240 1240	
• Molecule 5: CYTOCHI	ROME B-C1 COMP	LEX SUBUNIT R	RIESKE, MITOCHONDRIAL
Chain E: 22%	5%	73%	
MET LEU SER VAL ALA ALA ALA ARA CUY PHE PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO	SER ARG GLY GLY ALA ALA ALA ALA LEU PRO LEU CVAL CLEU ALA ALA	VAL PRO ALA ALA ALA GLU SER PRO PRO VAL LEU LEU LEU LYS	ARG VAL VAL LEU CYS ARG ALU ALA ALA ALA ALA
GLY ARG PRO LEU VAL LEU SER SER SER ALA ASN VAL ASN VAL ACA ATA ATA	S1 V7 P16 119 E27 A31 S36 S36	T42 V45 V54 V54 C58 F58 S61 S72	K73 ILE CLU CLU CLU CLU CLU CLU CLU CLU CLU CLU
MET ALA ALA ALA ALA TRP TRP CVAC CVAC CVAC CVAC ARG ARG ARG ARG ARG ARG TTRR ARG	GLU TILE ALA GLU GLU ALA ALA CLU CLU CLU CLU CLU ASP ASP	PRO GLN HIS ASP ASP CLU ASP CLU VAL LVS LVS PRO CLU	VAL VAL LEU TLE LEU TLE VAL CYS CYS CYS CYS VAL
LLE ALA ALA ALA ALA CLY CLY CLY TYR TYR TYR TYR TYR TYR HIS SER HIS	TYR ASP ALA SER SER GLY GLY GLY GLY GLY FRO ALA ALA ASN	LEU GLU VAL PRO SER TYR CLU PHE THR SER ASP MET	VAL TLE AL GLY
• Molecule 5: CYTOCHI	ROME B-C1 COMP	LEX SUBUNIT R	RIESKE, MITOCHONDRIAL
Chain I:	92%		
MET LEU SER VAL ALA ALA ALA ALA PHE PHE PHE PHE ALA ALA ALA THR	SER ARG GLY VAL ALA ALA ALA ALA PRO PRO PRO CLU CLEU ALA ALA	VAL VAL ALA ALA ALA SER GLU GLU VAL LEU LEU LEU LEU LYS	ALA VAL SER SER SEA SEA SEA SEA SEA CLN ALA ALA
GLY ARG PRO 164 164 866 866 866 866 866 866 866 866 871 77 77 77 77 877 77 888 77 888 77 888 77 888 77 888 77 888 77 8888	THIS ASP ASP ASP ILIE ARC ARC ARC ARC ARC ARC PRO	CLU L VAL ASP ASP ASP THR THR C VS SER SER SER SER	diu Ara Ara Ara Curs Phe Ser Trr Ala Ala Thr Thr Thr
THR VAL GLY VAL GLY AAL ALA ALA ALA ALA ASN VAL VAL SER SER SER SER	MET SER SER ALA SER ALA ASP VAL LEU MET MET SER LYS ILE GLU	LYS LEU SER SER ASP TLE PRO GLY GLY CYS ASN MET AET	LYS ARG GLY PRO CLEU VAL LEU VAL ARG ARG ARG ARG CVS
LYS GLU ILE ASP ASP GLU ALA ALA ALA ALA ALA ALA CLU VAL CLU VAL CLU CLU CLU CLU CLU CLU CLU CLU CLU CL	HIS ASP LEU GLU GLU CYS PXC PXC CLV GLU TRP TRP TRP TRP TRP TRP TLE LEU	GLY VAL CYS CYS THR HIS HEU CYS CYS CYS VAL PRO ILE ASN	ALA ASP ASP ASP ASP ASP ASP CLY CLY CLY CLY CLY CLY CLY CLY CLY CLY
HIS TYR ALA SER ALA ALA ARG LIJ PRO CLY PRO CLY CLU CLU	VAL PRO SER TYR GLU GLU ASP ASP ASP ASP ASP NET ILE VAL VAL GLY GLY		
• Molecule 5: CYTOCHI	ROME B-C1 COMP	LEX SUBUNIT R	RIESKE, MITOCHONDRIAL
Chain R:	56%	13% •	28%
MET LEU SER VAL ALA ALA ALA ALA ALA PHE PHE PHE PHC PHC PHC THA THA	SER ARG GLY VAL ALA ALA ALA PRO PRO PRO CALN ALA	VAL PRO ALA ALA SER SER CLU CVAL LEU LEU LYS	ARG SER VEL LLEU CYS CYS CYS CYS CLU CYS CLU ALA ALA ALA
GLY PRO PRO UAL UAL VAL SER SER VAL PRO PRO ALA VAL VAL TYR TYR	81 V7 V18 14 122 836 836	143 144 144 144 145 145 145 174 174 174 174 174	176 K77 K85 W91 W91 W91 W92 W98 W114
	W	ORLDWIDE	







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65	Depositor
Cell constants	129.90Å 129.90 Å 722.15 Å	Deperitor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	50.00 - 3.57	Depositor
Resolution (A)	49.81 - 3.57	EDS
% Data completeness	99.8 (50.00-3.57)	Depositor
(in resolution range)	99.9 (49.81 - 3.57)	EDS
R _{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.86 (at 3.57 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
D D	0.206 , 0.252	Depositor
Π, Π_{free}	0.207 , 0.251	DCC
R_{free} test set	3953 reflections $(4.86%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	122.6	Xtriage
Anisotropy	0.197	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.28, 79.3	EDS
L-test for twinning ²	$< L >=0.47, < L^2>=0.29$	Xtriage
Estimated twinning fraction	0.064 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	31051	wwPDB-VP
Average B, all atoms $(Å^2)$	135.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 1.68% 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: PO4, CDL, 4X9, HEC, PEE, HEM, FES, GOL

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).

Mol Chai		Bo	ond lengths	Bond angles		
	Unain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.46	1/3511~(0.0%)	0.69	5/4766~(0.1%)	
1	N	0.42	0/3503	0.70	7/4755~(0.1%)	
2	В	0.69	3/3224~(0.1%)	0.80	10/4375~(0.2%)	
3	С	0.50	0/3065	0.68	0/4196	
3	Р	0.48	1/3031~(0.0%)	0.67	0/4150	
4	D	0.42	0/1971	0.62	0/2676	
4	Q	0.42	0/1977	0.61	0/2684	
5	Е	0.41	0/557	0.62	0/752	
5	Ι	0.57	0/156	1.24	2/209~(1.0%)	
5	R	0.43	0/1552	0.78	7/2100~(0.3%)	
6	F	0.46	0/879	0.68	0/1180	
6	S	0.47	0/888	0.65	0/1191	
7	G	0.52	1/699~(0.1%)	1.26	6/946~(0.6%)	
7	Т	0.49	0/645	0.74	0/873	
8	Н	2.11	7/534~(1.3%)	1.96	8/718~(1.1%)	
8	U	1.48	6/543~(1.1%)	2.09	10/729~(1.4%)	
9	J	0.42	0/495	0.59	0/667	
9	W	0.43	0/500	0.60	0/675	
10	0	0.50	2/3197~(0.1%)	0.95	12/4336~(0.3%)	
11	V	0.58	0/129	0.86	0/177	
All	All	0.59	21/31056~(0.1%)	0.82	67/42155~(0.2%)	

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
1	А	0	1
1	N	0	1
2	В	0	2



Continued	from	previous	page
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Mol	Chain	#Chirality outliers	#Planarity outliers
7	G	0	1
8	Н	0	1
8	U	0	3
10	0	0	2
All	All	0	11

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	В	169	ARG	CZ-NH2	28.39	1.70	1.33
8	Н	43	ARG	CZ-NH1	26.86	1.68	1.33
8	Н	47	ARG	CZ-NH2	25.79	1.66	1.33
8	U	47	ARG	CZ-NH2	25.71	1.66	1.33
8	Н	43	ARG	NE-CZ	23.73	1.64	1.33
10	0	169	ARG	NE-CZ	15.59	1.53	1.33
1	А	408	ARG	CZ-NH2	13.97	1.51	1.33
2	В	169	ARG	CZ-NH1	-11.66	1.17	1.33
8	U	43	ARG	CZ-NH2	-10.62	1.19	1.33
8	U	43	ARG	CZ-NH1	9.93	1.46	1.33
8	Н	47	ARG	CD-NE	9.43	1.62	1.46
8	U	43	ARG	NE-CZ	8.60	1.44	1.33
10	0	169	ARG	CZ-NH1	7.78	1.43	1.33
2	В	169	ARG	NE-CZ	6.49	1.41	1.33
8	Н	42	GLU	CD-OE2	6.18	1.32	1.25
8	Н	47	ARG	CZ-NH1	-5.94	1.25	1.33
8	U	50	THR	CB-CG2	5.50	1.70	1.52
3	Р	220	PHE	CG-CD1	-5.38	1.30	1.38
8	Н	40	CYS	CB-SG	5.23	1.91	1.82
8	U	42	GLU	CD-OE2	5.08	1.31	1.25
7	G	74	PRO	N-CD	5.01	1.54	1.47

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
8	U	47	ARG	NE-CZ-NH2	-37.30	101.65	120.30
8	Н	47	ARG	NE-CZ-NH2	33.38	136.99	120.30
7	G	75	ALA	N-CA-CB	-19.29	83.10	110.10
8	U	43	ARG	NH1-CZ-NH2	-18.82	98.69	119.40
10	0	169	ARG	NH1-CZ-NH2	-17.91	99.70	119.40
8	U	43	ARG	NE-CZ-NH1	17.41	129.00	120.30
10	0	169	ARG	NE-CZ-NH2	17.25	128.93	120.30
8	Н	43	ARG	NE-CZ-NH2	-16.30	112.15	120.30



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
8	Н	43	ARG	NE-CZ-NH1	15.84	128.22	120.30
10	0	169	ARG	NE-CZ-NH1	15.61	128.10	120.30
2	В	390	GLY	N-CA-C	15.33	151.42	113.10
10	0	390	GLY	N-CA-C	15.25	151.24	113.10
8	Н	47	ARG	NH1-CZ-NH2	-14.99	102.92	119.40
7	G	74	PRO	N-CA-C	14.66	150.22	112.10
10	0	301	LYS	CB-CA-C	-14.42	81.56	110.40
8	U	47	ARG	NH1-CZ-NH2	13.47	134.21	119.40
10	0	168	TYR	CB-CA-C	-12.57	85.27	110.40
10	0	301	LYS	N-CA-C	12.53	144.84	111.00
2	В	301	LYS	N-CA-C	12.14	143.79	111.00
8	U	43	ARG	CB-CG-CD	-11.76	81.03	111.60
2	В	391	SER	N-CA-CB	11.69	128.03	110.50
10	0	169	ARG	N-CA-CB	-11.51	89.89	110.60
2	В	169	ARG	NE-CZ-NH1	11.35	125.97	120.30
8	U	43	ARG	CD-NE-CZ	-11.17	107.97	123.60
10	0	391	SER	N-CA-CB	11.11	127.16	110.50
2	В	301	LYS	CB-CA-C	-11.09	88.22	110.40
7	G	77	TYR	C-N-CA	10.54	148.06	121.70
10	0	169	ARG	N-CA-C	10.10	138.26	111.00
7	G	74	PRO	CB-CA-C	-9.99	87.02	112.00
8	Н	50	THR	CB-CA-C	-9.80	85.15	111.60
1	А	349	ALA	N-CA-CB	9.42	123.29	110.10
5	R	142	LEU	N-CA-C	-8.95	86.83	111.00
2	В	169	ARG	NE-CZ-NH2	-8.92	115.84	120.30
8	U	50	THR	CB-CA-C	-8.37	89.01	111.60
5	R	141	HIS	CB-CA-C	-8.23	93.95	110.40
5	Ι	53	GLU	N-CA-C	8.15	133.00	111.00
2	В	169	ARG	N-CA-CB	-8.15	95.94	110.60
1	Ν	349	ALA	N-CA-CB	8.13	121.48	110.10
8	Η	43	ARG	CB-CG-CD	-7.93	90.97	111.60
5	R	72	SER	N-CA-C	7.88	132.29	111.00
5	R	142	LEU	N-CA-CB	7.80	126.00	110.40
1	А	348	SER	CB-CA-C	7.54	124.42	110.10
8	Η	43	ARG	N-CA-CB	-7.47	97.14	110.60
1	A	349	ALA	N-CA-C	-7.33	91.20	111.00
8	Н	47	ARG	CD-NE-CZ	7.25	133.74	123.60
7	G	77	TYR	N-CA-C	7.24	$1\overline{30.54}$	111.00
5	Ι	$5\overline{2}$	ARG	CB-CA-C	6.95	124.29	110.40
1	N	349	ALA	N-CA-C	-6.93	92.29	111.00
1	A	348	SER	N-CA-C	-6.65	93.04	111.00
10	0	301	LYS	C-N-CA	6.42	135.79	122.30



Mol	Chain	\mathbf{Res}	Type	Atoms	\mathbf{Z}	$Observed(^{o})$	$Ideal(^{o})$
2	В	301	LYS	C-N-CA	6.40	135.75	122.30
7	G	73	ASN	C-N-CD	6.03	141.06	128.40
8	U	43	ARG	NE-CZ-NH2	5.98	123.29	120.30
1	N	445	ARG	NE-CZ-NH2	-5.96	117.32	120.30
5	R	73	LYS	N-CA-CB	5.89	121.20	110.60
5	R	72	SER	CB-CA-C	-5.87	98.94	110.10
10	0	169	ARG	CD-NE-CZ	-5.80	115.47	123.60
1	Ν	348	SER	N-CA-C	-5.67	95.68	111.00
2	В	169	ARG	NH1-CZ-NH2	-5.67	113.16	119.40
1	N	408	ARG	CB-CG-CD	-5.57	97.13	111.60
1	А	408	ARG	CG-CD-NE	5.51	123.37	111.80
1	N	348	SER	CB-CA-C	5.45	120.45	110.10
8	U	42	GLU	OE1-CD-OE2	5.44	129.83	123.30
8	U	47	ARG	NE-CZ-NH1	-5.42	117.59	120.30
2	В	168	TYR	CB-CA-C	-5.19	100.02	110.40
5	R	73	LYS	N-CA-C	-5.07	97.32	111.00
1	N	324	PHE	CB-CG-CD1	5.00	124.30	120.80

There are no chirality outliers.

