

Full wwPDB X-ray Structure Validation Report (i)

Nov 8, 2022 – 06:09 pm GMT

PDB ID	:	7Q5Y
Title	:	Structure of NADH:ubichinon oxidoreductase (complex I) of the hyperther-
		mophilic eubacterium Aquifex aeolicus
Authors	:	Warkentin, E.; Ermler, U.; Peng, G.
Deposited on	:	2021-11-05
Resolution	:	2.70 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
NIGH TODATY	•	
Mogul	:	1.8.4, CSD as 541 be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 2.70 Å.

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



Metric	Whole archive $(\#Entries)$	Similar resolution $(\#Entries, resolution range(Å))$
R _{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	632	82%	15%	••
1	G	632	83%	14%	
1	М	632	79%	18%	••
1	S	632	80%	17%	•••
2	В	586	9%	24%	•



Mol	Chain	Length	Quality of chain						
2	н	586	15%	240/					
	11	000	10%	24% •					
2	Ν	586	71%	27% ·					
2	Т	586	10%	27% •					
3	С	426	87%	11% •					
3	Ι	426	89%	9% •					
3	0	426	.% 87%	11% •					
3	U	426	% 87 %	12% •					
4	D	201	71%	24% ••					
4	J	201	68%	27% ••					
4	Р	201	16%	24% •••					
4	V	201	69%	26% ••					
5	Е	160	84%	13% •					
5	K	160	84%	11% ••					
5	Q	160	83%	14% •					
5	W	160	6% 80%	16% ••					
6	F	179	5%	. 25%					
6	I.	179	15% 40% 25%	. 25%					
6	B	170	15%	- 2570					
0	10	113	55% 18% 13%	• 25%					
6	Х	179	55% 18%	• 25%					



2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 69025 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

Mol	Chain	Residues		At	oms		ZeroOcc	AltConf	Trace		
1	Δ	626	Total	С	Ν	Ο	\mathbf{S}	0	0	0	
	A	020	5071	3250	846	946	29	0	0	0	
1	C	626	Total	С	Ν	0	S	0	0	0	
	G	020	5071	3250	846	946	29	0	0	0	
1	м	626	Total	С	Ν	0	S	0	0	0	
	111	020	5071	3250	846	946	29	0	0		
1	q	626	Total	С	Ν	Ο	S	0	0	0	
	G	020	5071	3250	846	946	29	0	0		

• Molecule 1 is a protein called NADH dehydrogenase I chain G.

• Molecule 2 is a protein called NADH-quinone oxidoreductase subunit C/D 2.

Mol	Chain	Residues		At	oms		ZeroOcc	AltConf	Trace		
9	P	595	Total	С	Ν	Ο	S	0	0	0	
	D	100	4789	3089	819	865	16	0	0	0	
0	и	595	Total	С	Ν	0	S	0	0	0	
	11	100	4789	3089	819	865	16	0	0	U	
0	N	EQE	Total	С	Ν	0	S	0	0	0	
	IN	505	4789	3089	819	865	16	0	0		
9	т	595	Total	С	Ν	0	S	0	0	0	
		000	4789	3089	819	865	16	0			

• Molecule 3 is a protein called NADH-quinone oxidoreductase subunit F.

Mol	Chain	Residues		At	oms		ZeroOcc	AltConf	Trace		
2	C	410	Total	С	Ν	0	\mathbf{S}	0	0	0	
່ <u>ບ</u>	U	419	3301	2122	550	615	14	0	0	0	
2	т	410	Total	С	Ν	0	S	0	0	0	
່ <u>ບ</u>	1	419	3301	2122	550	615	14	0	0		
9	0	0 410	Total	С	Ν	0	S	0	0	0	
່ <u>ບ</u>	0	419	3301	2122	550	615	14	0	0	0	
2	TT	410	Total	С	Ν	0	S	0	0	0	
່ງ	U	419	3301	2122	550	615	14	0	0	0	



Mol	Chain	Residues		At	oms		ZeroOcc	AltConf	Trace	
4	Л	107	Total	С	Ν	0	\mathbf{S}	0	0	0
4	D	197	1610	1029	280	286	15	0	0	0
4	т	107	Total	С	Ν	0	S	0	0	0
4	1	197	1610	1029	280	286	15	0	0	0
4	D	107	Total	С	Ν	0	S	0	0	0
4	1	197	1610	1029	280	286	15	0	0	0
4	V	107	Total	С	Ν	0	S	0	0	0
4	v	197	1610	1029	280	286	15	0	0	

• Molecule 4 is a protein called NADH-quinone oxidoreductase subunit I.

• Molecule 5 is a protein called NADH-quinone oxidoreductase subunit E.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
E E	Б	155	Total	С	Ν	0	\mathbf{S}	0	0	0
0	E	155	1259	816	203	231	9	0	0	0
E.	V	155	Total	С	Ν	0	S	0	0	0
0	n	155	1259	816	203	231	9	0	0	0
E E	0	155	Total	С	Ν	0	S	0	0	0
0	Q	155	1259	816	203	231	9	0	0	0
5	W/	155	Total	С	Ν	0	S	0	0	0
0	vv	100	1259	816	203	231	9	0		U

• Molecule 6 is a protein called NADH-quinone oxidoreductase subunit B.

Mol	Chain	Residues		A	toms			ZeroOcc	AltConf	Trace	
6	Б	125	Total	С	Ν	0	S	0	0	0	
0	Ľ	155	1033	665	180	178	10	0	0	0	
6	т	125	Total	С	Ν	0	S	0	0	0	
0		155	1033	665	180	178	10	0	0	0	
6	D	195	Total	С	Ν	0	S	0	0	0	
0	n	155	1033	665	180	178	10	0	0	0	
6	v	X 135	Total	С	Ν	0	S	0	0	0	
0	6 X		1033	665	180	178	10		U		





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	А	1	TotalFeS844	0	0
7	А	1	TotalFeS844	0	0
7	А	1	TotalFeS844	0	0
7	А	1	TotalFeS844	0	0
7	С	1	TotalFeS844	0	0
7	D	1	TotalFeS844	0	0
7	D	1	TotalFeS844	0	0
7	F	1	TotalFeS844	0	0
7	G	1	TotalFeS844	0	0
7	G	1	TotalFeS844	0	0
7	G	1	TotalFeS844	0	0
7	G	1	TotalFeS844	0	0
7	Ι	1	TotalFeS844	0	0
7	J	1	TotalFeS844	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	J	1	TotalFeS844	0	0
7	L	1	TotalFeS844	0	0
7	М	1	TotalFeS844	0	0
7	М	1	TotalFeS844	0	0
7	М	1	TotalFeS844	0	0
7	М	1	TotalFeS844	0	0
7	О	1	TotalFeS844	0	0
7	Р	1	TotalFeS844	0	0
7	Р	1	TotalFeS844	0	0
7	R	1	TotalFeS844	0	0
7	S	1	TotalFeS844	0	0
7	S	1	TotalFeS844	0	0
7	S	1	TotalFeS844	0	0
7	S	1	TotalFeS844	0	0
7	U	1	TotalFeS844	0	0
7	V	1	TotalFeS844	0	0
7	V	1	TotalFeS844	0	0
7	Х	1	Total Fe S 8 4 4	0	0

• Molecule 8 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	А	1	TotalFeS422	0	0
8	Е	1	TotalFeS422	0	0
8	G	1	TotalFeS422	0	0
8	Κ	1	Total Fe S 4 2 2	0	0
8	М	1	TotalFeS422	0	0
8	Q	1	TotalFeS422	0	0
8	S	1	TotalFeS422	0	0
8	W	1	TotalFeS422	0	0

• Molecule 9 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues		Ato	oms			ZeroOcc	AltConf	
0	С	1	Total	С	Ν	0	Р	0	0	
9	U	I	31	17	4	9	1	0	0	
0	т	1	Total	С	Ν	0	Р	0	0	
9	1	I	31	17	4	9	1	0	0	
0	0	1	Total	С	Ν	Ο	Р	0	0	
9	0	L	31	17	4	9	1	0	0	
0	TT	1	Total	С	Ν	Ο	Р	0	0	
9	U		31	17	4	9	1	0		

• Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	А	79	Total O 79 79	0	0
10	В	5	Total O 5 5	0	0
10	С	24	Total O 24 24	0	0
10	D	5	$\begin{array}{cc} \text{Total} & \text{O} \\ 5 & 5 \end{array}$	0	0
10	Е	14	Total O 14 14	0	0
10	G	38	Total O 38 38	0	0
10	Н	2	Total O 2 2	0	0
10	Ι	41	Total O 41 41	0	0



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	J	4	Total O 4 4	0	0
10	К	14	Total O 14 14	0	0
10	М	51	Total O 51 51	0	0
10	Ν	8	Total O 8 8	0	0
10	О	11	Total O 11 11	0	0
10	Р	3	Total O 3 3	0	0
10	Q	10	Total O 10 10	0	0
10	S	32	$\begin{array}{ccc} \text{Total} & \text{O} \\ 32 & 32 \end{array}$	0	0
10	Т	4	Total O 4 4	0	0
10	U	10	Total O 10 10	0	0
10	V	2	Total O 2 2	0	0
10	W	4	Total O 4 4	0	0