All (11)	planarity	outliers	are listed	below:
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Mol	Chain	Res	Type	Group
1	А	444	LEU	Peptide
2	В	169	ARG	Sidechain
2	В	301	LYS	Peptide
7	G	77	TYR	Peptide
8	Н	50	THR	Peptide
1	Ν	444	LEU	Peptide
10	0	169	ARG	Sidechain
10	0	301	LYS	Peptide
8	U	43	ARG	Sidechain
8	U	47	ARG	Sidechain
8	U	50	THR	Peptide

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	3439	0	3337	45	0
1	Ν	3432	0	3330	42	0
2	В	3164	0	3144	80	0
3	С	2968	0	3028	82	0
3	Р	2936	0	2996	71	0
4	D	1912	0	1861	42	0
4	Q	1918	0	1870	38	0
5	Ε	549	0	547	9	0
5	Ι	157	0	171	27	0
5	R	1518	0	1504	27	0
6	F	860	0	849	24	1
6	S	869	0	862	24	0
7	G	677	0	672	9	0
7	Т	624	0	630	8	0
8	Η	529	0	512	45	0
8	U	538	0	522	23	1
9	J	482	0	483	8	0
9	W	487	0	487	9	0
10	0	3140	0	3121	104	0
11	V	127	0	135	40	0
12	С	86	0	60	10	0
12	Р	86	0	60	10	0
13	С	28	0	14	6	0
13	Р	28	0	14	5	0
14	С	5	0	0	0	0
14	D	15	0	0	0	0
14	Ε	5	0	0	0	0
14	F	5	0	0	0	0
14	N	10	0	0	0	0
14	Q	10	0	0	0	0
14	S	5	0	0	0	0
15	С	49	0	72	1	0
15	D	26	0	26	0	0
15	Р	49	0	72	1	0
15	Q	51	0	82	3	0
16	D	43	0	32	12	0
16	Q	43	0	32	10	0
17	D	39	0	39	0	0
17	G	44	0	32	0	0
17	Q	39	0	39	1	0
17	Т	49	0	42	1	0
18	R	4	0	0	3	0
19	R	6	0	8	0	0



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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	31051	0	30685	645	1

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

All (645) 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)
8:H:43:ARG:CZ	8:H:43:ARG:NH1	1.68	1.56
2:B:169:ARG:CZ	2:B:169:ARG:NH2	1.70	1.49
8:H:47:ARG:CD	8:H:50:THR:HG21	1.35	1.44
8:H:47:ARG:CD	8:H:50:THR:CG2	2.07	1.32
8:H:47:ARG:HD2	8:H:50:THR:CG2	1.62	1.28
4:D:139:THR:OG1	8:H:41:ASP:OD1	1.55	1.22
8:H:44:VAL:CG2	8:H:47:ARG:HH21	1.53	1.20
10:O:168:TYR:O	10:O:173:ALA:HB2	1.41	1.17
1:N:284:TYR:CE1	11:V:73:PRO:HB3	1.80	1.16
8:H:47:ARG:HD2	8:H:50:THR:HG22	1.28	1.15
8:H:44:VAL:HG22	8:H:47:ARG:HH21	1.10	1.12
4:Q:139:THR:OG1	8:U:41:ASP:OD1	1.68	1.08
10:O:89:ILE:HD12	11:V:70:LEU:HD22	1.36	1.03
4:Q:37:CYS:SG	16:Q:501:HEC:CAB	2.48	1.02
8:H:47:ARG:CZ	8:H:50:THR:OG1	1.88	1.01
1:A:344:ARG:O	1:A:348:SER:O	1.79	1.01
8:U:37:LEU:O	8:U:41:ASP:HB2	1.61	1.01
10:O:85:ILE:HG22	11:V:70:LEU:HD13	1.43	0.99
4:D:40:CYS:SG	16:D:501:HEC:HBC3	2.02	0.99
10:O:90:GLU:HG2	11:V:71:ASN:OD1	1.64	0.97
2:B:168:TYR:HD2	2:B:172:LEU:HB2	1.27	0.96
8:H:37:LEU:O	8:H:41:ASP:HB2	1.64	0.96
8:H:44:VAL:HG22	8:H:47:ARG:NH2	1.80	0.94
10:O:168:TYR:HD2	10:O:172:LEU:HB2	1.33	0.93
3:C:376:LEU:HD12	6:F:20:TYR:HD2	1.33	0.93
1:N:344:ARG:O	1:N:348:SER:O	1.86	0.91
2:B:99:THR:CG2	5:I:67:SER:OG	2.19	0.91
8:U:43:ARG:O	8:U:47:ARG:HG2	1.72	0.89
10:O:85:ILE:HG22	11:V:70:LEU:CD1	2.02	0.89
4:Q:1:SER:HA	4:Q:155:GLY:HA2	1.54	0.88
4:D:178:THR:HG21	8:H:16:PRO:HD2	1.57	0.87
8:U:43:ARG:O	8:U:47:ARG:CG	2.23	0.87
8:H:44:VAL:CG2	8:H:47:ARG:NH2	2.36	0.86



Atom-1	Atom-2	Interatomic	Clash
		distance (A)	overlap (A)
3:C:376:LEU:CD1	6:F:20:TYR:HD2	1.90	0.84
2:B:99:THR:HG22	5:1:67:SER:OG	1.77	0.84
4:Q:37:CYS:SG	16:Q:501:HEC:CBB	2.66	0.83
3:P:276:PHE:HD1	3:P:277:ALA:N	1.74	0.83
4:D:37:CYS:SG	16:D:501:HEC:CAB	2.66	0.83
8:H:44:VAL:HG23	8:H:47:ARG:HH21	1.44	0.83
10:O:90:GLU:CG	11:V:71:ASN:OD1	2.26	0.83
3:C:376:LEU:HD12	6:F:20:TYR:CD2	2.14	0.82
3:C:276:PHE:HD1	3:C:277:ALA:N	1.78	0.82
2:B:168:TYR:CD2	2:B:172:LEU:HB2	2.14	0.81
10:O:169:ARG:HH21	10:O:238:LYS:HG2	1.45	0.81
8:H:50:THR:OG1	8:H:51:GLU:N	2.10	0.80
8:H:47:ARG:HH12	8:H:50:THR:C	1.85	0.80
10:O:168:TYR:CD2	10:O:172:LEU:HB2	2.17	0.80
8:U:50:THR:OG1	8:U:51:GLU:N	2.05	0.80
10:O:169:ARG:NH2	10:O:238:LYS:HG2	1.97	0.79
4:D:40:CYS:SG	16:D:501:HEC:CBC	2.69	0.79
3:C:145:VAL:HG21	3:C:268:ILE:HD12	1.64	0.79
8:H:47:ARG:NH1	8:H:50:THR:O	2.15	0.78
3:P:145:VAL:HG21	3:P:268:ILE:HD12	1.65	0.78
8:U:48:SER:C	8:U:49:GLN:HG2	2.04	0.78
4:D:37:CYS:SG	16:D:501:HEC:CBB	2.72	0.78
4:D:40:CYS:SG	16:D:501:HEC:CAC	2.71	0.78
12:C:502:HEM:HBC2	12:C:502:HEM:HMC2	1.64	0.77
4:D:140:GLY:HA3	8:H:53:ASP:HB3	1.64	0.76
4:D:37:CYS:SG	16:D:501:HEC:HBB3	2.25	0.76
10:O:89:ILE:HB	11:V:70:LEU:CD2	2.16	0.75
8:U:44:VAL:HG23	8:U:47:ARG:NH2	2.02	0.74
2:B:99:THR:HG23	5:I:67:SER:OG	1.87	0.74
2:B:169:ARG:NH2	2:B:238:LYS:HG2	2.03	0.74
4:D:120:ARG:NE	16:D:501:HEC:O1A	2.21	0.74
12:C:501:HEM:HMC1	12:C:501:HEM:HBC2	1.70	0.73
8:H:48:SER:C	8:H:49:GLN:HG2	2.09	0.73
5:I:53:GLU:O	5:I:53:GLU:HG3	1.88	0.73
13:P:503:4X9:C6	13:P:503:4X9:H16	2.18	0.72
7:G:77:TYR:O	7:G:80:ASP:O	2.07	0.72
10:O:89:ILE:CD1	11:V:70:LEU:HD22	2.16	0.72
6:F:20:TYR:HD1	6:F:20:TYR:O	1.73	0.72
2:B:78:LYS:HB2	2:B:129:ALA:HB1	1.72	0.71
3:C:106:SER:HB3	12:C:502:HEM:HBD2	1.71	0.71
8:H:43:ARG:O	8:H:47:ARG:HG2	1.90	0.71



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:B:438:GLU:OE2	10:O:169:ARG:NH1	2.23	0.71
12:P:501:HEM:HMC1	12:P:501:HEM:HBC2	1.71	0.71
2:B:227:ARG:HE	2:B:227:ARG:HA	1.55	0.70
2:B:168:TYR:O	2:B:173:ALA:HB2	1.92	0.70
3:C:205:SER:OG	13:C:503:4X9:H26B	1.91	0.70
1:N:253:VAL:HB	1:N:324:PHE:CE1	2.26	0.70
12:P:501:HEM:HMB1	12:P:501:HEM:HBB2	1.74	0.70
5:R:98:VAL:HG23	5:R:98:VAL:O	1.92	0.70
2:B:169:ARG:NH1	10:O:438:GLU:OE2	2.24	0.70
8:H:40:CYS:HA	8:H:43:ARG:HG2	1.74	0.70
4:Q:40:CYS:SG	16:Q:501:HEC:HBC3	2.31	0.69
8:H:47:ARG:NH2	8:H:50:THR:OG1	2.23	0.69
10:O:168:TYR:O	10:O:173:ALA:CB	2.30	0.69
1:A:21:ASN:O	1:A:221:GLY:O	2.10	0.69
10:O:78:LYS:HB2	10:O:129:ALA:HB1	1.75	0.69
3:P:276:PHE:CD1	3:P:277:ALA:N	2.60	0.69
10:O:227:ARG:HE	10:O:227:ARG:HA	1.57	0.68
8:H:44:VAL:HA	8:H:47:ARG:HE	1.58	0.68
10:O:304:HIS:O	10:O:305:GLU:HG3	1.93	0.68
4:Q:37:CYS:SG	16:Q:501:HEC:HBB3	2.33	0.68
2:B:29:LEU:HD23	2:B:30:PRO:HD2	1.75	0.67
3:P:276:PHE:HD1	3:P:276:PHE:C	1.97	0.67
11:V:72:VAL:HG13	11:V:73:PRO:HD2	1.77	0.67
3:C:187:PHE:CZ	3:P:184:ILE:CD1	2.78	0.66
3:C:276:PHE:CD1	3:C:277:ALA:N	2.61	0.66
3:C:201:HIS:CE1	13:C:503:4X9:H29	2.30	0.65
2:B:170:ASN:ND2	2:B:170:ASN:H	1.93	0.65
6:F:20:TYR:HD1	6:F:20:TYR:C	1.99	0.65
11:V:72:VAL:HG12	11:V:73:PRO:O	1.95	0.65
3:P:78:ILE:HD11	4:Q:204:MET:CE	2.27	0.65
3:C:220:PHE:HD1	3:C:220:PHE:O	1.80	0.65
5:R:163:SER:HA	5:R:174:GLY:HA3	1.79	0.65
8:H:43:ARG:O	8:H:47:ARG:CG	2.45	0.65
8:H:44:VAL:HA	8:H:47:ARG:NE	2.12	0.65
11:V:70:LEU:O	11:V:70:LEU:HG	1.97	0.65
10:O:29:LEU:HD23	10:O:30:PRO:HD2	1.78	0.64
1:A:253:VAL:HB	1:A:324:PHE:CE1	2.33	0.64
3:P:276:PHE:CD1	3:P:276:PHE:C	2.71	0.64
1:N:21:ASN:O	1:N:221:GLY:O	2.16	0.64
6:F:20:TYR:C	6:F:20:TYR:CD1	2.71	0.64
1:N:324:PHE:CE2	1:N:334:MET:HB3	2.33	0.64



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:C:78:ILE:HD11	4:D:204:MET:CE	2.28	0.64
5:I:70:LEU:HG	5:I:70:LEU:O	1.96	0.64
5:R:175:PRO:HG2	18:R:501:FES:S1	2.38	0.63
6:F:20:TYR:HE1	6:F:24:ALA:HB2	1.64	0.63
6:S:40:ASN:OD1	6:S:40:ASN:C	2.35	0.63
3:C:379:TRP:CE2	6:F:33:ARG:HD3	2.34	0.63
5:I:72:VAL:HG12	5:I:73:PRO:O	1.99	0.62
3:P:220:PHE:CD1	3:P:224:TYR:HB2	2.34	0.62
4:D:178:THR:HG21	8:H:16:PRO:CD	2.29	0.62
11:V:62:ARG:O	11:V:78:TYR:HB3	2.00	0.62
3:C:168:PHE:HE2	5:R:72:SER:HB2	1.65	0.62
10:O:98:VAL:O	11:V:67:SER:HA	2.00	0.62
3:P:103:TYR:HB2	3:P:325:PHE:HE2	1.65	0.61
3:C:276:PHE:HD1	3:C:276:PHE:C	2.03	0.61
1:A:293:PRO:O	1:A:297:ILE:HG12	2.01	0.61
2:B:261:SER:OG	2:B:262:ALA:N	2.32	0.61
1:N:284:TYR:CE1	11:V:73:PRO:CB	2.71	0.61
10:O:170:ASN:H	10:O:170:ASN:ND2	1.96	0.61
2:B:169:ARG:CD	10:O:435:PHE:CZ	2.83	0.61
10:O:169:ARG:HH21	10:O:238:LYS:CG	2.12	0.61
1:N:253:VAL:HB	1:N:324:PHE:HE1	1.64	0.61
2:B:435:PHE:CZ	10:O:169:ARG:CD	2.84	0.61
3:P:376:LEU:HB2	6:S:20:TYR:HD2	1.64	0.61
12:C:501:HEM:HBB2	12:C:501:HEM:HHC	1.83	0.60
11:V:76:VAL:HG12	11:V:76:VAL:O	2.01	0.60
3:C:277:ALA:HB1	3:C:294:LEU:CD1	2.31	0.60
9:W:58:LYS:C	9:W:59:TYR:HD1	2.05	0.60
5:I:72:VAL:HG13	5:I:73:PRO:HD2	1.83	0.60
2:B:134:ARG:NH2	6:S:49:ARG:O	2.34	0.60
2:B:169:ARG:HD3	10:O:435:PHE:CE2	2.36	0.60
3:P:277:ALA:HB1	3:P:294:LEU:CD1	2.32	0.60
3:P:376:LEU:CB	6:S:20:TYR:HD2	2.15	0.60
1:A:324:PHE:CE2	1:A:334:MET:HB3	2.37	0.59
4:D:178:THR:CG2	8:H:15:ASP:HA	2.32	0.59
1:A:443:TRP:CD1	1:A:444:LEU:HD23	2.37	0.59
3:C:220:PHE:O	3:C:220:PHE:CD1	2.55	0.59
10:O:89:ILE:HB	11:V:70:LEU:HD23	1.83	0.59
5:R:161:HIS:HB2	18:R:501:FES:S1	2.43	0.59
4:D:33:TYR:HA	4:D:37:CYS:SG	2.43	0.58
2:B:279:LEU:HA	2:B:294:SER:HB3	1.85	0.58
4:Q:181:GLN:HB2	8:U:77:LEU:HD22	1.85	0.58