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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: NADH dehydrogenase I chain G

• Molecule 1: NADH dehydrogenase I chain G



• Molecule 1: NADH dehydrogenase I chain G

Chain M:

79%









 \bullet Molecule 2: NADH-quinone oxidore ductase subunit C/D 2







DB ATA BANK



 \bullet Molecule 2: NADH-quinone oxidore ductase subunit C/D 2



• Molecule 3: NADH-quinone oxidoreductase subunit F











ILE PHE VAL PRO ARG GLU LEU LYS VAL



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants	132.88Å 240.24Å 230.92Å	Deperitor
a, b, c, α , β , γ	90.00° 95.57° 90.00°	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	29.95 - 2.70	Depositor
Resolution (A)	48.63 - 2.70	EDS
% Data completeness	98.4 (29.95-2.70)	Depositor
(in resolution range)	$98.4 \ (48.63-2.70)$	EDS
R_{merge}	(Not available)	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.46 (at 2.69 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.16_3549, PHENIX 1.16_3549	Depositor
B B.	0.169 , 0.209	Depositor
It, Itfree	0.170 , 0.209	DCC
R_{free} test set	19447 reflections $(5.02%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	64.9	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	(Not available), (Not available)	EDS
L-test for $twinning^2$	$< L > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	69025	wwPDB-VP
Average B, all atoms $(Å^2)$	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 11.27% 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: SF4, FMN, FES

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

Mal	Chain	Bo	ad lengths Bond angles		
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.56	2/5182~(0.0%)	0.78	5/7004~(0.1%)
1	G	0.53	2/5182~(0.0%)	0.74	0/7004
1	М	0.51	0/5182	0.74	0/7004
1	S	0.49	0/5182	0.74	2/7004~(0.0%)
2	В	0.39	0/4917	0.64	0/6657
2	Н	0.35	0/4917	0.61	0/6657
2	Ν	0.37	0/4917	0.61	0/6657
2	Т	0.38	0/4917	0.64	0/6657
3	С	0.49	0/3382	0.66	0/4574
3	Ι	0.52	0/3382	0.71	0/4574
3	0	0.46	0/3382	0.65	0/4574
3	U	0.43	0/3382	0.62	0/4574
4	D	0.41	0/1646	0.75	2/2216~(0.1%)
4	J	0.43	0/1646	0.69	0/2216
4	Р	0.39	0/1646	0.77	3/2216~(0.1%)
4	V	0.40	0/1646	0.72	1/2216~(0.0%)
5	Ε	0.49	0/1288	0.72	0/1740
5	Κ	0.52	0/1288	0.71	1/1740~(0.1%)
5	Q	0.43	0/1288	0.66	0/1740
5	W	0.40	0/1288	0.63	0/1740
6	F	0.42	0/1059	0.67	0/1442
6	L	0.34	0/1059	0.61	0/1442
6	R	0.37	0/1059	0.62	0/1442
6	Х	0.37	0/1059	0.62	0/1442
All	All	0.45	4/69896~(0.0%)	0.69	$14/\overline{94532}~(0.0\%)$

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
1	А	239	CYS	CB-SG	-6.75	1.70	1.82
1	G	112	CYS	CB-SG	-6.51	1.71	1.82



Contre	naca from	i prevu	Jus puge	•••			
Mol	Chain	\mathbf{Res}	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
1	А	154	CYS	CB-SG	-5.74	1.72	1.81
1	G	239	CYS	CB-SG	-5.00	1.73	1.81

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	Р	102	LEU	CA-CB-CG	10.14	138.63	115.30
4	D	15	LEU	CA-CB-CG	7.95	133.59	115.30
4	Р	15	LEU	CA-CB-CG	6.72	130.75	115.30
4	Р	165	LEU	CA-CB-CG	6.33	129.85	115.30
1	S	49	ARG	NE-CZ-NH2	6.17	123.39	120.30
5	Κ	139	VAL	N-CA-C	-6.06	94.64	111.00
1	А	526	ASP	CB-CG-OD1	5.79	123.51	118.30
1	А	153	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	А	137	ARG	NE-CZ-NH1	5.67	123.13	120.30
1	А	137	ARG	NE-CZ-NH2	-5.63	117.48	120.30
4	V	15	LEU	CA-CB-CG	5.41	127.74	115.30
1	A	101	LEU	CA-CB-CG	5.33	127.57	115.30
4	D	43	TYR	C-N-CD	-5.23	109.10	120.60
1	S	49	ARG	NE-CZ-NH1	-5.05	117.77	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	5071	0	5048	60	0
1	G	5071	0	5048	62	0
1	М	5071	0	5049	78	0
1	S	5071	0	5048	76	0
2	В	4789	0	4743	102	0
2	Н	4789	0	4743	99	0
2	N	4789	0	4743	104	0
2	Т	4789	0	4743	108	0
3	С	3301	0	3282	26	0



7Q5Y

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	I	3301	0	3282	27	0
3	0	3301	0	3282	29	0
3	U	3301	0	3282	30	0
4	D	1610	0	1623	36	0
4	J	1610	0	1623	43	0
4	P	1610	0	1623	43	0
4	V	1610	0	1623	37	0
5	E	1259	0	1263	15	0
5	K	1259	0	1263	15	0
5	Q	1259	0	1263	17	0
5	Ŵ	1259	0	1263	19	0
6	F	1033	0	1062	30	0
6	L	1033	0	1062	34	0
6	R	1033	0	1062	23	0
6	Х	1033	0	1062	25	0
7	А	32	0	0	1	0
7	С	8	0	0	0	0
7	D	16	0	0	0	0
7	F	8	0	0	0	0
7	G	32	0	0	1	0
7	Ι	8	0	0	0	0
7	J	16	0	0	0	0
7	L	8	0	0	0	0
7	М	32	0	0	0	0
7	0	8	0	0	0	0
7	Р	16	0	0	0	0
7	R	8	0	0	0	0
7	S	32	0	0	1	0
7	U	8	0	0	0	0
7	V	16	0	0	0	0
7	Х	8	0	0	0	0
8	A	4	0	0	0	0
8	E	4	0	0	0	0
8	G	4	0	0	0	0
8	K	4	0	0	0	0
8	М	4	0	0	0	0
8	Q	4	0	0	0	0
8	S	4	0	0	1	0
8	W	4	0	0	1	0
9	C	31	0	19	0	0
9	I	31	0	19	0	0
9	0	31	0	19	0	0



7Q5Y

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	U	31	0	19	0	0
10	А	79	0	0	1	0
10	В	5	0	0	0	0
10	С	24	0	0	0	0
10	D	5	0	0	0	0
10	Ε	14	0	0	1	0
10	G	38	0	0	0	0
10	Н	2	0	0	0	0
10	Ι	41	0	0	1	0
10	J	4	0	0	0	0
10	Κ	14	0	0	0	0
10	М	51	0	0	0	0
10	Ν	8	0	0	0	0
10	Ο	11	0	0	2	0
10	Р	3	0	0	0	0
10	Q	10	0	0	0	0
10	S	32	0	0	2	0
10	Т	4	0	0	0	0
10	U	10	0	0	1	0
10	V	2	0	0	0	0
10	W	4	0	0	0	0
All	All	69025	0	68161	1029	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 8.

All (1029) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:423:LYS:HG3	2:T:437:ILE:HD11	1.54	0.90
2:H:355:LEU:HB3	2:H:359:THR:HG21	1.54	0.89
2:B:355:LEU:HB3	2:B:359:THR:HG21	1.57	0.84
1:M:354:GLU:HG3	1:M:437:LYS:HG3	1.58	0.83
2:B:103:PRO:HD2	2:B:404:ASN:HB3	1.59	0.83
5:Q:138:MET:HG2	5:Q:143:GLU:HG3	1.61	0.82
1:G:137:ARG:NH2	1:G:182:SER:O	2.11	0.82
2:H:4:VAL:HG22	2:H:84:VAL:HG22	1.62	0.81
2:T:196:LYS:HD2	2:T:227:GLN:HG3	1.62	0.81
2:B:298:ARG:NH2	2:B:524:GLU:O	2.13	0.81
1:S:354:GLU:HG3	1:S:437:LYS:HG3	1.64	0.79
2:T:114:ASP:OD1	2:T:128:ARG:NH1	2.16	0.79