Atom-1	Atom-2	Interatomic	Clash
		distance (Å)	overlap (Å)
8:U:40:CYS:HA	8:U:43:ARG:HG2	1.84	0.58
3:C:375:LYS:O	6:F:17:ARG:NH1	2.36	0.58
7:G:59:TYR:CD1	7:G:59:TYR:C	2.75	0.58
5:I:64:LEU:HD21	5:I:76:VAL:HG13	1.84	0.58
3:C:106:SER:HB3	12:C:502:HEM:CBD	2.33	0.57
2:B:98:VAL:O	5:I:68:VAL:O	2.22	0.57
3:C:120:LEU:HG	3:C:124:MET:HE2	1.86	0.57
3:C:361:LEU:O	3:C:366:MET:HG3	2.04	0.57
3:C:220:PHE:CZ	13:C:503:4X9:H15	2.39	0.57
3:C:276:PHE:CD1	3:C:276:PHE:C	2.77	0.57
1:N:3:THR:HG23	1:N:6:GLN:H	1.69	0.57
8:U:47:ARG:HB2	8:U:50:THR:HG22	1.85	0.57
3:C:103:TYR:HB2	3:C:325:PHE:HE2	1.68	0.57
3:C:220:PHE:CD1	3:C:220:PHE:C	2.78	0.57
10:O:261:SER:OG	10:O:262:ALA:N	2.38	0.57
13:P:503:4X9:H16	13:P:503:4X9:H6	1.87	0.57
3:P:349:THR:HA	3:P:352:GLN:HG2	1.86	0.56
1:A:223:TYR:HB2	1:A:228:VAL:HG21	1.87	0.56
3:P:376:LEU:HB2	6:S:20:TYR:CD2	2.40	0.56
6:F:40:ASN:OD1	6:F:41:ASP:N	2.38	0.56
4:Q:40:CYS:SG	16:Q:501:HEC:CAC	2.93	0.56
2:B:71:LEU:HD23	5:I:68:VAL:HG11	1.88	0.56
6:F:49:ARG:O	10:O:134:ARG:NH2	2.39	0.56
3:P:18:PHE:O	3:P:220:PHE:HD2	1.88	0.56
4:Q:33:TYR:HA	4:Q:37:CYS:SG	2.45	0.56
1:A:253:VAL:HB	1:A:324:PHE:HE1	1.70	0.56
4:D:178:THR:HG21	8:H:15:ASP:HA	1.87	0.56
10:O:97:SER:HA	11:V:69:SER:OG	2.06	0.56
2:B:169:ARG:NH2	2:B:238:LYS:CG	2.69	0.56
5:E:58:PHE:O	5:E:61:SER:HB3	2.06	0.56
5:I:52:ARG:HD2	5:I:53:GLU:H	1.71	0.56
3:P:145:VAL:HG21	3:P:268:ILE:CD1	2.36	0.56
6:S:40:ASN:OD1	6:S:41:ASP:N	2.38	0.56
8:H:48:SER:C	8:H:49:GLN:CG	2.75	0.56
10:O:86:THR:HA	11:V:70:LEU:HD11	1.87	0.56
10:O:71:LEU:HD23	11:V:68:VAL:HG21	1.87	0.55
3:P:103:TYR:HD1	3:P:325:PHE:HD2	1.53	0.55
3:P:70:CYS:SG	3:P:80:ARG:HD3	2.46	0.55
8:H:40:CYS:CA	8:H:43:ARG:HG2	2.36	0.55
2:B:176:LEU:HD13	5:I:66:ALA:HB2	1.88	0.55
3:C:21:LEU:HD23	3:C:220:PHE:HD2	1.72	0.55



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
7:G:59:TYR:C	7:G:59:TYR:HD1	2.08	0.55
1:A:27:SER:HA	1:A:199:ALA:O	2.06	0.55
4:Q:1:SER:CA	4:Q:155:GLY:HA2	2.32	0.55
8:H:35:GLU:C	8:H:39:LEU:HD12	2.27	0.55
10:O:31:ASN:ND2	10:O:225:ASN:OD1	2.39	0.55
8:H:35:GLU:O	8:H:39:LEU:HD12	2.07	0.55
2:B:75:LEU:HD22	2:B:136:GLU:HB3	1.89	0.55
16:D:501:HEC:HBD2	16:D:501:HEC:HHA	1.88	0.55
3:C:105:GLY:HA2	3:C:107:TYR:CE2	2.42	0.55
4:Q:204:MET:HG2	15:Q:506:PEE:H2	1.88	0.55
1:A:3:THR:HG23	1:A:6:GLN:H	1.71	0.54
3:C:220:PHE:HD1	3:C:220:PHE:C	2.11	0.54
10:O:90:GLU:HA	11:V:71:ASN:HD21	1.71	0.54
16:D:501:HEC:HHA	16:D:501:HEC:CBD	2.37	0.54
6:F:40:ASN:OD1	6:F:40:ASN:C	2.44	0.54
5:I:53:GLU:O	5:I:53:GLU:CG	2.56	0.54
10:O:176:LEU:HD12	11:V:64:VAL:HG23	1.90	0.54
1:N:284:TYR:CD1	11:V:73:PRO:HB3	2.38	0.54
10:O:226:ILE:HD12	10:O:227:ARG:N	2.23	0.54
3:C:8:HIS:N	3:C:9:PRO:HD3	2.23	0.54
1:A:233:PRO:O	5:E:22:THR:HA	2.07	0.54
1:N:288:ALA:HB2	1:N:300:THR:HG22	1.90	0.54
2:B:169:ARG:HD3	10:O:435:PHE:CZ	2.43	0.53
8:U:48:SER:C	8:U:49:GLN:CG	2.77	0.53
3:C:75:TYR:CE2	5:E:57:GLN:HG2	2.42	0.53
2:B:99:THR:CG2	5:I:67:SER:HG	2.22	0.53
3:C:184:ILE:CD1	3:P:187:PHE:CZ	2.91	0.53
2:B:299:VAL:HG11	2:B:336:VAL:HG13	1.90	0.53
3:C:104:TYR:CD1	3:C:208:PRO:HA	2.43	0.53
3:P:221:HIS:ND1	3:P:222:PRO:HA	2.24	0.53
4:D:211:MET:HG2	9:J:35:PHE:CE2	2.43	0.53
7:T:59:TYR:CD1	7:T:59:TYR:C	2.82	0.53
3:P:376:LEU:HD12	6:S:20:TYR:CD2	2.44	0.53
1:N:219:LEU:HG	1:N:220:SER:O	2.08	0.53
3:C:11:MET:SD	3:C:11:MET:C	2.88	0.53
13:P:503:4X9:C6	13:P:503:4X9:C16	2.84	0.53
1:A:162:PRO:HD2	1:A:234:CYS:SG	2.48	0.52
8:H:44:VAL:HG23	8:H:47:ARG:NH2	2.14	0.52
2:B:157:ALA:O	2:B:161:GLU:HG2	2.09	0.52
2:B:168:TYR:CE2	2:B:172:LEU:HD12	2.44	0.52
1:N:106:LEU:HB3	1:N:107:PRO:HD3	1.91	0.52



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
10:O:299:VAL:HG11	10:O:336:VAL:HG13	1.91	0.52
3:P:375:LYS:O	6:S:17:ARG:NH1	2.37	0.52
4:Q:178:THR:HG21	8:U:16:PRO:HD2	1.90	0.52
1:N:283:THR:HB	11:V:74:ALA:HB3	1.91	0.52
6:F:107:TRP:HE1	10:O:87:ARG:HB3	1.75	0.52
3:C:11:MET:SD	3:C:11:MET:O	2.67	0.52
6:F:20:TYR:CE1	6:F:24:ALA:HB2	2.43	0.52
12:P:502:HEM:HMB1	12:P:502:HEM:HBB2	1.92	0.52
9:W:59:TYR:N	9:W:59:TYR:CD1	2.75	0.52
2:B:169:ARG:NH2	2:B:169:ARG:NH1	2.41	0.52
9:J:58:LYS:C	9:J:59:TYR:HD1	2.13	0.52
10:O:42:ALA:O	10:O:113:ARG:NH1	2.41	0.52
3:P:103:TYR:HD1	3:P:325:PHE:CD2	2.28	0.52
3:C:246:ALA:HB1	3:C:249:LEU:HB2	1.92	0.51
5:I:64:LEU:HD23	5:I:65:VAL:N	2.24	0.51
10:O:96:LEU:O	11:V:69:SER:HA	2.10	0.51
10:O:279:LEU:HA	10:O:294:SER:HB3	1.91	0.51
3:P:226:ILE:HA	3:P:229:ILE:HD12	1.92	0.51
3:P:361:LEU:O	3:P:366:MET:HG3	2.10	0.51
2:B:101:THR:HG1	2:B:103:GLU:H	1.57	0.51
3:C:277:ALA:HB1	3:C:294:LEU:HD12	1.92	0.51
4:D:141:VAL:HG23	8:H:53:ASP:OD2	2.10	0.51
2:B:435:PHE:CE2	10:O:169:ARG:HD3	2.45	0.51
10:O:49:LEU:HD23	10:O:127:THR:HG21	1.91	0.51
3:P:103:TYR:HB2	3:P:325:PHE:CE2	2.44	0.51
10:O:168:TYR:CE2	10:O:172:LEU:HD12	2.45	0.51
3:C:145:VAL:HG21	3:C:268:ILE:CD1	2.36	0.51
3:P:211:ILE:HD11	6:S:36:THR:HG22	1.93	0.51
7:T:73:ASN:HB3	7:T:75:ALA:H	1.76	0.51
2:B:226:ILE:HD12	2:B:227:ARG:N	2.25	0.51
5:I:65:VAL:HG23	5:I:77:ARG:HB2	1.91	0.51
10:O:85:ILE:HG22	11:V:70:LEU:HD11	1.90	0.51
2:B:435:PHE:CZ	10:O:169:ARG:HD2	2.46	0.51
5:I:76:VAL:HG12	5:I:76:VAL:O	2.10	0.51
1:N:27:SER:HA	1:N:199:ALA:O	2.11	0.51
3:C:181:PHE:HA	3:C:184:ILE:HG22	1.92	0.51
3:C:349:THR:HA	3:C:352:GLN:HG2	1.93	0.51
12:C:502:HEM:HBC2	12:C:502:HEM:CMC	2.38	0.51
3:P:246:ALA:HB1	3:P:249:LEU:HB2	1.92	0.51
3:P:277:ALA:HB1	3:P:294:LEU:HD12	1.93	0.51
3:C:120:LEU:HG	3:C:124:MET:CE	2.40	0.51



Atom_1	Atom_2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
10:O:75:LEU:HD22	10:O:136:GLU:HB3	1.93	0.51
3:P:120:LEU:HG	3:P:124:MET:HE2	1.93	0.51
1:A:244:ARG:CZ	7:G:10:VAL:HB	2.41	0.50
3:C:19:ILE:HG22	3:C:20:ASP:OD1	2.11	0.50
10:O:90:GLU:HG3	11:V:71:ASN:OD1	2.09	0.50
6:S:71:ARG:O	6:S:72:GLN:HB2	2.12	0.50
4:D:137:PRO:HA	4:D:149:PHE:CD2	2.46	0.50
10:O:98:VAL:HG22	10:O:107:TYR:CD1	2.46	0.50
17:Q:505:CDL:C42	17:T:501:CDL:C78	2.90	0.50
3:C:75:TYR:CD2	5:E:57:GLN:HG2	2.47	0.50
3:P:325:PHE:C	3:P:325:PHE:CD1	2.85	0.50
12:P:502:HEM:HBB2	12:P:502:HEM:CMB	2.42	0.50
4:Q:40:CYS:SG	16:Q:501:HEC:CBC	2.98	0.50
5:R:134:ILE:HD11	5:R:185:TYR:CG	2.47	0.50
2:B:177:TYR:OH	5:I:76:VAL:CG2	2.60	0.50
1:N:223:TYR:CB	1:N:228:VAL:HG21	2.41	0.49
1:N:293:PRO:O	1:N:297:ILE:HG12	2.12	0.49
10:O:157:ALA:O	10:O:161:GLU:HG2	2.12	0.49
6:S:12:TRP:CD1	6:S:13:LEU:HD23	2.47	0.49
3:C:226:ILE:HA	3:C:229:ILE:HD12	1.94	0.49
3:P:51:LEU:HD13	12:P:501:HEM:HBD1	1.94	0.49
5:R:150:ALA:O	5:R:157:TYR:HB2	2.12	0.49
10:O:385:GLN:O	10:O:389:ALA:O	2.29	0.49
3:P:14:VAL:HG12	3:P:14:VAL:O	2.11	0.49
3:P:137:GLN:OE1	3:P:260:ASN:N	2.45	0.49
1:A:288:ALA:HB2	1:A:300:THR:HG22	1.93	0.49
3:C:70:CYS:SG	3:C:80:ARG:HD3	2.52	0.49
1:N:3:THR:OG1	1:N:4:TYR:N	2.46	0.49
2:B:83:PHE:CZ	6:S:107:TRP:HD1	2.31	0.49
2:B:308:ASP:HB2	5:I:55:LEU:CB	2.42	0.49
2:B:435:PHE:CZ	10:O:169:ARG:HD3	2.47	0.49
5:R:171:ILE:HD11	5:R:176:ALA:HB3	1.95	0.49
1:A:106:LEU:HB3	1:A:107:PRO:HD3	1.95	0.49
1:A:223:TYR:CB	1:A:228:VAL:HG21	2.42	0.49
2:B:100:SER:O	5:I:66:ALA:O	2.30	0.49
3:C:10:LEU:HD12	3:C:10:LEU:C	2.32	0.49
4:D:231:LYS:O	6:F:71:ARG:HD3	2.13	0.49
4:Q:211:MET:HG2	9:W:35:PHE:CE2	2.48	0.49
5:R:140:THR:HB	5:R:177:PRO:HD2	1.95	0.49
1:A:223:TYR:HB2	1:A:228:VAL:CG2	2.42	0.49
2:B:316:TYR:CD1	2:B:316:TYR:N	2.80	0.49



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:B:380:ASP:O	2:B:384:SER:HB2	2.13	0.49
10:O:169:ARG:HH21	10:O:238:LYS:HB3	1.77	0.49
3:P:105:GLY:HA2	3:P:107:TYR:CE2	2.48	0.49
1:N:443:TRP:CD1	1:N:444:LEU:HD23	2.48	0.49
1:A:294:LEU:HD13	1:A:337:VAL:HG12	1.95	0.48
2:B:169:ARG:HD2	10:O:435:PHE:CZ	2.48	0.48
1:N:386:TYR:CD2	1:N:390:ILE:HD12	2.47	0.48
2:B:129:ALA:N	2:B:130:PRO:CD	2.77	0.48
9:J:59:TYR:CD1	9:J:59:TYR:N	2.82	0.48
10:O:95:LYS:HG3	11:V:72:VAL:CG2	2.44	0.48
10:O:164:HIS:NE2	10:O:316:TYR:OH	2.40	0.48
3:P:13:ILE:O	3:P:16:ASN:ND2	2.46	0.48
12:P:502:HEM:HBC2	12:P:502:HEM:HHD	1.95	0.48
4:Q:36:VAL:O	16:Q:501:HEC:HMC3	2.14	0.48
4:Q:149:PHE:CE1	4:Q:156:GLN:HB3	2.48	0.48
7:T:25:ALA:O	7:T:27:PRO:HD3	2.14	0.48
1:A:53:ASN:HD21	1:A:165:GLN:HB3	1.79	0.48
3:C:137:GLN:OE1	3:C:260:ASN:N	2.46	0.48
3:C:312:GLN:HG3	3:C:379:TRP:CZ3	2.47	0.48
2:B:49:LEU:HD23	2:B:127:THR:HG21	1.94	0.48
2:B:97:SER:HA	5:I:69:SER:HB3	1.96	0.48
3:C:103:TYR:HB2	3:C:325:PHE:CE2	2.48	0.48
10:O:95:LYS:HG3	11:V:72:VAL:HG23	1.95	0.48
3:P:120:LEU:HG	3:P:124:MET:CE	2.43	0.48
8:U:35:GLU:C	8:U:39:LEU:HD12	2.34	0.48
10:O:96:LEU:O	10:O:96:LEU:HG	2.13	0.48
10:O:229:GLY:O	10:O:230:LEU:C	2.51	0.48
6:S:20:TYR:O	6:S:20:TYR:CD1	2.66	0.48
1:A:40:TRP:CZ2	1:A:377:GLU:HA	2.49	0.48
3:C:15:ASN:N	3:C:15:ASN:OD1	2.46	0.48
4:D:140:GLY:CA	8:H:53:ASP:HB3	2.39	0.48
3:P:131:TYR:HA	12:P:501:HEM:HAA1	1.94	0.48
3:C:103:TYR:HD1	3:C:325:PHE:HD2	1.61	0.48
1:N:245:GLU:HG3	1:N:248:LEU:HG	1.96	0.48
2:B:209:LEU:CD2	2:B:375:SER:HB2	2.43	0.48
3:C:14:VAL:HG12	3:C:14:VAL:O	2.14	0.48
3:C:29:SER:O	3:C:32:ASN:HB2	2.13	0.48
16:D:501:HEC:CBB	16:D:501:HEC:HMB1	2.44	0.48
8:H:41:ASP:O	8:H:45:SER:OG	2.19	0.48
5:I:52:ARG:HD2	5:I:53:GLU:N	2.28	0.48
3:P:104:TYR:CD1	3:P:208:PRO:HA	2.48	0.48