	• • • • • •	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:N:103:PRO:HD2	2:N:404:ASN:HB3	1.64	0.79
2:N:56:ASP:HB2	2:N:548:ARG:HG3	1.66	0.78
2:H:264:ILE:HB	2:H:297:GLN:HG3	1.65	0.78
2:H:423:LYS:HG3	2:H:437:ILE:HD11	1.66	0.78
6:L:62:ARG:NH2	6:L:87:GLN:OE1	2.18	0.77
2:B:4:VAL:HG22	2:B:84:VAL:HG22	1.67	0.77
2:T:103:PRO:HD2	2:T:404:ASN:HB3	1.66	0.76
2:B:395:GLY:O	2:B:448:ARG:NH2	2.19	0.76
1:M:177:ASP:O	3:O:196:ARG:NH2	2.16	0.75
6:R:142:GLN:OE1	6:R:145:ARG:NH1	2.19	0.75
2:T:183:GLU:OE1	2:T:187:ARG:NH2	2.20	0.75
3:U:415:GLU:HG3	3:U:418:ARG:HD3	1.66	0.74
2:T:298:ARG:NH2	2:T:524:GLU:O	2.20	0.73
2:T:258:MET:HE1	2:T:547:ILE:HD13	1.68	0.73
4:P:12:LEU:O	4:P:13:ASN:HB2	1.88	0.73
1:S:368:LYS:O	1:S:422:ASN:ND2	2.21	0.72
1:M:468:GLU:OE2	1:M:471:LYS:NZ	2.21	0.72
1:G:95:LEU:HD22	1:G:155:VAL:HG22	1.69	0.72
1:G:97:THR:HG22	1:G:98:ARG:HG2	1.70	0.72
2:H:258:MET:HE1	2:H:547:ILE:HD13	1.72	0.72
4:V:171:ASP:OD2	4:V:175:ARG:NH1	2.23	0.72
1:S:97:THR:HG22	1:S:98:ARG:HG2	1.71	0.72
1:S:137:ARG:NH2	1:S:182:SER:O	2.23	0.72
1:M:324:GLU:OE2	1:M:547:THR:HG23	1.89	0.71
2:N:133:GLU:H	2:N:188:THR:HG22	1.52	0.71
2:T:395:GLY:O	2:T:448:ARG:NH2	2.23	0.71
5:E:138:MET:HG2	5:E:143:GLU:HG3	1.73	0.71
1:G:259:THR:HG21	1:G:271:GLY:O	1.89	0.71
2:N:206:LEU:HD23	6:R:80:MET:HG2	1.71	0.71
2:N:183:GLU:OE1	2:N:187:ARG:NH2	2.24	0.71
2:N:423:LYS:HG3	2:N:437:ILE:HD11	1.72	0.71
3:U:87:ARG:HG2	3:U:215:PRO:HB2	1.73	0.70
2:H:340:ARG:NH1	6:L:39:GLU:OE1	2.24	0.70
1:M:137:ARG:NH2	1:M:182:SER:O	2.24	0.70
1:M:101:LEU:HD22	2:N:498:LEU:HB2	1.73	0.70
4:V:12:LEU:O	4:V:13:ASN:HB2	1.91	0.70
2:T:355:LEU:HB3	2:T:359:THR:HG21	1.71	0.70
1:A:354:GLU:HG3	1:A:437:LYS:HG3	1.74	0.69
4:P:43:TYR:OH	4:P:149:GLU:OE1	2.09	0.69
1:G:180:PHE:HA	3:I:354:ARG:HG2	1.75	0.69
2:N:237:ARG:HH11	6:R:72:THR:HG21	1.58	0.69



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:M:592:ASN:HB3	1:M:594:ARG:HH21	1.55	0.68
4:P:134:VAL:HG21	4:P:144:MET:HG2	1.76	0.68
2:B:272:GLU:HG3	2:B:276:ARG:HH12	1.59	0.68
1:M:343:PRO:HG2	1:M:498:ASP:HB2	1.75	0.68
1:S:137:ARG:NH1	1:S:151:SER:O	2.26	0.67
3:C:83:ASN:O	3:C:87:ARG:NH1	2.28	0.67
2:N:264:ILE:HB	2:N:297:GLN:HG3	1.75	0.67
1:G:137:ARG:NH1	1:G:151:SER:O	2.26	0.67
2:T:388:LEU:HD22	2:T:392:LYS:HE3	1.76	0.67
1:G:354:GLU:HG3	1:G:437:LYS:HG3	1.77	0.67
4:D:43:TYR:OH	4:D:149:GLU:OE1	2.10	0.67
2:T:259:ASP:HB2	2:T:583:GLU:HG3	1.76	0.67
5:K:138:MET:HG2	5:K:143:GLU:HG3	1.78	0.66
1:M:259:THR:HG21	1:M:271:GLY:O	1.95	0.66
1:A:259:THR:HG21	1:A:271:GLY:O	1.95	0.66
2:H:388:LEU:HD22	2:H:392:LYS:HE3	1.78	0.66
1:A:416:LEU:HB3	1:A:446:LEU:HD21	1.78	0.65
2:H:367:ILE:HG23	2:H:460:VAL:HG13	1.77	0.65
2:H:272:GLU:HG3	2:H:276:ARG:NH1	2.10	0.65
2:B:206:LEU:HD23	6:F:80:MET:HG2	1.78	0.65
2:T:264:ILE:HB	2:T:297:GLN:HG3	1.78	0.65
1:M:97:THR:HG22	1:M:98:ARG:HG2	1.79	0.65
2:B:272:GLU:HG3	2:B:276:ARG:NH1	2.12	0.65
4:D:44:PRO:HG3	6:F:141:LEU:HD21	1.77	0.65
3:I:87:ARG:HG2	3:I:215:PRO:HB2	1.79	0.65
4:J:41:THR:HG21	4:J:48:LEU:HG	1.79	0.65
1:M:137:ARG:NH1	1:M:151:SER:O	2.29	0.65
3:I:8:PRO:HD3	5:K:143:GLU:HB3	1.79	0.64
2:N:355:LEU:HB3	2:N:359:THR:HG21	1.79	0.64
1:A:137:ARG:NH2	1:A:182:SER:O	2.25	0.64
2:N:213:THR:HG22	2:N:234:GLN:HB3	1.80	0.64
4:P:36:ARG:HH21	4:P:37:ARG:HB2	1.62	0.64
2:B:264:ILE:HB	2:B:297:GLN:HG3	1.79	0.64
2:H:369:ASP:HB3	2:H:373:ARG:HD2	1.79	0.64
6:R:62:ARG:NH2	6:R:87:GLN:OE1	2.31	0.64
2:H:133:GLU:H	2:H:188:THR:HB	1.62	0.64
2:T:398:THR:HG23	2:T:401:ASP:OD2	1.98	0.64
2:H:193:LEU:HD13	2:H:227:GLN:HE21	1.63	0.63
2:H:237:ARG:HD3	6:L:72:THR:HG21	1.79	0.63
2:N:258:MET:HE1	2:N:547:ILE:HD13	1.80	0.63
1:S:416:LEU:HB3	1:S:446:LEU:HD11	1.80	0.63



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:N:259:ASP:HB2	2:N:583:GLU:HG3	1.79	0.63
1:A:282:ARG:NH2	1:A:543:GLU:OE1	2.32	0.63
2:B:196:LYS:HD2	2:B:227:GLN:HG3	1.80	0.63
6:F:27:TRP:HE1	6:F:56:ILE:HD12	1.64	0.63
3:U:8:PRO:HD3	5:W:143:GLU:HB3	1.79	0.63
1:S:259:THR:HG21	1:S:271:GLY:O	1.97	0.63
1:S:78:HIS:O	1:S:85:ARG:NH1	2.33	0.62
1:S:343:PRO:HG2	1:S:498:ASP:HB2	1.79	0.62
3:U:374:GLU:OE2	3:U:418:ARG:NH2	2.32	0.62
2:H:324:ARG:HH12	4:J:34:LEU:HD11	1.64	0.62
6:L:39:GLU:HG2	6:L:131:PRO:O	1.99	0.62
2:H:272:GLU:HG3	2:H:276:ARG:HH12	1.63	0.62
6:X:117:ASP:HA	6:X:120:ILE:O	1.99	0.62
1:A:324:GLU:OE2	1:A:547:THR:HG23	2.00	0.62
4:J:43:TYR:OH	4:J:149:GLU:OE1	2.14	0.62
4:P:62:VAL:HG13	4:P:83:ALA:HA	1.81	0.62
6:L:28:PRO:HB3	6:L:66:VAL:HB	1.81	0.62
2:T:39:LYS:NZ	2:T:100:ASP:OD2	2.29	0.62
2:B:262:SER:HA	2:B:297:GLN:NE2	2.15	0.62
1:G:396:LYS:NZ	1:G:403:ASP:OD2	2.32	0.62
2:N:114:ASP:OD1	2:N:128:ARG:NH1	2.31	0.61
5:Q:74:ASP:OD2	5:Q:121:LYS:NZ	2.33	0.61
5:W:74:ASP:OD2	5:W:121:LYS:NZ	2.33	0.61
5:K:23:PHE:HE2	5:K:32:LEU:HD12	1.66	0.61
1:A:368:LYS:O	1:A:422:ASN:ND2	2.33	0.61
3:0:147:ASP:0	3:O:151:GLU:HG3	2.00	0.61
2:B:56:ASP:HB2	2:B:548:ARG:HG3	1.83	0.61
2:B:383:ARG:HH12	4:D:24:LEU:HD12	1.66	0.61
4:J:36:ARG:HH21	4:J:37:ARG:HD2	1.65	0.61
1:M:180:PHE:HA	3:O:354:ARG:HG2	1.82	0.61
1:G:343:PRO:HG2	1:G:498:ASP:HB2	1.81	0.61
3:C:87:ARG:HG2	3:C:215:PRO:HB2	1.81	0.61
6:X:72:THR:HA	6:X:100:CYS:HB3	1.83	0.61
2:B:445:VAL:HG13	2:B:576:SER:HB3	1.82	0.60
2:T:237:ARG:HH11	6:X:72:THR:HG21	1.64	0.60
2:H:182:LEU:HD21	6:L:83:LEU:HB2	1.83	0.60
4:P:13:ASN:HB3	4:P:15:LEU:HB2	1.83	0.60
1:A:330:LEU:HD22	1:A:469:VAL:HG13	1.82	0.60
6:F:85:TRP:HA	6:F:88:MET:HE3	1.83	0.60
$1:\overline{S:155:VAL:HG13}$	1:S:155:VAL:O	2.02	0.60
1:S:426:LEU:HD23	1:S:455:ILE:HB	1.84	0.60



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
4:J:106:GLU:HB2	4:J:119:ARG:HB3	1.84	0.60
2:T:61:ASP:OD1	2:T:68:ARG:HD3	2.02	0.60
3:C:6:ALA:HB3	5:E:142:ASP:HB3	1.83	0.59
3:0:8:PRO:HD3	5:Q:143:GLU:HB3	1.84	0.59
1:M:373:VAL:HG11	1:M:416:LEU:HD21	1.82	0.59
4:V:184:TRP:CE2	4:V:190:ARG:HG3	2.38	0.59
2:H:343:SER:O	4:J:55:ARG:NH1	2.24	0.59
5:K:130:ALA:HB3	5:K:136:VAL:HG21	1.85	0.59
2:T:445:VAL:HG13	2:T:576:SER:HB3	1.84	0.59
2:N:272:GLU:HG3	2:N:276:ARG:NH1	2.17	0.59
6:X:28:PRO:HB3	6:X:66:VAL:HB	1.83	0.59
2:T:56:ASP:HB2	2:T:548:ARG:HG3	1.84	0.59
2:B:8:THR:HG22	2:B:11:ARG:HH21	1.68	0.58
1:M:95:LEU:HD22	1:M:155:VAL:HG22	1.86	0.58
1:G:416:LEU:HB3	1:G:446:LEU:HD11	1.86	0.58
1:S:432:LEU:HB2	1:S:436:ILE:HG12	1.84	0.58
4:V:27:LEU:HD21	4:V:31:LEU:HD12	1.85	0.58
2:B:383:ARG:HH21	4:D:27:LEU:HD22	1.67	0.58
2:T:324:ARG:HH11	2:T:373:ARG:HH22	1.51	0.58
6:X:74:VAL:HG12	6:X:76:LYS:H	1.67	0.58
1:G:218:TYR:CD2	4:J:115:LYS:HB2	2.38	0.58
2:T:367:ILE:HD12	2:T:460:VAL:HG13	1.85	0.58
6:F:28:PRO:HB3	6:F:66:VAL:HB	1.85	0.58
2:H:56:ASP:HB2	2:H:548:ARG:HG3	1.86	0.58
6:X:27:TRP:HE1	6:X:56:ILE:HD12	1.68	0.58
3:C:374:GLU:OE2	3:C:418:ARG:NH2	2.37	0.57
2:B:46:LYS:HG3	2:B:52:LEU:HA	1.84	0.57
2:B:61:ASP:OD1	2:B:68:ARG:HD3	2.04	0.57
4:D:106:GLU:HB2	4:D:119:ARG:HB3	1.85	0.57
6:X:27:TRP:NE1	6:X:56:ILE:HD12	2.18	0.57
4:D:62:VAL:HG13	4:D:83:ALA:HA	1.86	0.57
1:G:343:PRO:HA	1:G:477:LEU:HD22	1.87	0.57
2:H:395:GLY:O	2:H:448:ARG:NH2	2.38	0.57
2:N:395:GLY:O	2:N:448:ARG:NH2	2.37	0.57
2:B:423:LYS:HG3	2:B:437:ILE:HD11	1.87	0.57
2:N:201:LEU:HD22	2:N:220:LEU:HD11	1.87	0.57
4:P:99:MET:O	4:P:102:LEU:HD13	2.04	0.57
2:B:201:LEU:HD22	2:B:220:LEU:HD11	1.85	0.57
1:G:112:CYS:HB3	1:G:115:GLN:HB3	1.86	0.57
6:F:50:LEU:HD11	6:F:57:PHE:HE2	1.70	0.57
2:T:272:GLU:HG3	2:T:276:ARG:NH1	2.20	0.57



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:G:368:LYS:O	1:G:422:ASN:ND2	2.37	0.57
2:B:258:MET:HE1	2:B:547:ILE:HD13	1.86	0.56
2:B:327:GLU:OE2	2:B:340:ARG:NH2	2.37	0.56
1:G:178:ARG:NH2	3:I:178:GLY:O	2.37	0.56
6:L:138:TYR:HA	6:L:141:LEU:HD22	1.87	0.56
1:A:291:ARG:NH2	1:A:293:GLU:OE2	2.36	0.56
2:H:298:ARG:NH2	2:H:524:GLU:O	2.38	0.56
5:Q:23:PHE:HE2	5:Q:32:LEU:HD12	1.69	0.56
5:W:138:MET:HG2	5:W:143:GLU:HG3	1.87	0.56
6:X:62:ARG:NH2	6:X:87:GLN:OE1	2.38	0.56
4:J:62:VAL:HG13	4:J:83:ALA:HA	1.87	0.56
2:N:280:VAL:HG22	2:N:484:HIS:CD2	2.40	0.56
3:U:101:PHE:CZ	5:W:132:SER:HB3	2.39	0.56
2:H:166:ASP:OD1	2:H:166:ASP:N	2.33	0.56
5:Q:159:TYR:O	5:Q:160:THR:HB	2.06	0.56
6:R:28:PRO:HD2	6:R:57:PHE:H	1.71	0.56
2:B:580:VAL:HG12	2:B:582:GLY:H	1.70	0.56
2:H:206:LEU:HD23	6:L:80:MET:HG2	1.88	0.56
2:N:340:ARG:NH1	6:R:39:GLU:OE1	2.39	0.56
2:T:73:TYR:CE2	2:T:98:VAL:HG21	2.40	0.56
2:H:50:ARG:NH2	2:H:52:LEU:HD21	2.20	0.56
2:N:399:ARG:HD3	2:N:417:VAL:HG22	1.86	0.56
1:S:261:PRO:HB3	1:S:267:ILE:HB	1.88	0.56
6:F:142:GLN:OE1	6:F:145:ARG:NH1	2.33	0.56
2:H:262:SER:HA	2:H:297:GLN:NE2	2.20	0.56
2:T:383:ARG:HH21	4:V:27:LEU:HD22	1.70	0.56
4:V:71:LEU:HG	4:V:139:VAL:HG13	1.87	0.56
2:H:61:ASP:OD1	2:H:68:ARG:HD3	2.05	0.56
2:N:384:ASN:HB2	2:N:387:TRP:HE1	1.71	0.56
4:P:43:TYR:CG	4:P:43:TYR:O	2.59	0.56
1:S:508:PHE:HA	1:S:511:LEU:HB2	1.88	0.56
3:I:354:ARG:NH1	10:I:601:HOH:O	2.38	0.55
3:O:412:GLU:CD	3:O:412:GLU:H	2.09	0.55
4:J:71:LEU:HG	4:J:139:VAL:HG13	1.88	0.55
2:N:133:GLU:H	2:N:188:THR:CG2	2.18	0.55
1:A:97:THR:HG22	1:A:98:ARG:HG2	1.86	0.55
2:B:24:GLU:HG2	2:B:29:LYS:HG2	1.87	0.55
6:F:67:LEU:HB2	6:F:88:MET:HE1	1.89	0.55
1:G:324:GLU:OE2	1:G:547:THR:HG23	2.06	0.55
4:D:187:ASP:O	4:D:191:GLU:HG3	2.07	0.55
1:M:107:ASP:OD2	1:M:217:LYS:HA	2.06	0.55