Atom-1	Atom-2	Interatomic	Clash
	1100111-2	distance (Å)	overlap (Å)
1:A:386:TYR:CD2	1:A:390:ILE:HD12	2.49	0.48
2:B:229:GLY:O	2:B:230:LEU:C	2.53	0.48
3:C:325:PHE:CD1	3:C:325:PHE:C	2.87	0.48
10:O:243:GLU:HA	10:O:424:MET:O	2.13	0.48
10:O:312:PHE:HD1	10:O:313:ASN:N	2.11	0.48
6:S:20:TYR:CD1	6:S:20:TYR:C	2.85	0.48
4:D:225:HIS:CE1	7:G:20:PRO:HB2	2.49	0.47
1:N:85:HIS:HB2	1:N:100:LYS:HB2	1.96	0.47
10:O:85:ILE:CG2	11:V:70:LEU:HD13	2.29	0.47
3:P:75:TYR:CE2	5:R:57:GLN:HG2	2.49	0.47
1:A:3:THR:OG1	1:A:4:TYR:N	2.47	0.47
2:B:29:LEU:CD2	2:B:30:PRO:HD2	2.43	0.47
2:B:385:GLN:O	2:B:389:ALA:O	2.32	0.47
1:A:267:ASN:O	1:A:271:GLN:HG2	2.15	0.47
3:C:211:ILE:HD11	6:F:36:THR:HG22	1.95	0.47
4:D:211:MET:HG2	9:J:35:PHE:HE2	1.79	0.47
10:O:301:LYS:HG3	10:O:301:LYS:O	2.13	0.47
10:O:316:TYR:CD1	10:O:316:TYR:N	2.80	0.47
3:P:10:LEU:HD12	3:P:10:LEU:C	2.35	0.47
4:Q:3:LEU:HD21	8:U:56:GLU:HG3	1.96	0.47
2:B:227:ARG:HA	2:B:227:ARG:NE	2.26	0.47
4:D:218:LEU:O	4:D:221:ALA:HB3	2.13	0.47
2:B:354:ASN:N	2:B:355:PRO:HD2	2.30	0.47
10:O:86:THR:HA	11:V:70:LEU:HD21	1.97	0.47
3:P:14:VAL:O	3:P:14:VAL:CG1	2.63	0.47
3:P:77:TRP:CZ3	3:P:78:ILE:HG13	2.50	0.47
16:Q:501:HEC:CBB	16:Q:501:HEC:HMB1	2.45	0.47
5:R:98:VAL:O	5:R:98:VAL:CG2	2.62	0.47
8:U:35:GLU:O	8:U:39:LEU:HD12	2.15	0.47
2:B:435:PHE:N	2:B:435:PHE:CD1	2.82	0.47
5:R:45:VAL:HG13	9:W:28:ALA:HA	1.96	0.47
11:V:62:ARG:HB3	11:V:63:PRO:HD2	1.97	0.47
15:Q:506:PEE:H11	5:R:53:ASN:OD1	2.15	0.47
7:T:59:TYR:C	7:T:59:TYR:HD1	2.17	0.47
10:O:209:LEU:CD2	10:O:375:SER:HB2	2.45	0.46
12:P:501:HEM:HHA	12:P:501:HEM:CBA	2.45	0.46
5:R:171:ILE:CD1	5:R:176:ALA:HB3	2.45	0.46
13:C:503:4X9:C6	13:C:503:4X9:C12	2.89	0.46
5:E:31:ALA:HB2	9:J:7:ALA:HB2	1.96	0.46
3:P:379:TRP:CE3	6:S:33:ARG:HD3	2.51	0.46
4:D:138:PRO:HG3	8:H:55:THR:HA	1.98	0.46



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
3:P:358:TYR:HE1	3:P:362:ILE:HD11	1.80	0.46
8:H:40:CYS:O	8:H:43:ARG:CG	2.64	0.46
1:N:294:LEU:HD13	1:N:337:VAL:HG12	1.97	0.46
10:O:34:VAL:HG11	10:O:386:ALA:HB1	1.98	0.46
12:P:501:HEM:HBB2	12:P:501:HEM:CMB	2.42	0.46
3:C:373:GLU:HA	6:F:20:TYR:HE2	1.80	0.46
8:U:17:LEU:HD11	8:U:21:ARG:NE	2.30	0.46
1:N:442:PHE:CD1	1:N:442:PHE:C	2.89	0.46
5:R:91:TRP:HZ3	5:R:136:ILE:HD11	1.81	0.46
1:A:245:GLU:HG3	1:A:248:LEU:HG	1.97	0.46
2:B:308:ASP:HB2	5:I:55:LEU:HB2	1.97	0.46
4:D:138:PRO:HD3	4:D:149:PHE:CE2	2.50	0.46
4:D:181:GLN:OE1	8:H:77:LEU:HB3	2.16	0.46
3:P:103:TYR:CD1	3:P:325:PHE:CD2	3.04	0.46
2:B:87:ARG:HB3	6:S:107:TRP:NE1	2.30	0.46
3:C:186:PRO:HG2	12:C:501:HEM:HMC3	1.96	0.46
1:A:77:LYS:HE3	2:B:291:ALA:HB1	1.97	0.46
2:B:70:ARG:HG2	5:I:68:VAL:HB	1.98	0.46
2:B:109:VAL:HB	2:B:119:LEU:HD12	1.98	0.46
1:N:219:LEU:O	1:N:220:SER:C	2.54	0.46
10:O:169:ARG:HH21	10:O:238:LYS:CB	2.29	0.46
10:O:354:ASN:N	10:O:355:PRO:HD2	2.31	0.45
3:P:319:PRO:HD2	6:S:20:TYR:CE1	2.51	0.45
3:C:14:VAL:O	3:C:14:VAL:CG1	2.64	0.45
12:C:502:HEM:HBB2	12:C:502:HEM:CMB	2.47	0.45
4:D:40:CYS:SG	16:D:501:HEC:C3C	3.04	0.45
10:O:26:PHE:CE2	10:O:391:SER:HA	2.52	0.45
10:O:99:THR:HG23	11:V:67:SER:OG	2.15	0.45
4:Q:149:PHE:CD1	4:Q:156:GLN:HB3	2.50	0.45
3:C:10:LEU:HD21	3:P:202:GLU:HG3	1.99	0.45
3:C:233:LEU:HD22	4:D:216:LEU:HG	1.98	0.45
4:D:37:CYS:HG	16:D:501:HEC:HBB3	1.80	0.45
8:H:17:LEU:HD11	8:H:21:ARG:NE	2.31	0.45
1:N:442:PHE:C	1:N:442:PHE:HD1	2.20	0.45
10:O:213:HIS:N	10:O:214:PRO:CD	2.79	0.45
4:Q:137:PRO:HA	4:Q:149:PHE:CD2	2.52	0.45
10:O:129:ALA:N	10:O:130:PRO:CD	2.80	0.45
3:P:103:TYR:CD1	3:P:325:PHE:HD2	2.34	0.45
4:Q:3:LEU:CD2	8:U:56:GLU:HG3	2.47	0.45
4:D:216:LEU:N	4:D:217:PRO:HD2	2.31	0.45
1:N:77:LYS:HE3	10:O:291:ALA:HB1	1.98	0.45



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:111:GLU:HG3	1:A:215:HIS:CE1	2.52	0.45
2:B:303:VAL:HG23	2:B:303:VAL:O	2.16	0.45
7:G:75:ALA:O	7:G:77:TYR:CD2	2.69	0.45
1:N:233:PRO:O	5:R:22:THR:HA	2.17	0.45
10:O:291:ALA:HA	10:O:297:GLN:NE2	2.31	0.45
6:S:68:LEU:HD11	6:S:75:LEU:HG	1.99	0.45
3:C:221:HIS:ND1	3:C:222:PRO:HA	2.32	0.45
8:H:73:LEU:O	8:H:73:LEU:HD23	2.17	0.45
5:I:70:LEU:O	5:I:70:LEU:CG	2.64	0.45
3:P:103:TYR:CE2	15:P:505:PEE:H2	2.51	0.45
1:A:140:GLU:OE2	5:I:52:ARG:O	2.35	0.45
2:B:87:ARG:HB3	6:S:107:TRP:HE1	1.82	0.45
3:P:15:ASN:OD1	3:P:15:ASN:N	2.49	0.45
6:F:26:PHE:HD1	6:F:27:ASN:N	2.15	0.44
6:F:77:LYS:HA	6:F:80:TRP:CE2	2.52	0.44
13:P:503:4X9:H6	13:P:503:4X9:C16	2.47	0.44
5:R:175:PRO:CG	18:R:501:FES:S1	3.04	0.44
3:C:144:THR:O	3:C:148:ASN:HB2	2.17	0.44
5:E:45:VAL:HG13	9:J:28:ALA:HA	1.99	0.44
8:H:40:CYS:CB	8:H:54:CYS:SG	3.05	0.44
10:O:227:ARG:HA	10:O:227:ARG:NE	2.28	0.44
10:O:325:TYR:HD1	10:O:326:THR:N	2.14	0.44
8:U:73:LEU:HD23	8:U:73:LEU:O	2.17	0.44
1:A:84:ALA:HB1	1:A:100:LYS:O	2.18	0.44
1:A:149:VAL:HG23	1:A:425:PHE:CB	2.47	0.44
4:Q:31:GLN:O	4:Q:35:GLN:HG2	2.17	0.44
1:A:120:CYS:SG	1:A:122:LEU:HG	2.57	0.44
5:E:72:SER:HB2	3:P:168:PHE:HE2	1.81	0.44
8:U:40:CYS:O	8:U:43:ARG:HG3	2.18	0.44
2:B:164:HIS:NE2	2:B:316:TYR:OH	2.43	0.44
13:C:503:4X9:C6	13:C:503:4X9:H12	2.47	0.44
10:O:58:GLU:OE1	10:O:63:LEU:HA	2.16	0.44
10:O:85:ILE:O	11:V:70:LEU:HD21	2.17	0.44
10:O:151:ALA:HB2	11:V:76:VAL:HG21	1.98	0.44
2:B:31:ASN:ND2	2:B:225:ASN:OD1	2.51	0.44
2:B:34:VAL:HG11	2:B:386:ALA:HB1	1.99	0.44
2:B:213:HIS:N	2:B:214:PRO:CD	2.81	0.44
3:C:312:GLN:HG3	3:C:379:TRP:HZ3	1.82	0.44
10:O:70:ARG:NE	11:V:66:ALA:HB3	2.33	0.44
10:O:124:LEU:HD22	10:O:224:LEU:HD12	2.00	0.44
3:P:29:SER:O	3:P:32:ASN:HB2	2.18	0.44



Atom_1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:P:181:PHE:HA	3:P:184:ILE:HG22	2.00	0.44
4:Q:138:PRO:HD3	4:Q:149:PHE:CE2	2.53	0.44
2:B:83:PHE:CZ	6:S:107:TRP:CD1	3.06	0.44
3:C:103:TYR:HD1	3:C:325:PHE:CD2	2.35	0.44
3:C:220:PHE:CE2	13:C:503:4X9:H15	2.52	0.44
1:N:41:ILE:HG12	1:N:195:MET:HG2	1.99	0.44
3:P:219:PRO:HB2	3:P:221:HIS:O	2.17	0.44
1:N:162:PRO:HD2	1:N:234:CYS:SG	2.58	0.44
10:O:168:TYR:N	10:O:168:TYR:CD1	2.86	0.44
10:O:208:GLY:HA3	10:O:216:LEU:HD11	2.00	0.44
2:B:98:VAL:HG22	2:B:107:TYR:CD1	2.53	0.43
3:C:50:PHE:HE2	5:E:58:PHE:HB3	1.82	0.43
3:C:99:GLY:O	3:C:100:ARG:C	2.57	0.43
1:N:84:ALA:HB1	1:N:100:LYS:O	2.18	0.43
5:R:72:SER:O	5:R:92:ARG:NE	2.50	0.43
1:A:442:PHE:CD1	1:A:442:PHE:C	2.91	0.43
2:B:47:ILE:HD11	2:B:116:VAL:HG12	1.99	0.43
12:C:501:HEM:HBC2	12:C:501:HEM:CMC	2.43	0.43
3:P:26:ASN:ND2	3:P:208:PRO:HD2	2.33	0.43
4:Q:178:THR:HG21	8:U:15:ASP:HA	2.00	0.43
2:B:291:ALA:HA	2:B:297:GLN:NE2	2.33	0.43
3:C:358:TYR:HE1	3:C:362:ILE:HD11	1.83	0.43
4:Q:48:TYR:CE2	4:Q:65:ALA:HA	2.54	0.43
1:A:369:LEU:HD12	1:A:392:LEU:HD21	2.00	0.43
2:B:299:VAL:O	2:B:299:VAL:HG12	2.18	0.43
4:D:137:PRO:HA	4:D:149:PHE:HD2	1.83	0.43
1:N:252:HIS:CE1	1:N:325:VAL:HG22	2.54	0.43
5:R:75:GLU:OE1	5:R:75:GLU:HA	2.19	0.43
10:O:47:ILE:HD11	10:O:116:VAL:HG12	1.99	0.43
2:B:243:GLU:HA	2:B:424:MET:O	2.18	0.43
1:N:267:ASN:O	1:N:271:GLN:HG2	2.18	0.43
1:A:41:ILE:HD13	1:A:190:TYR:CE1	2.54	0.43
4:D:240:PRO:O	4:D:241:LYS:HG3	2.19	0.43
5:I:68:VAL:HG12	5:I:69:SER:N	2.34	0.43
1:A:192:ALA:N	1:A:193:PRO:HD2	2.34	0.43
2:B:26:PHE:CE1	2:B:391:SER:HA	2.54	0.43
3:C:77:TRP:CZ3	3:C:78:ILE:HG13	2.54	0.43
10:O:37:SER:HA	10:O:208:GLY:O	2.19	0.43
3:P:94:LEU:O	3:P:98:VAL:HG23	2.19	0.43
1:A:246:ASP:OD2	7:G:9:ARG:HA	2.18	0.43
1:A:430:GLN:O	1:A:431:LEU:C	2.56	0.42