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
6:L:72:THR:HA	6:L:100:CYS:HB3	1.88	0.55
1:M:416:LEU:HB3	1:M:446:LEU:HD11	1.88	0.55
2:N:8:THR:HG22	2:N:11:ARG:HH21	1.72	0.55
6:R:28:PRO:HB3	6:R:66:VAL:HB	1.88	0.55
4:V:42:GLU:CD	4:V:42:GLU:H	2.08	0.55
1:G:164:CYS:SG	1:G:170:THR:HG23	2.47	0.55
2:N:199:LEU:HD12	2:N:200:VAL:H	1.70	0.55
2:T:425:GLN:NE2	2:T:522:ALA:O	2.29	0.55
2:B:555:LEU:HG	2:B:579:PRO:HB3	1.89	0.55
5:E:119:LYS:HE2	5:E:160:THR:HG23	1.87	0.55
4:J:44:PRO:HG3	6:L:141:LEU:HD21	1.88	0.55
2:N:433:VAL:HG11	2:N:462:ILE:HG23	1.87	0.55
3:O:354:ARG:NH1	10:O:603:HOH:O	2.40	0.55
1:M:261:PRO:HB3	1:M:267:ILE:HB	1.89	0.55
2:N:196:LYS:HD2	2:N:227:GLN:HG3	1.87	0.55
2:B:2:LYS:NZ	2:B:80:GLU:O	2.31	0.55
2:N:383:ARG:HH12	4:P:24:LEU:HA	1.70	0.55
2:T:332:ILE:HA	4:V:183:ILE:HD11	1.89	0.55
5:W:38:GLN:HB2	5:W:44:ILE:HG13	1.89	0.55
1:A:426:LEU:HD23	1:A:455:ILE:HB	1.89	0.54
1:G:485:GLU:OE1	1:G:514:LYS:HE3	2.08	0.54
4:D:146:ASP:OD2	4:D:175:ARG:NH2	2.40	0.54
1:S:164:CYS:SG	1:S:170:THR:HG23	2.47	0.54
3:C:402:LEU:O	3:C:406:THR:HG23	2.07	0.54
4:D:71:LEU:HD22	4:D:139:VAL:HG13	1.90	0.54
2:H:344:CYS:O	2:H:347:ARG:NH2	2.40	0.54
6:R:74:VAL:HG12	6:R:76:LYS:H	1.71	0.54
1:M:39:HIS:ND1	1:M:40:PRO:HD2	2.23	0.54
1:M:150:TYR:HB3	1:M:153:ARG:HG3	1.88	0.54
3:U:97:GLU:HG2	3:U:98:PRO:HD2	1.90	0.54
1:G:36:PHE:HE2	1:G:50:MET:HE3	1.73	0.54
4:J:57:ALA:HB2	4:J:150:LEU:HD11	1.90	0.54
1:A:261:PRO:HB3	1:A:267:ILE:HB	1.89	0.54
5:E:100:LEU:HD22	5:E:111:PRO:HG3	1.89	0.54
2:H:51:PHE:CE2	2:H:84:VAL:HG23	2.42	0.54
1:S:218:TYR:CD2	4:V:115:LYS:HB2	2.43	0.54
1:S:95:LEU:HD22	1:S:155:VAL:HG22	1.90	0.53
3:I:374:GLU:OE2	3:I:418:ARG:NH2	2.41	0.53
4:V:43:TYR:OH	4:V:149:GLU:OE1	2.22	0.53
6:F:39:GLU:HG2	6:F:131:PRO:O	2.08	0.53
1:G:39:HIS:ND1	1:G:40:PRO:HD2	2.23	0.53



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:H:379:THR:O	2:H:383:ARG:HB2	2.08	0.53
3:I:99:GLY:HA2	5:K:131:CYS:SG	2.48	0.53
2:N:262:SER:HA	2:N:297:GLN:NE2	2.23	0.53
4:P:55:ARG:HB3	4:P:144:MET:HE3	1.91	0.53
6:X:44:ALA:HA	6:X:50:LEU:HD22	1.90	0.53
2:B:51:PHE:CE2	2:B:84:VAL:HG23	2.43	0.53
2:H:260:TYR:CB	6:L:35:CYS:HB3	2.39	0.53
2:N:166:ASP:OD1	2:N:166:ASP:N	2.42	0.53
1:A:180:PHE:HA	3:C:354:ARG:HG2	1.89	0.53
1:G:101:LEU:HA	2:H:501:MET:HE1	1.90	0.53
3:U:142:TYR:OH	10:U:601:HOH:O	2.18	0.53
4:J:171:ASP:OD2	4:J:175:ARG:NH1	2.42	0.53
6:L:142:GLN:OE1	6:L:145:ARG:NH1	2.40	0.53
3:O:129:GLU:HG2	3:O:172:TYR:HE1	1.74	0.53
1:M:374:PHE:CE1	1:M:426:LEU:HD12	2.44	0.53
6:R:23:ARG:O	6:R:23:ARG:HG2	2.09	0.53
2:T:24:GLU:HG2	2:T:29:LYS:HG2	1.91	0.53
2:T:73:TYR:HE2	2:T:98:VAL:HG21	1.75	0.53
5:E:130:ALA:HB3	5:E:136:VAL:HG21	1.91	0.52
2:H:46:LYS:HB2	2:H:102:TRP:CZ2	2.44	0.52
2:H:127:ARG:HD2	2:H:133:GLU:OE1	2.08	0.52
2:H:183:GLU:OE2	2:H:187:ARG:NH2	2.38	0.52
6:X:39:GLU:HG2	6:X:131:PRO:O	2.10	0.52
2:T:383:ARG:NH2	4:V:27:LEU:HD22	2.23	0.52
4:D:130:CYS:SG	4:D:132:LEU:HG	2.49	0.52
1:S:301:LEU:HD13	1:S:534:ILE:HD11	1.91	0.52
5:W:41:TYR:O	5:W:78:LYS:HE3	2.08	0.52
1:A:6:LYS:HE2	1:A:8:TYR:OH	2.10	0.52
6:F:23:ARG:O	6:F:23:ARG:HG2	2.10	0.52
1:G:576:GLU:O	1:G:579:LYS:HE3	2.09	0.52
2:H:129:MET:HG3	2:H:130:PHE:CD1	2.44	0.52
5:Q:138:MET:CG	5:Q:143:GLU:HG3	2.37	0.52
2:T:360:LEU:HD22	2:T:467:VAL:HG13	1.91	0.52
1:A:101:LEU:HA	2:B:501:MET:HE2	1.92	0.52
1:A:458:PRO:HG3	1:A:464:LEU:HG	1.91	0.52
3:O:47:LEU:HD12	3:O:163:LEU:HD12	1.90	0.52
2:T:97:THR:HG22	2:T:99:GLU:H	1.73	0.52
2:N:51:PHE:CE2	2:N:84:VAL:HG23	2.45	0.52
2:N:367:ILE:HG23	2:N:460:VAL:HG13	1.91	0.52
1:S:180:PHE:HA	3:U:354:ARG:HG2	1.92	0.52
1:G:101:LEU:HD22	2:H:498:LEU:HB2	1.92	0.52



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Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:G:359:ASP:OD1	1:G:447:LYS:HE2	2.10	0.52
6:L:89:PRO:HB2	6:L:91:PRO:HD2	1.91	0.52
1:A:270:LYS:HA	1:A:614:LEU:HD11	1.92	0.52
2:B:295:GLU:OE2	2:B:298:ARG:NH1	2.42	0.52
4:D:158:GLU:OE2	6:F:127:PRO:HG3	2.10	0.52
5:Q:100:LEU:HD22	5:Q:111:PRO:HG3	1.91	0.52
3:C:8:PRO:HD3	5:E:143:GLU:HB3	1.91	0.51
6:L:74:VAL:HG12	6:L:76:LYS:H	1.74	0.51
1:M:501:GLU:OE1	1:M:595:ARG:NH1	2.43	0.51
6:R:22:ARG:HD2	6:R:148:LYS:NZ	2.25	0.51
6:X:97:MET:HA	6:X:126:ILE:HB	1.92	0.51
1:A:343:PRO:HG2	1:A:498:ASP:HB2	1.90	0.51
1:G:98:ARG:HG3	1:G:180:PHE:HZ	1.75	0.51
1:S:282:ARG:NH2	1:S:543:GLU:OE1	2.44	0.51
1:G:270:LYS:HA	1:G:614:LEU:HD11	1.92	0.51
3:I:325:LEU:HG	5:K:93:LEU:HD21	1.93	0.51
1:M:426:LEU:HD23	1:M:455:ILE:HB	1.92	0.51
2:N:325:GLU:CD	2:N:373:ARG:HE	2.14	0.51
1:S:324:GLU:OE2	1:S:547:THR:HG23	2.09	0.51
2:N:495:PHE:HB3	4:P:68:PRO:HB2	1.91	0.51
6:R:117:ASP:HA	6:R:120:ILE:O	2.10	0.51
2:B:522:ALA:HB1	2:B:529:GLU:HG3	1.92	0.51
1:S:170:THR:HG21	7:S:704:SF4:S3	2.50	0.51
2:T:129:MET:HG3	2:T:130:PHE:CD1	2.45	0.51
1:A:142:TRP:CE2	1:A:149:TYR:HB2	2.46	0.51
3:C:101:PHE:CZ	5:E:132:SER:HB3	2.46	0.51
4:D:27:LEU:HG	4:D:31:LEU:HB2	1.93	0.51
3:I:153:LYS:HE3	3:I:170:GLU:OE2	2.10	0.51
1:M:98:ARG:HG3	1:M:180:PHE:CZ	2.45	0.51
2:N:97:THR:HG22	2:N:99:GLU:H	1.76	0.51
4:V:52:LYS:HE3	4:V:176:ARG:O	2.11	0.51
4:V:186:ASN:OD1	4:V:188:GLU:N	2.41	0.51
2:B:183:GLU:OE2	2:B:187:ARG:NH2	2.44	0.51
3:I:94:ASP:O	3:I:135:ARG:HB3	2.11	0.51
4:P:41:THR:HG21	4:P:48:LEU:HG	1.93	0.51
1:S:438:GLU:OE1	1:S:438:GLU:N	2.33	0.51
3:U:88:TYR:HE2	3:U:214:LYS:HG3	1.75	0.51
3:I:129:GLU:HG2	3:I:172:TYR:HE1	1.75	0.51
2:T:46:LYS:HB2	2:T:102:TRP:CZ2	2.46	0.51
3:O:257:LYS:HA	3:O:284:LEU:HD12	1.93	0.50
4:P:13:ASN:C	4:P:15:LEU:H	2.14	0.50