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
3:C:187:PHE:HZ	3:P:184:ILE:CD1	2.31	0.42
6:F:20:TYR:O	6:F:21:TYR:C	2.57	0.42
1:N:192:ALA:N	1:N:193:PRO:HD2	2.33	0.42
3:P:201:HIS:NE2	13:P:503:4X9:H29	2.35	0.42
6:S:18:LYS:HA	6:S:83:TYR:CD2	2.54	0.42
1:A:185:TYR:CD1	1:A:189:HIS:CD2	3.07	0.42
3:P:11:MET:SD	3:P:11:MET:C	2.97	0.42
1:N:123:GLU:HB2	1:N:126:GLN:HB2	2.00	0.42
1:N:379:ILE:HG12	1:N:389:ARG:CD	2.49	0.42
3:P:75:TYR:CD2	5:R:57:GLN:HG2	2.55	0.42
5:R:141:HIS:O	5:R:141:HIS:CG	2.72	0.42
1:A:21:ASN:HB2	1:A:221:GLY:CA	2.49	0.42
2:B:42:ALA:O	2:B:113:ARG:NH1	2.49	0.42
4:Q:216:LEU:N	4:Q:217:PRO:HD2	2.35	0.42
2:B:169:ARG:HH22	2:B:238:LYS:HG2	1.78	0.42
2:B:312:PHE:HD1	2:B:313:ASN:N	2.17	0.42
1:N:204:GLU:O	1:N:205:HIS:C	2.57	0.42
3:C:21:LEU:HD23	3:C:220:PHE:CD2	2.53	0.42
10:O:299:VAL:HG21	10:O:340:ALA:HB2	2.01	0.42
3:P:174:THR:O	3:P:177:ARG:HG2	2.20	0.42
4:Q:105:ASN:HD22	16:Q:501:HEC:HMD3	1.85	0.42
8:U:44:VAL:HA	8:U:47:ARG:CZ	2.49	0.42
3:C:26:ASN:ND2	3:C:208:PRO:HD2	2.35	0.42
3:C:310:SER:HA	3:C:374:ASN:HD21	1.85	0.42
10:O:26:PHE:HZ	10:O:390:GLY:O	2.01	0.42
10:O:83:PHE:CE1	10:O:87:ARG:HG3	2.55	0.42
3:P:17:ALA:O	3:P:18:PHE:CD1	2.72	0.42
3:P:19:ILE:HG22	3:P:20:ASP:OD1	2.19	0.42
1:A:270:LEU:HD21	1:A:414:TYR:HD2	1.85	0.42
2:B:208:GLY:HA3	2:B:216:LEU:HD11	2.01	0.42
4:D:149:PHE:CD1	4:D:156:GLN:HB3	2.55	0.42
3:P:16:ASN:N	3:P:16:ASN:HD22	2.17	0.42
4:D:143:LEU:HD11	4:D:149:PHE:HB2	2.02	0.42
4:Q:126:TYR:CD1	4:Q:126:TYR:C	2.93	0.42
4:Q:182:VAL:HG12	4:Q:183:ALA:N	2.35	0.42
3:C:140:PHE:C	3:C:140:PHE:CD1	2.93	0.42
10:O:240:HIS:ND1	10:O:241:GLY:O	2.52	0.42
5:R:44:THR:HG21	9:W:24:ILE:HD13	2.02	0.42
1:A:46:ARG:NH1	1:A:93:GLU:OE2	2.49	0.41
2:B:51:ILE:HG12	2:B:204:MET:HG2	2.02	0.41
4:Q:118:ARG:HD2	4:Q:194:ALA:O	2.20	0.41


A + a 1	A + ama - D	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
4:Q:224:ARG:HG3	7:T:26:PHE:CE1	2.55	0.41
3:C:284:ILE:HD12	3:C:293:ALA:HB2	2.01	0.41
4:D:48:TYR:CE2	4:D:65:ALA:HA	2.55	0.41
1:N:280:TYR:HB3	1:N:307:PHE:CE2	2.55	0.41
10:O:96:LEU:C	11:V:69:SER:HB3	2.41	0.41
3:P:310:SER:HA	3:P:374:ASN:HD21	1.85	0.41
2:B:299:VAL:HG21	2:B:340:ALA:HB2	2.02	0.41
3:C:13:ILE:O	3:C:16:ASN:ND2	2.52	0.41
1:N:40:TRP:CZ2	1:N:377:GLU:HA	2.56	0.41
1:N:327:ASP:OD1	1:N:328:HIS:N	2.53	0.41
10:O:435:PHE:CD1	10:O:435:PHE:N	2.88	0.41
4:Q:237:TYR:HB2	6:S:60:PHE:CD1	2.54	0.41
5:R:113:GLU:OE1	5:R:115:SER:N	2.52	0.41
3:C:17:ALA:O	3:C:18:PHE:CD1	2.74	0.41
3:C:193:ALA:O	3:C:196:HIS:HB3	2.21	0.41
1:N:149:VAL:HG23	1:N:425:PHE:CB	2.50	0.41
4:Q:131:LEU:HD11	16:Q:501:HEC:HMB2	2.02	0.41
1:A:442:PHE:C	1:A:442:PHE:HD1	2.23	0.41
4:D:28:ARG:HA	4:D:31:GLN:HE21	1.85	0.41
4:D:198:HIS:ND1	4:D:198:HIS:C	2.73	0.41
11:V:70:LEU:O	11:V:70:LEU:CG	2.66	0.41
3:C:187:PHE:CZ	3:P:184:ILE:HD11	2.56	0.41
10:O:303:VAL:HG23	10:O:303:VAL:O	2.20	0.41
10:O:417:PHE:CD1	10:O:417:PHE:C	2.94	0.41
4:Q:110:PRO:HA	4:Q:111:PRO:HD2	1.97	0.41
7:T:34:ILE:N	7:T:35:PRO:HD2	2.35	0.41
1:A:37:VAL:HG23	1:A:199:ALA:HB2	2.03	0.41
1:A:41:ILE:HG12	1:A:195:MET:HG2	2.03	0.41
4:D:140:GLY:HA3	8:H:53:ASP:CB	2.42	0.41
7:G:79:ASN:ND2	8:H:52:GLU:OE2	2.53	0.41
10:O:172:LEU:HD13	10:O:316:TYR:CD2	2.56	0.41
3:P:186:PRO:HG2	12:P:501:HEM:HMC3	2.03	0.41
4:Q:204:MET:HE3	15:Q:506:PEE:O4	2.21	0.41
1:A:294:LEU:HG	1:A:307:PHE:CZ	2.56	0.41
3:C:30:TRP:NE1	15:C:505:PEE:O4	2.53	0.41
3:C:311:LYS:HE2	3:C:379:TRP:CD1	2.56	0.41
12:C:502:HEM:HBB2	12:C:502:HEM:HMB1	2.02	0.41
6:F:71:ARG:O	6:F:72:GLN:HB2	2.20	0.41
1:N:246:ASP:OD2	7:T:9:ARG:HA	2.20	0.41
10:O:86:THR:N	11:V:70:LEU:HD11	2.36	0.41
10:O:144:LEU:HB2	10:O:183:ILE:HG23	2.02	0.41



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
10:O:166:ALA:HB2	10:O:244:ILE:HG13	2.03	0.41
5:R:14:ARG:NH1	5:R:18:VAL:O	2.52	0.41
5:R:137:GLY:O	5:R:146:PRO:HD2	2.21	0.41
5:R:188:THR:HG23	5:R:192:MET:HB2	2.02	0.41
4:D:7:PRO:HA	4:D:8:PRO:HD3	1.92	0.41
5:R:82:PRO:HD2	5:R:85:LYS:HD3	2.03	0.41
8:U:47:ARG:CD	8:U:50:THR:CG2	2.99	0.41
2:B:209:LEU:HD23	2:B:375:SER:HB2	2.02	0.40
4:D:27:ARG:NH1	9:J:59:TYR:CE2	2.90	0.40
6:F:18:LYS:HG3	6:F:83:TYR:HD2	1.86	0.40
10:O:74:SER:CB	11:V:70:LEU:HD12	2.51	0.40
3:P:376:LEU:CD1	6:S:20:TYR:CD2	3.03	0.40
4:Q:60:GLU:OE2	9:W:59:TYR:HB3	2.20	0.40
2:B:365:LYS:HG2	2:B:399:LEU:HD23	2.03	0.40
4:D:179:MET:HB3	8:H:15:ASP:OD2	2.21	0.40
5:E:16:PRO:HA	5:E:19:LEU:HD12	2.03	0.40
6:F:18:LYS:HA	6:F:83:TYR:CD2	2.57	0.40
4:Q:204:MET:HE3	4:Q:204:MET:HB3	1.86	0.40
4:Q:211:MET:HG2	9:W:35:PHE:HE2	1.84	0.40
9:W:58:LYS:C	9:W:59:TYR:CD1	2.90	0.40
4:D:19:SER:HA	9:J:47:ASN:OD1	2.21	0.40
1:N:244:ARG:CZ	7:T:10:VAL:HB	2.51	0.40
10:O:109:VAL:HB	10:O:119:LEU:HD12	2.02	0.40
10:O:309:VAL:HA	10:O:325:TYR:O	2.20	0.40
3:P:17:ALA:O	3:P:18:PHE:HD1	2.04	0.40
3:P:276:PHE:CE1	3:P:277:ALA:HB2	2.57	0.40
8:U:40:CYS:O	8:U:43:ARG:CG	2.69	0.40
9:W:4:THR:HG22	9:W:5:LEU:H	1.86	0.40
1:A:26:ALA:O	1:A:198:ALA:HA	2.21	0.40
2:B:240:HIS:ND1	2:B:241:GLY:O	2.54	0.40
3:C:138:MET:HE2	3:C:138:MET:HA	2.03	0.40
3:C:186:PRO:O	3:C:189:ILE:HB	2.21	0.40
6:F:68:LEU:HD11	6:F:75:LEU:HG	2.04	0.40
10:O:29:LEU:CD2	10:O:30:PRO:HD2	2.47	0.40
10:O:89:ILE:CG1	11:V:70:LEU:HD22	2.52	0.40
6:S:77:LYS:HA	6:S:80:TRP:CE2	2.56	0.40
7:G:79:ASN:ND2	7:G:79:ASN:H	2.19	0.40
10:O:51:ILE:HD13	10:O:199:PHE:CE2	2.55	0.40

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



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:57:ASP:OD2	8:U:42:GLU:OE2[1_655]	1.73	0.47

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
1	А	442/480~(92%)	405 (92%)	35~(8%)	2~(0%)	29	67
1	N	442/480~(92%)	407 (92%)	33~(8%)	2~(0%)	29	67
2	В	420/453~(93%)	375~(89%)	44 (10%)	1 (0%)	47	80
3	С	372/379~(98%)	347 (93%)	23~(6%)	2(0%)	29	67
3	Р	368/379~(97%)	337 (92%)	30 (8%)	1 (0%)	41	74
4	D	238/265~(90%)	216 (91%)	21 (9%)	1 (0%)	34	71
4	Q	239/265~(90%)	218 (91%)	20 (8%)	1 (0%)	34	71
5	Е	71/274~(26%)	64 (90%)	7 (10%)	0	100	100
5	Ι	17/274~(6%)	12 (71%)	5 (29%)	0	100	100
5	R	194/274~(71%)	174 (90%)	19 (10%)	1 (0%)	29	67
6	F	$96/111 \ (86\%)$	87 (91%)	9 (9%)	0	100	100
6	S	97/111 ($87%$)	89 (92%)	8 (8%)	0	100	100
7	G	78/82~(95%)	67~(86%)	10 (13%)	1 (1%)	12	49
7	Т	72/82~(88%)	62 (86%)	10 (14%)	0	100	100
8	Н	63/91~(69%)	59 (94%)	4 (6%)	0	100	100
8	U	64/91~(70%)	61 (95%)	3 (5%)	0	100	100
9	J	56/64~(88%)	51 (91%)	5 (9%)	0	100	100
9	W	57/64~(89%)	51 (90%)	6 (10%)	0	100	100
10	Ο	417/453 (92%)	376 (90%)	41 (10%)	0	100	100
11	V	15/274~(6%)	12 (80%)	3 (20%)	0	100	100
All	All	3818/4946 (77%)	3470 (91%)	336 (9%)	12 (0%)	41	74



Mol	Chain	Res	Type
1	А	267	ASN
1	Ν	267	ASN
3	Р	107	TYR
5	R	177	PRO
3	С	107	TYR
2	В	394	PRO
7	G	74	PRO
1	N	260	PRO
4	D	240	PRO
1	А	260	PRO
3	С	266	PRO
4	Q	240	PRO

All (12) Ramachandran outliers are listed below:

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Perce	entiles
1	А	368/394~(93%)	350~(95%)	18 (5%)	25	59
1	Ν	367/394~(93%)	347~(95%)	20~(5%)	22	57
2	В	331/355~(93%)	309~(93%)	22~(7%)	16	51
3	С	322/327~(98%)	301 (94%)	21 (6%)	17	51
3	Р	318/327~(97%)	297~(93%)	21 (7%)	16	51
4	D	205/218~(94%)	196 (96%)	9 (4%)	28	63
4	Q	206/218~(94%)	196~(95%)	10 (5%)	25	59
5	Ε	63/228~(28%)	57~(90%)	6 (10%)	8	37
5	Ι	19/228~(8%)	13~(68%)	6 (32%)	0	2
5	R	168/228~(74%)	158 (94%)	10 (6%)	19	54
6	F	90/99~(91%)	82 (91%)	8 (9%)	9	40
6	S	$9\overline{1/99}~(92\%)$	84 (92%)	7(8%)	13	44
7	G	$\overline{71/72}\ (99\%)$	64 (90%)	7 (10%)	8	35
7	Т	66/72 (92%)	59 (89%)	7 (11%)	6	33



Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
8	Н	62/85~(73%)	54 (87%)	8 (13%)	4 24
8	U	63/85~(74%)	56~(89%)	7 (11%)	6 31
9	J	49/54~(91%)	45 (92%)	4 (8%)	11 42
9	W	49/54~(91%)	44 (90%)	5 (10%)	7 34
10	Ο	328/355~(92%)	304 (93%)	24 (7%)	14 46
11	V	15/228~(7%)	12 (80%)	3(20%)	1 8
All	All	3251/4120~(79%)	3028 (93%)	223 (7%)	15 49

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All (223) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	51	LYS
1	А	58	PHE
1	А	150	PHE
1	А	156	THR
1	А	185	TYR
1	А	186	LEU
1	А	203	LEU
1	А	206	ARG
1	А	230	THR
1	А	305	GLN
1	А	324	PHE
1	А	348	SER
1	А	388	ARG
1	А	397	SER
1	А	416	TYR
1	А	442	PHE
1	А	444	LEU
1	А	445	ARG
2	В	33	LEU
2	В	96	LEU
2	В	97	SER
2	В	99	THR
2	В	101	THR
2	В	108	THR
2	В	116	VAL
2	В	150	VAL
2	В	158	HIS
2	В	170	ASN
2	В	189	VAL



Mol	Chain	Res	Type
2	В	224	LEU
2	В	226	ILE
2	В	230	LEU
2	В	301	LYS
2	В	310	SER
2	В	312	PHE
2	В	316	TYR
2	В	324	PHE
2	В	325	TYR
2	В	417	PHE
2	В	436	ILE
3	С	10	LEU
3	С	11	MET
3	С	15	ASN
3	С	21	LEU
3	С	35	SER
3	С	63	PHE
3	С	64	SER
3	С	78	ILE
3	С	140	PHE
3	С	156	ILE
3	С	171	ASP
3	С	220	PHE
3	С	257	THR
3	С	268	ILE
3	С	276	PHE
3	С	296	PHE
3	С	310	SER
3	С	311	LYS
3	С	325	PHE
3	С	349	THR
3	С	358	TYR
4	D	3	LEU
4	D	17	LEU
4	D	19	SER
4	D	37	CYS
4	D	68	VAL
4	D	178	THR
4	D	182	VAL
4	D	216	LEU
4	D	232	SER
5	Е	7	VAL



Mol	Chain	Res	Type
5	Е	27	GLU
5	Е	36	SER
5	Е	42	THR
5	Е	54	VAL
5	Е	72	SER
6	F	20	TYR
6	F	26	PHE
6	F	40	ASN
6	F	78	GLU
6	F	83	TYR
6	F	91	GLU
6	F	94	LEU
6	F	95	LYS
7	G	9	ARG
7	G	17	SER
7	G	18	LEU
7	G	41	THR
7	G	46	LEU
7	G	59	TYR
7	G	60	THR
8	Н	14	VAL
8	Н	43	ARG
8	Н	44	VAL
8	Н	47	ARG
8	Н	49	GLN
8	Н	50	THR
8	Н	51	GLU
8	Н	55	THR
5	Ι	50	LEU
5	Ι	54	SER
5	Ι	56	ARG
5	Ι	65	VAL
5	Ι	67	SER
5	I	70	LEU
9	J	13	LEU
9	J	20	PHE
9	J	37	GLN
9	J	59	TYR
1	N	27	SER
1	N	51	LYS
1	N	58	PHE
1	Ν	150	PHE



Mol	Chain	Res	Type
1	N	156	THR
1	Ν	185	TYR
1	N	186	LEU
1	N	203	LEU
1	N	206	ARG
1	N	230	THR
1	N	305	GLN
1	N	324	PHE
1	N	327	ASP
1	N	348	SER
1	N	388	ARG
1	N	397	SER
1	N	416	TYR
1	N	442	PHE
1	N	444	LEU
1	N	445	ARG
10	0	33	LEU
10	0	96	LEU
10	0	97	SER
10	0	99	THR
10	0	101	THR
10	0	108	THR
10	0	116	VAL
10	0	126	VAL
10	0	150	VAL
10	0	158	HIS
10	0	170	ASN
10	0	189	VAL
10	0	224	LEU
10	0	226	ILE
10	0	230	LEU
10	0	301	LYS
10	0	310	SER
10	0	312	PHE
10	0	316	TYR
10	0	324	PHE
10	0	325	TYR
10	0	407	ASP
10	Ō	417	PHE
10	0	436	ILE
3	P	10	LEU
3	Р	11	MET



Mol	Chain	Res	Type
3	Р	15	ASN
3	Р	21	LEU
3	Р	35	SER
3	Р	63	PHE
3	Р	64	SER
3	Р	78	ILE
3	Р	90	PHE
3	Р	140	PHE
3	Р	156	ILE
3	Р	257	THR
3	Р	268	ILE
3	Р	276	PHE
3	Р	296	PHE
3	Р	310	SER
3	Р	311	LYS
3	Р	325	PHE
3	Р	349	THR
3	Р	358	TYR
3	Р	379	TRP
4	Q	3	LEU
4	Q	17	LEU
4	Q	37	CYS
4	Q	40	CYS
4	Q	68	VAL
4	Q	126	TYR
4	Q	178	THR
4	Q	182	VAL
4	Q	216	LEU
4	Q	232	SER
5	R	7	VAL
5	R	27	GLU
5	R	36	SER
5	R	42	THR
5	R	54	VAL
5	R	72	SER
5	R	113	GLU
5	R	136	ILE
5	R	140	THR
5	R	160	CYS
6	S	26	PHE
6	S	40	ASN
6	S	78	GLU



Mol	Chain	Res	Type
6	S	83	TYR
6	S	91	GLU
6	S	94	LEU
6	S	95	LYS
7	Т	9	ARG
7	Т	17	SER
7	Т	18	LEU
7	Т	41	THR
7	Т	46	LEU
7	Т	59	TYR
7	Т	60	THR
8	U	14	VAL
8	U	43	ARG
8	U	47	ARG
8	U	49	GLN
8	U	50	THR
8	U	51	GLU
8	U	55	THR
11	V	65	VAL
11	V	67	SER
11	V	70	LEU
9	W	4	THR
9	W	13	LEU
9	W	20	PHE
9	W	37	GLN
9	W	59	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	53	ASN
1	А	118	GLN
1	А	189	HIS
1	А	215	HIS
1	А	271	GLN
2	В	22	GLN
2	В	104	ASN
2	В	170	ASN
2	В	290	ASN
2	В	297	GLN
2	В	343	GLN
2	В	400	GLN



Mol	Chain	Res	Type
3	С	8	HIS
3	С	16	ASN
4	D	225	HIS
7	G	73	ASN
7	G	79	ASN
1	Ν	118	GLN
1	N	189	HIS
1	Ν	215	HIS
1	N	271	GLN
10	0	104	ASN
10	0	297	GLN
10	0	400	GLN
3	Р	16	ASN
4	Q	31	GLN
6	S	79	GLN

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5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

29 ligands are modelled in this entry.

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



Mal	Tuno	Chain	Dog	Link	В	Bond lengths			Bond angles		
	туре	Unam	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2	
19	GOL	R	502	-	$5,\!5,\!5$	0.33	0	$5,\!5,\!5$	0.45	0	
12	HEM	С	501	3	41,50,50	1.43	6 (14%)	45,82,82	1.96	12 (26%)	
15	PEE	С	505	-	48,48,50	1.27	4 (8%)	$51,\!53,\!55$	1.03	4 (7%)	
16	HEC	D	501	4	32,50,50	2.21	12 (37%)	24,82,82	2.74	9 (37%)	
16	HEC	Q	501	4	32,50,50	2.23	11 (34%)	24,82,82	2.29	6 (25%)	
14	PO4	С	504	-	4,4,4	0.95	0	6,6,6	0.43	0	
14	PO4	S	501	_	4,4,4	0.86	0	6,6,6	0.48	0	
14	PO4	D	503	-	4,4,4	0.88	0	6,6,6	0.67	0	
15	PEE	Q	506	-	50,50,50	1.30	4 (8%)	53,55,55	1.29	6 (11%)	
17	CDL	G	501	-	43,43,99	1.55	4 (9%)	49,55,111	1.57	8 (16%)	
12	HEM	Р	502	3	41,50,50	1.45	7 (17%)	45,82,82	1.94	15 (33%)	
12	HEM	Р	501	3	41,50,50	1.38	6 (14%)	45,82,82	1.96	16 (35%)	
14	PO4	Q	1002	-	4,4,4	0.89	0	6,6,6	0.48	0	
12	HEM	С	502	3	41,50,50	1.49	7 (17%)	45,82,82	1.69	9 (20%)	
17	CDL	D	505	-	38,38,99	1.27	3 (7%)	43,47,111	1.16	4 (9%)	
14	PO4	D	504	-	4,4,4	0.85	0	6,6,6	0.58	0	
14	PO4	Q	1001	-	4,4,4	0.87	0	6,6,6	0.47	0	
14	PO4	F	501	-	4,4,4	0.87	0	6,6,6	0.62	0	
13	4X9	Р	503	-	30,30,30	2.79	6 (20%)	43,44,44	1.90	8 (18%)	
17	CDL	Q	505	-	38,38,99	1.27	3 (7%)	43,47,111	1.19	5 (11%)	
17	CDL	Т	501	-	48,48,99	1.39	4 (8%)	54,60,111	1.18	4 (7%)	
14	PO4	D	502	-	4,4,4	0.76	0	6,6,6	0.63	0	
15	PEE	Р	505	-	48,48,50	1.34	4 (8%)	51,53,55	0.93	1 (1%)	
13	4X9	С	503	-	30,30,30	2.97	7 (23%)	43,44,44	1.43	3 (6%)	
14	PO4	N	501	-	4,4,4	0.72	0	6,6,6	0.98	0	
14	PO4	N	1001	-	4,4,4	0.81	0	6,6,6	0.78	0	
18	FES	R	501	5	0,4,4	-	-	-			
14	PO4	Е	501	-	4,4,4	0.69	0	6,6,6	0.81	0	
15	PEE	D	506	-	25,25,50	1.49	2 (8%)	28,30,55	1.46	4 (14%)	

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	PEE	С	505	-	1/1/4/8	25/52/52/54	-
19	GOL	R	502	-	-	2/4/4/4	-



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	PEE	Р	505	-	1/1/4/8	22/52/52/54	-
16	HEC	D	501	4	-	8/10/54/54	-
13	4X9	С	503	-	-	5/13/13/13	0/3/3/3
17	CDL	Т	501	-	-	28/57/57/110	-
12	HEM	С	502	3	-	6/12/54/54	-
12	HEM	С	501	3	-	4/12/54/54	-
16	HEC	Q	501	4	-	5/10/54/54	-
17	CDL	D	505	-	-	21/43/43/110	-
15	PEE	Q	506	-	1/1/4/8	24/54/54/54	-
17	CDL	G	501	-	-	25/52/52/110	-
18	FES	R	501	5	-	-	0/1/1/1
17	CDL	Q	505	-	-	13/43/43/110	-
13	4X9	Р	503	-	-	3/13/13/13	0/3/3/3
12	HEM	Р	502	3	-	7/12/54/54	-
12	HEM	Р	501	3	-	8/12/54/54	-
15	PEE	D	506	-	1/1/4/8	13/29/29/54	-

All (90) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	Р	503	4X9	C19-C20	8.52	1.50	1.38
13	С	503	4X9	C17-C18	8.10	1.50	1.40
13	С	503	4X9	C19-C20	7.70	1.49	1.38
13	С	503	4X9	C17-C22	7.65	1.49	1.40
16	D	501	HEC	C3C-C2C	6.89	1.47	1.40
13	Р	503	4X9	C17-C18	6.76	1.48	1.40
13	Р	503	4X9	C17-C22	6.73	1.48	1.40
16	Q	501	HEC	C3C-C2C	6.57	1.47	1.40
13	С	503	4X9	C18-C19	5.96	1.49	1.39
17	G	501	CDL	OA6-CA5	5.25	1.47	1.35
16	Q	501	HEC	C2B-C3B	5.22	1.46	1.40
16	D	501	HEC	C2B-C3B	5.06	1.46	1.40
15	D	506	PEE	O3-C30	5.00	1.48	1.33
17	Т	501	CDL	OB6-CB5	4.95	1.48	1.34
17	G	501	CDL	OB6-CB5	4.89	1.48	1.34
17	Q	505	CDL	OA6-CA5	4.87	1.48	1.34
17	G	501	CDL	OB8-CB7	4.85	1.47	1.33
15	Р	505	PEE	O2-C10	4.84	1.48	1.34
15	Q	506	PEE	O2-C10	4.78	1.47	1.34



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	Р	503	4X9	O28-C18	-4.78	1.25	1.37
17	D	505	CDL	OA6-CA5	4.76	1.47	1.34
17	Т	501	CDL	OB8-CB7	4.73	1.47	1.33
15	Р	505	PEE	O3-C30	4.70	1.47	1.33
17	Т	501	CDL	OA6-CA5	4.68	1.45	1.35
15	С	505	PEE	O2-C10	4.66	1.47	1.34
13	С	503	4X9	O28-C18	-4.56	1.26	1.37
17	Q	505	CDL	OA8-CA7	4.54	1.46	1.33
15	D	506	PEE	O2-C10	4.53	1.47	1.34
13	Р	503	4X9	C18-C19	4.50	1.46	1.39
17	D	505	CDL	OA8-CA7	4.49	1.46	1.33
15	Q	506	PEE	O3-C30	4.28	1.45	1.33
12	С	501	HEM	C1B-NB	-4.22	1.33	1.40
15	С	505	PEE	O3-C30	4.12	1.45	1.33
12	С	502	HEM	C1B-NB	-4.10	1.33	1.40
15	Q	506	PEE	C18-C19	3.87	1.54	1.31
15	С	505	PEE	C18-C19	3.81	1.53	1.31
15	Р	505	PEE	C39-C38	3.80	1.53	1.31
15	Р	505	PEE	C18-C19	3.80	1.53	1.31
15	С	505	PEE	C39-C38	3.77	1.53	1.31
15	Q	506	PEE	C39-C38	3.73	1.53	1.31
12	Р	502	HEM	C1B-NB	-3.67	1.34	1.40
12	Р	501	HEM	C1B-NB	-3.63	1.34	1.40
16	D	501	HEC	C4B-C3B	3.39	1.49	1.43
12	С	502	HEM	C4D-ND	-3.38	1.34	1.40
16	Q	501	HEC	C2A-C3A	3.30	1.47	1.37
12	С	501	HEM	C4D-ND	-3.28	1.34	1.40
16	D	501	HEC	C2A-C3A	3.27	1.47	1.37
13	Р	503	4X9	C19-CL	3.23	1.79	1.72
16	Q	501	HEC	C3D-C2D	3.19	1.47	1.37
16	Q	501	HEC	C3A-C4A	3.11	1.49	1.42
17	G	501	CDL	OA8-CA7	3.01	1.48	1.33
16	Q	501	HEC	C2A-C1A	3.00	1.49	1.42
16	Q	501	HEC	C4B-C3B	2.97	1.48	1.43
12	Р	501	HEM	C4D-ND	-2.97	1.35	1.40
16	D	501	HEC	C3D-C2D	2.96	1.46	1.37
12	Р	502	HEM	FE-NB	2.93	2.11	1.96
13	С	503	4X9	C19-CL	2.88	1.79	1.72
12	С	502	HEM	C4B-NB	-2.82	1.33	1.38
16	D	501	HEC	C1C-CHC	2.73	1.48	1.41
12	С	502	HEM	C1D-ND	-2.73	1.33	1.38
12	P	$50\overline{2}$	HEM	C4D-ND	-2.73	1.35	1.40



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
12	Р	501	HEM	CHB-C1B	2.68	1.41	1.35
16	D	501	HEC	C3A-C4A	2.67	1.48	1.42
12	Р	501	HEM	FE-NB	2.65	2.10	1.96
16	D	501	HEC	C3C-C4C	2.64	1.47	1.43
16	Q	501	HEC	C1B-CHB	2.62	1.48	1.41
12	С	501	HEM	FE-NB	2.59	2.09	1.96
17	Q	505	CDL	PB2-OB5	2.58	1.64	1.54
12	С	501	HEM	C4B-NB	-2.58	1.33	1.38
12	Р	501	HEM	C4B-NB	-2.56	1.33	1.38
12	С	502	HEM	C3B-C4B	2.55	1.50	1.44
12	Р	502	HEM	C4B-NB	-2.48	1.33	1.38
16	Q	501	HEC	C1C-CHC	2.48	1.47	1.41
17	Т	501	CDL	OA8-CA7	2.47	1.45	1.33
17	D	505	CDL	PB2-OB5	2.45	1.64	1.54
16	Q	501	HEC	C3C-C4C	2.42	1.47	1.43
12	С	502	HEM	FE-NB	2.36	2.08	1.96
16	Q	501	HEC	C1D-CHD	2.35	1.47	1.41
13	С	503	4X9	O3-C1	2.33	1.44	1.31
12	Р	501	HEM	C1D-C2D	2.32	1.49	1.44
16	D	501	HEC	C1B-CHB	2.30	1.47	1.41
16	D	501	HEC	C1D-CHD	2.29	1.47	1.41
12	Р	502	HEM	C1D-ND	-2.27	1.34	1.38
12	Р	502	HEM	C4D-C3D	2.18	1.48	1.45
12	С	501	HEM	C1D-ND	-2.08	1.34	1.38
16	D	501	HEC	C4D-CHA	2.06	1.46	1.41
12	С	501	HEM	CHB-C1B	2.05	1.40	1.35
12	С	502	HEM	C3C-C2C	-2.05	1.37	1.40
12	Р	502	HEM	C1D-C2D	2.01	1.48	1.44
16	D	501	HEC	C2A-C1A	2.01	1.47	1.42