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
6:R:39:GLU:HG2	6:R:131:PRO:O	2.11	0.50
2:B:25:THR:HG22	2:B:26:LYS:N	2.26	0.50
2:B:154:LEU:HB3	6:F:118:ARG:HD3	1.94	0.50
6:F:149:GLU:HG2	6:F:152:ILE:HG21	1.93	0.50
1:G:142:TRP:CD1	1:G:186:PRO:HD3	2.46	0.50
2:T:180:PRO:O	6:X:79:PRO:HG3	2.11	0.50
5:Q:130:ALA:HB3	5:Q:136:VAL:HG21	1.93	0.50
1:S:142:TRP:CE2	1:S:149:TYR:HB2	2.46	0.50
2:B:355:LEU:HB3	2:B:359:THR:CG2	2.35	0.50
6:L:117:ASP:HA	6:L:120:ILE:O	2.10	0.50
2:T:321:TYR:OH	4:V:34:LEU:HG	2.12	0.50
4:V:134:VAL:HG21	4:V:144:MET:HG2	1.92	0.50
6:X:142:GLN:OE1	6:X:145:ARG:NH1	2.38	0.50
1:G:103:CYS:H	2:H:501:MET:HE3	1.77	0.50
1:M:119:ALA:HB3	2:N:506:ARG:HG3	1.94	0.50
1:A:478:PRO:HD3	1:A:593:LEU:HD12	1.92	0.50
1:G:261:PRO:HB3	1:G:267:ILE:HB	1.93	0.50
4:J:14:ILE:O	4:J:16:GLU:N	2.43	0.50
1:M:98:ARG:HG3	1:M:180:PHE:HZ	1.76	0.50
2:B:97:THR:HG22	2:B:99:GLU:H	1.76	0.50
2:B:156:SER:OG	2:B:159:GLU:HG2	2.12	0.50
6:L:23:ARG:O	6:L:23:ARG:HG2	2.11	0.50
2:N:63:PRO:HA	2:N:68:ARG:HG2	1.94	0.50
2:T:496:HIS:ND1	2:T:497:ASP:OD2	2.33	0.50
2:H:237:ARG:HH11	6:L:72:THR:HG21	1.77	0.49
2:H:497:ASP:HB2	2:H:499:GLU:OE1	2.12	0.49
1:M:142:TRP:CE2	1:M:149:TYR:HB2	2.47	0.49
2:T:4:VAL:HG22	2:T:84:VAL:HG22	1.93	0.49
2:B:16:PHE:O	2:B:20:VAL:HG22	2.12	0.49
3:I:336:LEU:HA	3:I:364:LEU:HD13	1.94	0.49
4:P:43:TYR:N	4:P:44:PRO:HD3	2.27	0.49
2:T:355:LEU:HB3	2:T:359:THR:CG2	2.42	0.49
3:C:94:ASP:O	3:C:135:ARG:HB3	2.12	0.49
6:F:74:VAL:HG12	6:F:76:LYS:H	1.76	0.49
1:G:155:VAL:O	1:G:155:VAL:HG13	2.12	0.49
1:M:282:ARG:NH2	1:M:543:GLU:OE1	2.45	0.49
2:N:59:CYS:HB2	2:N:116:PHE:CD2	2.47	0.49
2:N:445:VAL:HG13	2:N:576:SER:HB3	1.92	0.49
2:T:63:PRO:HA	2:T:68:ARG:HG2	1.93	0.49
2:T:115:MET:HB3	2:T:140:LEU:HB2	1.94	0.49
4:V:78:MET:HE2	4:V:115:LYS:HB3	1.95	0.49



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Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:B:220:LEU:HA	2:B:224:LYS:O	2.12	0.49
4:J:21:ILE:O	4:J:25:LYS:HG2	2.13	0.49
3:O:6:ALA:HB3	5:Q:142:ASP:HB3	1.94	0.49
3:O:196:ARG:HD3	3:O:198:HIS:NE2	2.26	0.49
4:P:133:CYS:HB2	4:P:142:LEU:CD2	2.42	0.49
2:T:300:ASN:HB2	2:T:329:ILE:HG21	1.93	0.49
1:A:119:ALA:HB3	2:B:506:ARG:HG3	1.93	0.49
4:D:78:MET:CE	4:D:115:LYS:HB3	2.42	0.49
1:M:270:LYS:HA	1:M:614:LEU:HD11	1.94	0.49
2:N:398:THR:HG23	2:N:401:ASP:OD2	2.12	0.49
2:H:103:PRO:HD2	2:H:404:ASN:HB3	1.93	0.49
2:H:433:VAL:HG11	2:H:462:ILE:HG23	1.94	0.49
1:M:343:PRO:HA	1:M:477:LEU:HD22	1.95	0.49
3:O:97:GLU:HG2	3:O:98:PRO:HD2	1.93	0.49
6:R:27:TRP:NE1	6:R:56:ILE:HD12	2.28	0.49
2:T:51:PHE:CE2	2:T:77:ASN:HB2	2.48	0.49
2:T:166:ASP:OD1	2:T:166:ASP:N	2.45	0.49
2:T:399:ARG:HD3	2:T:417:VAL:HG22	1.94	0.49
1:A:78:HIS:O	1:A:85:ARG:NH1	2.46	0.49
2:B:304:LEU:HD21	6:F:38:ILE:HD12	1.95	0.49
1:S:478:PRO:HD3	1:S:593:LEU:HD12	1.95	0.49
1:S:539:SER:OG	1:S:567:ASP:HB2	2.13	0.49
4:V:48:LEU:HD11	6:X:47:ARG:NH2	2.28	0.49
5:W:103:LEU:HD23	5:W:152:LEU:HD21	1.93	0.49
2:N:268:LEU:O	2:N:272:GLU:HB2	2.12	0.49
2:T:527:ARG:HD3	2:T:578:ASP:O	2.12	0.49
4:V:121:ASP:HA	4:V:160:LEU:O	2.12	0.49
2:H:24:GLU:HG2	2:H:29:LYS:HG2	1.94	0.49
2:H:52:LEU:O	2:H:102:TRP:NE1	2.46	0.49
6:R:133:PRO:O	6:R:137:ILE:HG13	2.13	0.49
1:S:35:TYR:HB2	8:S:705:FES:S2	2.53	0.49
1:S:485:GLU:HA	1:S:514:LYS:HD2	1.93	0.49
2:B:213:THR:OG1	2:B:581:VAL:HG21	2.12	0.49
2:B:421:LEU:HB2	2:B:524:GLU:HG2	1.93	0.49
2:H:316:LEU:HD12	2:H:316:LEU:H	1.78	0.49
2:T:184:ASP:O	2:T:188:THR:HG22	2.13	0.49
6:F:27:TRP:NE1	6:F:56:ILE:HD12	2.27	0.48
6:L:97:MET:HA	6:L:126:ILE:HB	1.95	0.48
1:M:142:TRP:CD1	1:M:186:PRO:HD3	2.48	0.48
1:M:478:PRO:HD3	1:M:593:LEU:HD12	1.95	0.48
2:T:51:PHE:CE2	2:T:84:VAL:HG23	2.48	0.48



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:97:THR:HG21	3:C:359:GLU:CG	2.44	0.48
1:A:346:VAL:HG11	1:A:502:PHE:CE1	2.48	0.48
2:B:123:HIS:HB3	2:B:126:LEU:HB2	1.94	0.48
2:B:166:ASP:OD1	2:B:166:ASP:N	2.42	0.48
1:G:98:ARG:HG3	1:G:180:PHE:CZ	2.48	0.48
2:N:553:TYR:O	2:N:556:SER:OG	2.31	0.48
2:B:38:LEU:HD23	2:B:96:PRO:HD2	1.95	0.48
2:H:25:THR:HG22	2:H:26:LYS:N	2.28	0.48
2:B:2:LYS:HG3	2:B:82:GLU:HG2	1.94	0.48
1:M:218:TYR:CD2	4:P:115:LYS:HB2	2.49	0.48
1:S:99:HIS:O	1:S:135:LYS:HG2	2.12	0.48
2:B:25:THR:HG22	2:B:26:LYS:H	1.78	0.48
1:M:396:LYS:HG3	1:M:397:ILE:N	2.28	0.48
4:P:106:GLU:HB2	4:P:119:ARG:HB3	1.96	0.48
4:D:62:VAL:CG1	4:D:83:ALA:HA	2.44	0.48
4:D:78:MET:HE2	4:D:115:LYS:HB3	1.96	0.48
6:L:137:ILE:O	6:L:141:LEU:HD13	2.13	0.48
3:U:402:LEU:O	3:U:406:THR:HG23	2.14	0.48
2:B:261:ILE:HG23	2:B:304:LEU:HD23	1.96	0.48
1:G:281:LYS:NZ	5:Q:119:LYS:HE2	2.27	0.48
6:R:93:TRP:CE2	6:R:147:ILE:HG12	2.49	0.48
2:B:343:SER:O	4:D:55:ARG:NH1	2.37	0.48
2:B:433:VAL:HG11	2:B:462:ILE:HG23	1.93	0.48
1:S:112:CYS:HB3	1:S:115:GLN:HB3	1.95	0.48
1:G:246:GLY:HA3	1:G:253:LYS:O	2.14	0.48
2:H:295:GLU:OE2	2:H:298:ARG:NH1	2.47	0.48
2:H:445:VAL:HG13	2:H:576:SER:HB3	1.96	0.48
4:P:146:ASP:OD2	4:P:175:ARG:NH2	2.47	0.48
1:S:137:ARG:HH12	1:S:154:CYS:HB3	1.78	0.48
2:T:139:PRO:HA	2:T:144:PHE:CD2	2.49	0.48
2:T:199:LEU:HD12	2:T:200:VAL:H	1.79	0.48
2:T:512:GLU:H	2:T:512:GLU:CD	2.17	0.48
4:D:89:ALA:HB2	4:D:117:VAL:HG22	1.96	0.48
6:L:31:ILE:HG13	6:L:67:LEU:HD11	1.96	0.48
1:S:212:ILE:HD12	1:S:212:ILE:HA	1.74	0.48
2:T:463:ILE:O	2:T:467:VAL:HG23	2.13	0.48
2:T:198:GLU:OE1	2:T:221:GLU:HA	2.14	0.47
1:A:339:TYR:CE1	1:A:587:VAL:HG22	2.49	0.47
2:B:54:PHE:HB2	2:B:102:TRP:CD1	2.49	0.47
3:I:381:ASP:OD2	3:I:385:ARG:NH2	2.47	0.47
4:P:78:MET:CE	4:P:115:LYS:HB3	2.44	0.47



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:S:388:TYR:O	1:S:391:LYS:HE2	2.14	0.47
1:G:170:THR:HG21	7:G:704:SF4:S3	2.54	0.47
4:J:184:TRP:CE2	4:J:190:ARG:HG3	2.48	0.47
1:M:155:VAL:O	1:M:155:VAL:HG13	2.13	0.47
4:P:89:ALA:HB3	4:P:115:LYS:HE2	1.97	0.47
1:S:52:VAL:HG11	3:U:390:THR:HG22	1.96	0.47
2:T:260:TYR:CB	6:X:35:CYS:HB3	2.44	0.47
1:G:156:VAL:HG22	1:G:156:VAL:O	2.15	0.47
2:H:420:ASP:OD1	2:H:524:GLU:HG3	2.13	0.47
5:K:38:GLN:HB2	5:K:44:ILE:HG13	1.97	0.47
1:M:339:TYR:CE1	1:M:587:VAL:HG22	2.49	0.47
4:P:71:LEU:HG	4:P:139:VAL:HG13	1.97	0.47
3:U:6:ALA:HB3	5:W:142:ASP:HB3	1.95	0.47
3:I:97:GLU:HG2	3:I:98:PRO:HD2	1.96	0.47
4:V:42:GLU:O	4:V:46:GLU:HB3	2.14	0.47
2:B:398:THR:HG22	2:B:401:ASP:OD2	2.14	0.47
5:E:27:ARG:NH1	10:E:301:HOH:O	2.47	0.47
5:E:159:TYR:O	5:E:160:THR:HB	2.15	0.47
1:G:150:TYR:HB3	1:G:153:ARG:HG3	1.95	0.47
1:G:177:ASP:O	3:I:196:ARG:NH2	2.35	0.47
2:H:46:LYS:HB2	2:H:102:TRP:HZ2	1.80	0.47
2:H:71:GLY:O	2:H:87:LYS:HA	2.15	0.47
2:H:213:THR:OG1	2:H:581:VAL:HG21	2.15	0.47
1:M:112:CYS:HB3	1:M:115:GLN:HB3	1.96	0.47
2:N:5:ASN:HD21	2:N:8:THR:HG23	1.80	0.47
2:N:61:ASP:OD1	2:N:68:ARG:HD3	2.14	0.47
4:P:62:VAL:HG22	4:P:84:LYS:C	2.35	0.47
3:U:90:ILE:HB	3:U:218:VAL:HG22	1.96	0.47
2:B:332:ILE:HA	4:D:183:ILE:HD11	1.96	0.47
3:C:16:LEU:HD13	3:C:249:PRO:HB3	1.97	0.47
4:J:30:THR:O	4:J:34:LEU:N	2.47	0.47
1:M:322:PRO:HB3	1:M:546:GLY:HA3	1.97	0.47
2:N:39:LYS:HB3	2:N:40:PRO:HD3	1.96	0.47
2:T:110:ARG:HD2	2:T:129:MET:HE2	1.96	0.47
2:T:129:MET:HG3	2:T:130:PHE:CE1	2.50	0.47
2:B:285:LYS:HB3	2:B:478:PRO:O	2.15	0.47
4:D:41:THR:HG21	4:D:48:LEU:HG	1.96	0.47
2:H:143:ASP:OD1	2:H:143:ASP:N	2.42	0.47
2:H:311:LEU:HD12	2:H:319:PHE:CD1	2.50	0.47
2:H:369:ASP:O	2:H:373:ARG:HG3	2.15	0.47
6:L:36:CYS:SG	6:L:98:GLY:HA3	2.55	0.47



	the case page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:S:6:LYS:HE2	1:S:8:TYR:OH	2.15	0.47
6:X:22:ARG:HD2	6:X:148:LYS:NZ	2.29	0.47
3:C:271:THR:OG1	3:C:274:GLU:HG3	2.15	0.47
4:D:13:ASN:C	4:D:15:LEU:H	2.17	0.47
1:M:97:THR:HG21	3:O:359:GLU:CG	2.45	0.47
2:N:57:MET:HG3	2:N:108:ALA:HB1	1.95	0.47
2:N:103:PRO:HB2	2:N:405:TYR:CE2	2.50	0.47
1:S:142:TRP:CD1	1:S:186:PRO:HD3	2.50	0.47
3:U:313:PRO:HB2	3:U:314:LEU:HD22	1.97	0.47
1:A:374:PHE:CE1	1:A:426:LEU:HD12	2.50	0.46
2:B:259:ASP:HB2	2:B:583:GLU:HG3	1.96	0.46
5:E:23:PHE:HE2	5:E:32:LEU:HD12	1.79	0.46
2:N:192:ARG:HG3	2:N:229:ASP:OD2	2.15	0.46
3:O:86:PRO:HD2	3:O:214:LYS:HD3	1.97	0.46
2:T:142:LYS:HE3	2:T:543:TYR:CZ	2.50	0.46
2:H:199:LEU:HD12	2:H:200:VAL:H	1.80	0.46
1:M:101:LEU:N	1:M:101:LEU:HD23	2.31	0.46
5:Q:14:THR:O	5:Q:18:GLU:HG3	2.15	0.46
2:T:123:HIS:CD2	2:T:126:LEU:HA	2.50	0.46
2:T:253:PRO:O	2:T:257:ARG:NH1	2.49	0.46
2:B:180:PRO:O	6:F:79:PRO:HG3	2.16	0.46
3:C:22:ARG:NH1	3:C:37:ASP:OD2	2.48	0.46
2:H:123:HIS:HB3	2:H:126:LEU:HB2	1.96	0.46
1:M:359:ASP:OD1	1:M:447:LYS:HE2	2.15	0.46
2:N:139:PRO:HA	2:N:144:PHE:CD2	2.51	0.46
4:P:25:LYS:O	4:P:29:VAL:HG23	2.16	0.46
2:T:344:CYS:O	2:T:347:ARG:NH2	2.48	0.46
4:D:163:GLU:H	4:D:163:GLU:CD	2.19	0.46
4:J:71:LEU:HD11	4:J:86:ARG:HB3	1.98	0.46
1:S:343:PRO:HA	1:S:477:LEU:HD22	1.98	0.46
1:G:435:GLU:O	1:G:439:VAL:HG23	2.16	0.46
2:H:109:GLU:OE1	2:H:123:HIS:ND1	2.44	0.46
2:H:506:ARG:NH1	2:H:513:ASP:OD2	2.48	0.46
1:M:396:LYS:HD3	1:M:400:SER:HB2	1.98	0.46
1:M:428:THR:HB	1:M:430:HIS:CE1	2.50	0.46
2:N:115:MET:HB3	2:N:140:LEU:HB2	1.98	0.46
2:N:162:HIS:CG	2:N:164:ARG:HH21	2.32	0.46
3:O:287:LYS:HD3	3:O:328:GLU:OE1	2.16	0.46
2:T:262:SER:HA	2:T:297:GLN:OE1	2.16	0.46
3:U:60:LYS:HD3	3:U:235:TRP:CE2	2.51	0.46
2:B:140:LEU:HD23	2:B:140:LEU:HA	1.77	0.46