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All (114) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
13	Р	503	4X9	C20-C19-C18	-7.02	118.33	122.79
16	Q	501	HEC	C1D-C2D-C3D	-6.86	102.23	107.00
16	D	501	HEC	CBA-CAA-C2A	6.42	123.43	112.60
16	D	501	HEC	C1D-C2D-C3D	-6.10	102.75	107.00
16	D	501	HEC	CMC-C2C-C3C	5.18	131.91	125.82
15	D	506	PEE	O2-C10-C11	5.07	122.42	111.50
13	Р	503	4X9	C20-C19-CL	5.04	128.27	121.14
12	С	501	HEM	C1B-NB-C4B	5.02	110.26	105.07
12	Р	502	HEM	CAD-C3D-C4D	4.87	133.17	124.66



Mol	Chain	\mathbf{Res}	Type	Atoms	Z	Observed(°)	Ideal(°)
12	P	501	HEM	CHC-C4B-NB	4.84	129.69	124.43
13	C	503	4X9	C20-C19-C18	-4.82	119.73	122.79
17	G	501	CDL	OA6-CA5-C11	4.81	119.95	111.09
12	Р	501	HEM	C1B-NB-C4B	4.69	109.92	105.07
12	С	501	HEM	CBA-CAA-C2A	-4.63	104.71	112.62
15	Q	506	PEE	C2-O2-C10	4.63	129.18	117.79
12	P	502	HEM	CHD-C1D-ND	4.51	129.33	124.43
17	G	501	CDL	OB6-CB5-C51	4.51	123.37	110.80
16	Q	501	HEC	CMB-C2B-C3B	4.46	131.07	125.82
12	С	502	HEM	C1B-NB-C4B	4.36	109.57	105.07
17	Т	501	CDL	OA6-CA5-C11	4.22	118.85	111.09
13	Р	503	4X9	C18-C19-CL	-4.18	113.39	118.08
16	D	501	HEC	CMB-C2B-C3B	4.08	130.62	125.82
17	D	505	CDL	OA6-CA5-C11	3.98	120.08	111.50
17	G	501	CDL	OB8-CB7-C71	3.95	124.29	111.91
12	Р	502	HEM	CHC-C4B-NB	3.86	128.63	124.43
12	Р	501	HEM	CMD-C2D-C1D	3.81	130.85	125.04
16	Q	501	HEC	CMC-C2C-C3C	3.80	130.29	125.82
15	Q	506	PEE	O2-C10-C11	3.80	119.68	111.50
17	Q	505	CDL	OA6-CA5-C11	3.76	119.61	111.50
17	Т	501	CDL	OB6-CB5-C51	3.74	119.55	111.50
12	С	501	HEM	CHC-C4B-NB	3.71	128.47	124.43
12	С	501	HEM	CHB-C1B-NB	3.67	128.92	124.38
13	С	503	4X9	C18-C17-C22	-3.60	116.06	119.57
12	Р	502	HEM	CBA-CAA-C2A	-3.55	106.57	112.62
12	С	502	HEM	CHA-C4D-ND	3.45	128.65	124.38
12	С	502	HEM	CHC-C4B-NB	3.44	128.17	124.43
17	D	505	CDL	OA8-CA7-C31	3.42	122.63	111.91
12	С	502	HEM	CHD-C1D-ND	3.41	128.13	124.43
12	Р	502	HEM	C1B-NB-C4B	3.38	108.56	105.07
15	Р	505	PEE	O2-C10-C11	3.35	118.73	111.50
16	D	501	HEC	CAA-CBA-CGA	-3.29	104.54	113.76
12	Р	501	HEM	CHA-C4D-ND	3.24	128.39	124.38
13	С	503	4X9	C22-N30-C20	3.21	124.37	119.64
12	С	501	HEM	CHD-C1D-ND	3.19	127.90	124.43
15	D	506	PEE	O3-C30-C31	3.14	121.75	111.91
12	С	502	HEM	CHA-C4D-C3D	-3.09	119.52	125.33
13	Р	503	4X9	C29-C22-C17	-3.07	117.85	122.33
12	P	502	HEM	CHB-C1B-NB	3.03	128.12	124.38
13	Р	503	4X9	C29-C22-N30	3.03	121.18	116.49
17	G	501	CDL	CA6-OA8-CA7	2.97	124.55	117.10
15	С	505	PEE	O2-C10-C11	2.96	117.88	111.50



4D	6T
4D	υI

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	$Ideal(^{o})$
15	С	505	PEE	O3-C30-C31	2.94	121.15	111.91
15	Q	506	PEE	O3-C3-C2	2.93	116.95	108.43
12	С	501	HEM	CHD-C1D-C2D	-2.91	120.43	124.98
17	Т	501	CDL	OB8-CB7-C71	2.87	120.92	111.91
12	Р	502	HEM	CAD-C3D-C2D	-2.81	122.65	127.88
17	Q	505	CDL	OA8-CA7-C31	2.80	120.70	111.91
12	Р	501	HEM	CHB-C1B-NB	2.80	127.84	124.38
17	G	501	CDL	OB8-CB6-CB4	2.79	116.56	108.43
17	D	505	CDL	OA8-CA7-OA9	-2.73	116.71	123.59
12	С	502	HEM	CHD-C1D-C2D	-2.71	120.74	124.98
12	Р	501	HEM	CHD-C1D-C2D	-2.70	120.76	124.98
15	Q	506	PEE	O3-C30-C31	2.69	120.34	111.91
15	D	506	PEE	O2-C10-O4	-2.67	117.25	123.70
13	Р	503	4X9	C22-N30-C20	2.66	123.56	119.64
17	Т	501	CDL	OA6-CA5-OA7	-2.62	117.76	122.96
12	Р	501	HEM	CHA-C4D-C3D	-2.61	120.43	125.33
17	G	501	CDL	OB6-CB5-OB7	-2.59	117.44	123.70
12	С	502	HEM	CHB-C1B-NB	2.59	127.58	124.38
12	Р	501	HEM	CHD-C1D-ND	2.58	127.24	124.43
15	С	505	PEE	O3-C30-O5	-2.56	117.12	123.59
17	Q	505	CDL	OB4-PB2-OB3	2.55	120.68	110.68
17	Q	505	CDL	OA8-CA7-OA9	-2.55	117.16	123.59
12	С	501	HEM	CMB-C2B-C1B	2.50	128.85	125.04
12	С	501	HEM	CAB-C3B-C2B	-2.50	120.36	128.60
12	Р	501	HEM	O2D-CGD-CBD	2.49	122.04	114.03
12	Р	501	HEM	CAD-CBD-CGD	-2.48	108.27	113.60
17	G	501	CDL	OB8-CB7-OB9	-2.46	117.40	123.59
16	D	501	HEC	CAD-CBD-CGD	-2.44	106.91	113.76
16	Q	501	HEC	CAD-CBD-CGD	-2.42	106.97	113.76
12	С	501	HEM	CAD-C3D-C4D	2.38	128.81	124.66
12	Р	501	HEM	O2A-CGA-CBA	2.37	121.65	114.03
12	Р	502	HEM	CHA-C4D-ND	2.35	127.28	124.38
12	Р	501	HEM	CAD-C3D-C4D	2.31	128.70	124.66
16	D	501	HEC	C4C-C3C-C2C	-2.31	103.86	106.35
12	Р	502	HEM	C4D-ND-C1D	2.30	107.45	105.07
17	G	501	CDL	OA8-CA7-C31	2.30	122.39	112.38
12	Р	501	HEM	C4A-C3A-C2A	2.28	108.58	107.00
12	Р	502	HEM	CMD-C2D-C1D	2.26	128.48	125.04
17	Q	505	CDL	PB2-OB2-CB2	2.24	124.48	118.30
16	Q	501	HEC	CBA-CAA-C2A	2.24	116.38	112.60
12	Р	502	HEM	CHD-C1D-C2D	-2.23	121.50	124.98
12	С	502	HEM	CBA-CAA-C2A	-2.22	108.84	112.62



Mol	Chain	\mathbf{Res}	Type	Atoms		$Observed(^{o})$	$ $ Ideal $(^{o})$ $ $
12	Р	501	HEM	CMA-C3A-C4A	-2.16	125.14	128.46
12	С	501	HEM	CHA-C4D-C3D	-2.16	121.27	125.33
12	С	502	HEM	O2A-CGA-CBA	2.14	120.91	114.03
17	D	505	CDL	OB4-PB2-OB3	2.12	119.00	110.68
12	Р	502	HEM	CMA-C3A-C4A	-2.12	125.20	128.46
13	Р	503	4X9	C26-C20-C19	-2.12	121.79	123.01
12	Р	501	HEM	C4B-C3B-C2B	-2.11	105.44	107.11
12	Р	502	HEM	C3C-C4C-NC	-2.11	106.97	110.94
15	Q	506	PEE	O3-C30-O5	-2.10	118.29	123.59
12	Р	502	HEM	CHB-C1B-C2B	-2.10	120.92	126.72
13	Р	503	4X9	O28-C18-C17	2.09	124.34	119.56
15	Q	506	PEE	C40-C39-C38	-2.09	108.67	124.73
15	D	506	PEE	O3-C30-O5	-2.09	118.33	123.59
16	D	501	HEC	O2A-CGA-CBA	2.08	120.73	114.03
16	Q	501	HEC	CAA-CBA-CGA	-2.06	107.97	113.76
16	D	501	HEC	CMA-C3A-C2A	2.06	128.82	124.94
12	Р	502	HEM	C4B-C3B-C2B	-2.04	105.50	107.11
12	Р	501	HEM	C1D-C2D-C3D	-2.04	104.81	106.96
12	С	501	HEM	C4B-CHC-C1C	2.03	125.23	122.56
12	С	501	HEM	CMB-C2B-C3B	-2.02	123.37	128.30
15	C	505	PEE	C3-C2-C1	-2.00	107.06	111.79

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
15	С	505	PEE	C2
15	D	506	PEE	C2
15	Р	505	PEE	C2
15	Q	506	PEE	C2

All (219) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	С	502	HEM	C2D-C3D-CAD-CBD
12	С	502	HEM	C4D-C3D-CAD-CBD
12	Р	501	HEM	C1A-C2A-CAA-CBA
12	Р	501	HEM	C3A-C2A-CAA-CBA
15	D	506	PEE	C1-O3P-P-O2P
15	D	506	PEE	C5-C4-O4P-P
15	D	506	PEE	O4P-C4-C5-N
15	Р	505	PEE	O4P-C4-C5-N
15	Q	506	PEE	C17-C18-C19-C20



Mol	Chain	Res	Type	Atoms
15	Q	506	PEE	C1-O3P-P-O2P
16	D	501	HEC	C1A-C2A-CAA-CBA
16	D	501	HEC	C2D-C3D-CAD-CBD
16	D	501	HEC	C4D-C3D-CAD-CBD
16	Q	501	HEC	C1A-C2A-CAA-CBA
16	Q	501	HEC	C3A-C2A-CAA-CBA
17	D	505	CDL	CB2-OB2-PB2-OB4
17	D	505	CDL	CB2-OB2-PB2-OB5
17	G	501	CDL	O1-C1-CB2-OB2
17	G	501	CDL	CA2-C1-CB2-OB2
17	G	501	CDL	CA3-OA5-PA1-OA4
17	G	501	CDL	CB4-CB3-OB5-PB2
17	G	501	CDL	C51-CB5-OB6-CB4
17	Q	505	CDL	CB2-OB2-PB2-OB3
17	Q	505	CDL	CB2-OB2-PB2-OB4
17	Q	505	CDL	CB2-OB2-PB2-OB5
17	Т	501	CDL	O1-C1-CB2-OB2
17	Т	501	CDL	CA3-OA5-PA1-OA3
17	Т	501	CDL	CB2-OB2-PB2-OB3
17	Т	501	CDL	CB2-OB2-PB2-OB5
17	Т	501	CDL	CB3-OB5-PB2-OB2
17	Т	501	CDL	CB3-OB5-PB2-OB3
17	Т	501	CDL	CB3-OB5-PB2-OB4
19	R	502	GOL	C1-C2-C3-O3
17	Т	501	CDL	C11-CA5-OA6-CA4
17	Q	505	CDL	OA9-CA7-OA8-CA6
17	Т	501	CDL	OA7-CA5-OA6-CA4
17	G	501	CDL	OB7-CB5-OB6-CB4
17	Q	505	CDL	C31-CA7-OA8-CA6
17	G	501	CDL	C11-CA5-OA6-CA4
15	С	505	PEE	C37-C38-C39-C40
12	Р	502	HEM	C4D-C3D-CAD-CBD
17	G	501	CDL	O1-C1-CA2-OA2
17	Т	501	CDL	OA9-CA7-OA8-CA6
17	Т	501	CDL	C31-CA7-OA8-CA6
13	С	503	4X9	F23-C1-O3-C4
17	D	505	CDL	CA2-C1-CB2-OB2
17	G	501	CDL	CB2-C1-CA2-OA2
15	D	506	PEE	C31-C30-O3-C3
15	D	506	PEE	O5-C30-O3-C3
17	G	501	CDL	OA6-CA4-CA6-OA8
17	D	505	CDL	C31-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
15	Р	505	PEE	C10-C11-C12-C13
15	Q	506	PEE	C10-C11-C12-C13
17	Q	505	CDL	CA7-C31-C32-C33
17	Т	501	CDL	CB4-CB3-OB5-PB2
15	Р	505	PEE	C30-C31-C32-C33
12	С	502	HEM	C3D-CAD-CBD-CGD
15	Р	505	PEE	C11-C10-O2-C2
17	G	501	CDL	OA7-CA5-OA6-CA4
17	D	505	CDL	O1-C1-CB2-OB2
15	Р	505	PEE	C37-C38-C39-C40
12	Р	502	HEM	C2D-C3D-CAD-CBD
15	D	506	PEE	C1-O3P-P-O4P
15	D	506	PEE	C4-O4P-P-O3P
15	Р	505	PEE	C1-O3P-P-O4P
17	G	501	CDL	CA3-OA5-PA1-OA2
17	Т	501	CDL	CA2-OA2-PA1-OA5
17	Т	501	CDL	CA2-C1-CB2-OB2
15	Р	505	PEE	O4-C10-O2-C2
15	С	505	PEE	C21-C22-C23-C24
15	Q	506	PEE	C31-C32-C33-C34
17	D	505	CDL	OA9-CA7-OA8-CA6
15	С	505	PEE	C30-C31-C32-C33
13	С	503	4X9	F24-C1-O3-C4
15	Q	506	PEE	C22-C23-C24-C25
15	С	505	PEE	C20-C21-C22-C23
15	Р	505	PEE	C13-C14-C15-C16
15	Q	506	PEE	C32-C33-C34-C35
15	С	505	PEE	C15-C16-C17-C18
15	Р	505	PEE	C34-C35-C36-C37
15	Q	506	PEE	C21-C22-C23-C24
15	Q	506	PEE	C11-C12-C13-C14
17	Q	505	CDL	C38-C39-C40-C41
15	С	505	PEE	C42-C43-C44-C45
15	Р	505	PEE	C42-C43-C44-C45
17	Т	501	CDL	C73-C74-C75-C76
15	Q	506	PEE	O4P-C4-C5-N
15	Р	505	PEE	C32-C33-C34-C35
15	Q	506	PEE	C34-C35-C36-C37
17	Т	501	CDL	C52-C53-C54-C55
12	Р	501	HEM	C2A-CAA-CBA-CGA
13	С	503	4X9	F25-C1-O3-C4
17	D	505	CDL	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
15	Р	505	PEE	C1-C2-C3-O3
17	Т	501	CDL	C72-C73-C74-C75
15	Q	506	PEE	C19-C20-C21-C22
15	Q	506	PEE	C39-C40-C41-C42
15	С	505	PEE	C40-C41-C42-C43
17	Q	505	CDL	C34-C35-C36-C37
17	G	501	CDL	C31-CA7-OA8-CA6
17	D	505	CDL	CA4-CA3-OA5-PA1
15	D	506	PEE	C11-C10-O2-C2
17	D	505	CDL	C37-C38-C39-C40
15	Р	505	PEE	C16-C17-C18-C19
15	С	505	PEE	O4-C10-O2-C2
15	С	505	PEE	C10-C11-C12-C13
17	Т	501	CDL	CB7-C71-C72-C73
17	G	501	CDL	C71-CB7-OB8-CB6
15	С	505	PEE	C11-C10-O2-C2
17	D	505	CDL	C11-CA5-OA6-CA4
15	Р	505	PEE	O2-C2-C3-O3
17	Q	505	CDL	C36-C37-C38-C39
15	С	505	PEE	C19-C20-C21-C22
15	D	506	PEE	O4-C10-O2-C2
17	G	501	CDL	OB5-CB3-CB4-CB6
16	Q	501	HEC	C3D-CAD-CBD-CGD
15	Р	505	PEE	C12-C13-C14-C15
17	G	501	CDL	OB9-CB7-OB8-CB6
15	Р	505	PEE	C23-C24-C25-C26
15	Q	506	PEE	C42-C43-C44-C45
15	С	505	PEE	C31-C30-O3-C3
15	Р	505	PEE	C1-C2-O2-C10
17	D	505	CDL	CB2-OB2-PB2-OB3
15	D	506	PEE	O3P-C1-C2-O2
17	D	505	CDL	OA5-CA3-CA4-OA6
12	P	501	HEM	C3D-CAD-CBD-CGD
17	D	505	CDL	OA7-CA5-OA6-CA4
15	C	505	PEE	C22-C23-C24-C25
17	D	505	CDL	C36-C37-C38-C39
15	D	506	PEE	O3P-C1-C2-C3
15	Q	506	PEE	O3P-C1-C2-C3
17	D	505	CDL	OA5-CA3-CA4-CA6
17	Т	501	CDL	C51-C52-C53-C54
15	Р	505	PEE	C33-C34-C35-C36
15	Р	505	PEE	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
17	Q	505	CDL	C33-C34-C35-C36
12	С	501	HEM	C3D-CAD-CBD-CGD
17	G	501	CDL	CA3-CA4-CA6-OA8
15	С	505	PEE	C1-O3P-P-O4P
15	Q	506	PEE	C1-O3P-P-O4P
19	R	502	GOL	O2-C2-C3-O3
17	G	501	CDL	OB5-CB3-CB4-OB6
15	С	505	PEE	O5-C30-O3-C3
17	Т	501	CDL	C75-C76-C77-C78
17	G	501	CDL	OA9-CA7-OA8-CA6
15	С	505	PEE	O3P-C1-C2-C3
15	С	505	PEE	C12-C13-C14-C15
16	D	501	HEC	C2A-CAA-CBA-CGA
15	Q	506	PEE	C1-C2-O2-C10
13	Р	503	4X9	F24-C1-O3-C4
17	D	505	CDL	C33-C34-C35-C36
12	С	501	HEM	C4B-C3B-CAB-CBB
17	Т	501	CDL	C71-CB7-OB8-CB6
17	G	501	CDL	C72-C73-C74-C75
15	D	506	PEE	C4-O4P-P-O1P
15	Р	505	PEE	C1-O3P-P-O1P
15	Q	506	PEE	C1-O3P-P-O1P
17	Т	501	CDL	CA2-OA2-PA1-OA4
15	Р	505	PEE	C5-C4-O4P-P
15	С	505	PEE	O3P-C1-C2-O2
17	G	501	CDL	OA5-CA3-CA4-OA6
15	Q	506	PEE	C40-C41-C42-C43
17	Т	501	CDL	OB9-CB7-OB8-CB6
15	С	505	PEE	C1-C2-O2-C10
17	Т	501	CDL	OA5-CA3-CA4-CA6
$1\overline{7}$	Т	501	CDL	OA5-CA3-CA4-OA6
15	Q	506	PEE	C41-C42-C43-C44
15	C	505	PEE	C4-O4P-P-O3P
17	G	501	CDL	CB2-OB2-PB2-OB5
17	Q	505	CDL	CA3-OA5-PA1-OA2
17	D	505	CDL	C34-C35-C36-C37
15	Q	506	PEE	C1-C2-C3-O3
17	Q	505	CDL	C37-C38-C39-C40
15	C	505	PEE	O4P-C4-C5-N
12	С	502	HEM	CAA-CBA-CGA-O1A
12	Р	502	HEM	CAA-CBA-CGA-O1A
12	Р	502	HEM	C3D-CAD-CBD-CGD

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Mol	Chain	Res	Type	Atoms
17	Т	501	CDL	C71-C72-C73-C74
13	С	503	4X9	C5-C4-O3-C1
17	D	505	CDL	CA3-CA4-CA6-OA8
15	С	505	PEE	C16-C17-C18-C19
15	Р	505	PEE	C19-C20-C21-C22
17	G	501	CDL	C1-CA2-OA2-PA1
13	С	503	4X9	C9-C4-O3-C1
12	С	502	HEM	CAA-CBA-CGA-O2A
12	Р	502	HEM	CAA-CBA-CGA-O2A
15	С	505	PEE	C36-C37-C38-C39
15	Q	506	PEE	C13-C14-C15-C16
12	Р	501	HEM	CAA-CBA-CGA-O2A
12	Р	501	HEM	CAD-CBD-CGD-O2D
17	G	501	CDL	OA5-CA3-CA4-CA6
16	D	501	HEC	CAD-CBD-CGD-O2D
15	Q	506	PEE	O2-C2-C3-O3
17	Т	501	CDL	C53-C54-C55-C56
16	D	501	HEC	CAD-CBD-CGD-O1D
15	D	506	PEE	C32-C33-C34-C35
17	G	501	CDL	C74-C75-C76-C77
12	С	501	HEM	CAD-CBD-CGD-O2D
12	Р	501	HEM	CAA-CBA-CGA-O1A
13	Р	503	4X9	F25-C1-O3-C4
17	D	505	CDL	C35-C36-C37-C38
12	Р	501	HEM	CAD-CBD-CGD-O1D
12	Р	502	HEM	CAD-CBD-CGD-O2D
12	Р	502	HEM	CAD-CBD-CGD-O1D
16	Q	501	HEC	CAD-CBD-CGD-O2D
12	С	501	HEM	CAD-CBD-CGD-O1D
16	Q	501	HEC	CAD-CBD-CGD-O1D
15	Q	506	PEE	C38-C39-C40-C41
15	С	505	PEE	C13-C14-C15-C16
17	D	505	CDL	C12-C11-CA5-OA6
15	С	505	PEE	C1-O3P-P-O1P
17	Q	505	CDL	CA3-OA5-PA1-OA3
16	D	501	HEC	CAA-CBA-CGA-O2A
16	D	501	HEC	CAA-CBA-CGA-O1A
13	Р	503	4X9	F23-C1-O3-C4
15	Q	506	PEE	C18-C19-C20-C21
12	C	502	HEM	CAD-CBD-CGD-O1D
17	Т	501	\overline{CDL}	C74-C75-C76-C77
17	D	505	CDL	C12-C11-CA5-OA7

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There are no ring outliers.

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	С	501	HEM	4	0
15	С	505	PEE	1	0
16	D	501	HEC	12	0
16	Q	501	HEC	10	0
15	Q	506	PEE	3	0
12	Р	502	HEM	3	0
12	Р	501	HEM	7	0
12	С	502	HEM	6	0
13	Р	503	4X9	5	0
17	Q	505	CDL	1	0
17	Т	501	CDL	1	0
15	Р	505	PEE	1	0
13	С	503	4X9	6	0
18	R	501	FES	3	0

14 monomers are involved in 62 short contacts:

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.













































5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	$\langle RSRZ \rangle$	# RSRZ > 2	$\mathbf{OWAB}(\mathbf{\AA}^2)$	Q < 0.9
1	А	444/480~(92%)	-0.14	9 (2%) 65 48	92, 150, 191, 255	0
1	Ν	444/480~(92%)	-0.33	7 (1%) 72 55	87, 132, 176, 243	0
2	В	422/453~(93%)	0.13	29 (6%) 16 9	108, 157, 200, 247	0
3	С	374/379~(98%)	-0.50	0 100 100	77, 103, 137, 225	0
3	Р	370/379~(97%)	-0.44	1 (0%) 94 88	79, 112, 148, 183	0
4	D	240/265~(90%)	-0.31	2 (0%) 86 73	92, 121, 153, 178	0
4	Q	241/265~(90%)	-0.10	6 (2%) 57 39	86, 131, 168, 211	0
5	Е	73/274~(26%)	-0.36	1 (1%) 75 59	93, 130, 158, 170	0
5	Ι	21/274~(7%)	0.63	1 (4%) 30 18	146, 192, 220, 228	0
5	R	196/274~(71%)	-0.15	2 (1%) 82 69	91, 150, 193, 230	0
6	F	98/111 (88%)	-0.44	2 (2%) 65 48	91, 124, 157, 171	0
6	S	99/111 (89%)	-0.44	0 100 100	85, 122, 168, 182	0
7	G	80/82~(97%)	-0.29	1 (1%) 77 61	88, 119, 189, 293	0
7	Т	74/82~(90%)	-0.40	2 (2%) 54 36	83, 124, 181, 200	0
8	Н	65/91~(71%)	-0.48	0 100 100	103, 136, 171, 223	0
8	U	66/91~(72%)	0.09	5 (7%) 13 7	132, 163, 213, 245	0
9	J	58/64~(90%)	-0.06	0 100 100	103, 137, 165, 175	0
9	W	59/64~(92%)	-0.19	1 (1%) 70 53	102, 121, 153, 162	0
10	Ο	419/453~(92%)	-0.21	7 (1%) 70 53	97, 146, 193, 250	0
11	V	17/274~(6%)	1.19	$3\ (17\%)\ 1\ 0$	176, 209, 228, 268	0
All	All	$386\overline{0/4946}$ (78%)	-0.23	79 (2%) 65 48	77, 133, 189, 293	0

All (79) RSRZ outliers are listed below:



Mol	Chain	Res	Type	RSRZ
1	А	226	ASP	5.9
11	V	62	ARG	4.8
2	В	232	LEU	4.7
1	Ν	225	GLU	4.2
2	В	21	PRO	4.0
10	0	232	LEU	4.0
2	В	36	ALA	4.0
8	U	44	VAL	3.8
8	U	50	THR	3.7
2	В	23	ASP	3.7
11	V	63	PRO	3.6
1	Ν	243	HIS	3.6
2	В	19	PRO	3.4
8	U	51	GLU	3.4
10	0	231	GLY	3.4
10	0	233	SER	3.4
10	0	234	GLY	3.3
5	Е	73	LYS	3.3
2	В	274	VAL	3.3
4	Q	1	SER	3.1
1	А	225	GLU	3.1
1	Ν	226	ASP	3.0
2	В	272	PHE	3.0
2	В	208	GLY	3.0
4	D	241	LYS	3.0
6	F	109	LYS	3.0
5	Ι	77	ARG	3.0
4	Q	143	LEU	2.9
2	В	439	LEU	2.9
9	W	2	ALA	2.9
2	В	276	GLN	2.8
2	В	322	PHE	2.8
2	В	233	SER	2.8
2	В	220	ALA	2.7
2	В	417	PHE	2.7
4	Q	146	GLY	2.7
8	U	78	LYS	2.7
2	В	352	LEU	2.7
1	А	127	ILE	2.7
2	В	275	LEU	2.6
1	А	177	LEU	2.6
2	В	407	ASP	2.5
2	В	38	LEU	2.5



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Mol	Chain	Res	Type	RSRZ
1	А	182	LEU	2.5
2	В	344	VAL	2.4
11	V	70	LEU	2.4
6	F	106	GLU	2.4
2	В	229	GLY	2.3
10	0	41	TYR	2.3
3	Р	168	PHE	2.3
2	В	231	GLY	2.3
4	Q	142	SER	2.3
7	Т	74	PRO	2.3
1	А	83	GLY	2.3
1	А	303	LEU	2.3
10	0	122	PHE	2.3
2	В	20	HIS	2.2
5	R	77	LYS	2.2
7	Т	14	ILE	2.2
2	В	311	ALA	2.2
1	А	126	GLN	2.2
1	N	394	GLU	2.2
1	N	424	GLY	2.2
1	N	425	PHE	2.2
2	В	227	ARG	2.2
4	Q	167	GLU	2.1
7	G	76	ALA	2.1
2	В	410	VAL	2.1
5	R	98	VAL	2.1
2	В	347	ILE	2.1
4	Q	149	PHE	2.1
1	А	84	ALA	2.1
4	D	180	SER	2.1
2	В	313	ASN	2.1
8	U	52	GLU	2.1
10	0	229	GLY	2.1
2	В	43	PRO	2.0
2	В	217	LYS	2.0
1	N	393	ALA	2.0

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

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


6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(Å^2)$	Q<0.9
14	PO4	S	501	5/5	0.39	0.52	225,226,243,252	0
14	PO4	F	501	5/5	0.51	0.58	242,243,245,246	0
14	PO4	D	504	5/5	0.57	0.23	179,190,194,195	0
14	PO4	Q	1001	5/5	0.66	0.20	194,205,216,232	0
14	PO4	N	501	5/5	0.67	0.45	112,126,127,137	0
14	PO4	D	502	5/5	0.71	0.27	176,192,199,203	0
14	PO4	Q	1002	5/5	0.72	0.20	210,211,220,230	0
19	GOL	R	502	6/6	0.72	1.89	169,181,193,193	0
14	PO4	Е	501	5/5	0.74	0.32	124,134,144,145	0
14	PO4	С	504	5/5	0.82	0.39	121,121,134,149	0
14	PO4	D	503	5/5	0.82	0.61	168,169,177,181	0
13	4X9	Р	503	28/28	0.88	0.32	109,147,226,261	0
15	PEE	Q	506	51/51	0.90	0.40	100,134,171,187	0
13	4X9	С	503	28/28	0.90	0.39	116,143,206,215	0
17	CDL	D	505	39/100	0.91	0.27	85,124,146,148	0
15	PEE	С	505	49/51	0.91	0.49	94,116,135,137	0
17	CDL	Т	501	49/100	0.92	0.31	93,129,160,167	0
17	CDL	G	501	44/100	0.92	0.28	95,115,153,168	0
15	PEE	Р	505	49/51	0.93	0.33	100,122,154,156	0
17	CDL	Q	505	39/100	0.93	0.28	100,126,146,148	0
14	PO4	N	1001	5/5	0.93	0.42	120,127,135,137	0
15	PEE	D	506	26/51	0.93	0.26	107,127,169,176	0
18	FES	R	501	4/4	0.97	0.13	125,158,164,170	0
12	HEM	С	502	43/43	0.98	0.26	71,85,99,106	0
12	HEM	Р	501	43/43	0.98	0.30	86,101,116,124	0
12	HEM	Р	502	43/43	0.98	0.23	74,89,104,106	0
12	HEM	С	501	43/43	0.98	0.27	89,99,107,115	0
16	HEC	D	501	43/43	0.98	0.24	80,111,127,138	0
16	HEC	Q	501	43/43	0.98	0.28	106,117,136,143	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.