	the case page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:B:192:ARG:HG3	2:B:229:ASP:OD2	2.15	0.46
2:B:383:ARG:NH2	4:D:27:LEU:HD22	2.30	0.46
4:D:62:VAL:HG22	4:D:84:LYS:C	2.36	0.46
1:M:103:CYS:HB2	2:N:501:MET:HE3	1.97	0.46
1:M:318:SER:HB2	1:M:495:PHE:O	2.14	0.46
1:M:520:VAL:HG23	1:M:532:ALA:HB2	1.98	0.46
1:S:446:LEU:HD13	1:S:452:PHE:CD2	2.51	0.46
2:B:98:VAL:HG12	2:B:101:LEU:HD12	1.97	0.46
3:C:17:ASN:OD1	3:C:24:LYS:NZ	2.48	0.46
1:M:39:HIS:CE1	1:M:40:PRO:HD2	2.51	0.46
1:M:150:TYR:CB	1:M:153:ARG:HG3	2.45	0.46
1:M:226:GLU:OE1	1:M:251:ARG:NH2	2.35	0.46
1:S:137:ARG:NH1	1:S:154:CYS:HB3	2.31	0.46
1:S:345:SER:HA	1:S:349:PHE:HB2	1.97	0.46
1:A:438:GLU:OE1	1:A:438:GLU:N	2.43	0.46
2:H:37:PHE:C	2:H:40:PRO:HD2	2.35	0.46
6:L:94:CYS:HB3	6:L:122:VAL:HA	1.98	0.46
1:M:404:GLU:HB3	1:M:628:TYR:HB2	1.98	0.46
2:N:512:GLU:CD	2:N:512:GLU:H	2.18	0.46
1:A:36:PHE:CE2	1:A:50:MET:HE3	2.51	0.46
2:H:268:LEU:O	2:H:272:GLU:HB2	2.16	0.46
4:J:62:VAL:HG22	4:J:84:LYS:C	2.36	0.46
1:M:521:VAL:HA	1:M:536:ILE:O	2.15	0.46
3:O:153:LYS:HE3	3:O:170:GLU:OE2	2.16	0.46
6:R:72:THR:HA	6:R:100:CYS:HB3	1.98	0.46
1:A:218:TYR:CD2	4:D:115:LYS:HB2	2.51	0.46
2:B:63:PRO:HA	2:B:68:ARG:HG2	1.96	0.46
6:F:122:VAL:HG22	6:F:125:TYR:CZ	2.51	0.46
2:H:215:TRP:HB3	2:H:231:ILE:O	2.16	0.46
2:N:255:THR:HA	2:N:258:MET:HG3	1.98	0.46
2:B:39:LYS:NZ	2:B:100:ASP:OD1	2.48	0.45
2:H:2:LYS:HG3	2:H:82:GLU:HG2	1.98	0.45
2:H:68:ARG:HD2	2:H:69:PHE:CZ	2.51	0.45
6:R:95:ILE:HG12	6:R:124:VAL:HB	1.98	0.45
1:A:164:CYS:SG	1:A:170:THR:HG23	2.57	0.45
5:E:138:MET:CG	5:E:143:GLU:HG3	2.44	0.45
6:F:82:LYS:HE3	6:F:86:ASP:OD2	2.16	0.45
2:H:261:ILE:HB	2:H:527:ARG:HH12	1.82	0.45
6:L:85:TRP:HA	6:L:88:MET:HE3	1.98	0.45
4:P:71:LEU:HG	4:P:139:VAL:HG22	1.98	0.45
1:S:101:LEU:HA	2:T:501:MET:HE1	1.96	0.45



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:514:LYS:HE2	1:A:514:LYS:HB2	1.72	0.45
3:C:274:GLU:O	3:C:278:LYS:HB3	2.16	0.45
2:H:288:TYR:CZ	2:H:469:LYS:HG2	2.51	0.45
3:I:101:PHE:CZ	5:K:132:SER:HB3	2.52	0.45
2:N:283:PRO:HD3	2:N:481:ASN:HB2	1.98	0.45
2:T:220:LEU:HA	2:T:224:LYS:O	2.15	0.45
4:V:17:SER:HA	4:V:20:PHE:HB3	1.98	0.45
1:A:339:TYR:CD1	1:A:587:VAL:HG22	2.51	0.45
1:A:346:VAL:O	1:A:350:LYS:HD2	2.16	0.45
2:B:422:ARG:HG3	2:B:524:GLU:HB2	1.99	0.45
2:H:534:ILE:HG23	2:H:545:THR:HG22	1.99	0.45
4:J:126:ASN:HA	6:L:105:GLY:HA2	1.99	0.45
4:V:62:VAL:HG13	4:V:83:ALA:HA	1.99	0.45
4:V:133:CYS:HB2	4:V:142:LEU:HD23	1.99	0.45
6:F:44:ALA:HA	6:F:50:LEU:HD22	1.98	0.45
2:H:298:ARG:HA	2:H:526:PRO:HG3	1.99	0.45
2:H:580:VAL:HG12	2:H:582:GLY:H	1.82	0.45
2:T:57:MET:HG3	2:T:108:ALA:HB1	1.98	0.45
2:T:164:ARG:HB3	4:V:156:ARG:NH2	2.31	0.45
2:T:374:LEU:HD23	2:T:374:LEU:HA	1.84	0.45
1:G:99:HIS:O	1:G:135:LYS:HG2	2.17	0.45
2:N:24:GLU:HG2	2:N:29:LYS:HG2	1.99	0.45
2:N:51:PHE:CD2	2:N:77:ASN:HB2	2.51	0.45
2:N:355:LEU:HB3	2:N:359:THR:CG2	2.47	0.45
2:T:407:LEU:HD11	2:T:557:ILE:HD12	1.99	0.45
2:B:201:LEU:HB3	2:B:218:PHE:HB2	1.99	0.45
1:G:464:LEU:HD23	1:G:464:LEU:HA	1.80	0.45
2:H:123:HIS:HD2	2:H:126:LEU:HA	1.81	0.45
2:N:46:LYS:HB2	2:N:102:TRP:CZ2	2.52	0.45
2:N:57:MET:HA	2:N:72:VAL:O	2.17	0.45
2:N:211:HIS:CD2	2:N:579:PRO:HG2	2.52	0.45
2:N:522:ALA:HB1	2:N:529:GLU:HG3	1.99	0.45
2:N:571:ILE:HD12	2:N:571:ILE:H	1.81	0.45
3:U:83:ASN:O	3:U:87:ARG:NH1	2.50	0.45
5:Q:128:LEU:HD12	5:Q:136:VAL:HG12	1.99	0.45
2:T:497:ASP:HB2	2:T:499:GLU:OE1	2.16	0.45
1:A:25:VAL:HG21	1:A:69:VAL:HG11	1.98	0.45
2:H:355:LEU:HB3	2:H:359:THR:CG2	2.36	0.45
2:T:51:PHE:CD2	2:T:77:ASN:HB2	2.51	0.45
4:V:55:ARG:HB3	4:V:144:MET:HE3	1.99	0.45
4:V:130:CYS:SG	4:V:132:LEU:HG	2.57	0.45



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Atom-1	Atom-2	distance (Å)	overlap (Å)
1:G:103:CYS:SG	2:H:501:MET:HE2	2.57	0.45
3:I:348:GLY:HA2	3:I:354:ARG:HG3	1.98	0.45
2:N:304:LEU:HD13	2:N:323:PHE:CZ	2.52	0.45
2:N:420:ASP:OD1	2:N:524:GLU:HG3	2.17	0.45
1:S:373:VAL:HG11	1:S:416:LEU:HD21	1.99	0.45
2:B:114:ASP:OD1	2:B:128:ARG:NH1	2.41	0.44
2:B:288:TYR:CZ	2:B:469:LYS:HG2	2.52	0.44
4:D:67:GLU:HG3	4:D:86:ARG:NE	2.32	0.44
6:F:117:ASP:HB3	6:F:122:VAL:HG13	1.99	0.44
3:I:7:ILE:HG21	3:I:7:ILE:HD13	1.74	0.44
5:K:128:LEU:HD12	5:K:136:VAL:HG12	1.99	0.44
1:M:514:LYS:HE2	1:M:514:LYS:HB2	1.83	0.44
2:N:360:LEU:HD22	2:N:467:VAL:HG13	1.99	0.44
1:S:107:ASP:OD2	1:S:217:LYS:HA	2.17	0.44
2:T:54:PHE:HB2	2:T:102:TRP:CD1	2.53	0.44
4:V:128:LEU:HG	6:X:106:PRO:HB3	1.99	0.44
2:B:340:ARG:NH1	6:F:39:GLU:OE1	2.50	0.44
1:G:478:PRO:HD3	1:G:593:LEU:HD12	1.99	0.44
4:J:71:LEU:HG	4:J:139:VAL:CG1	2.46	0.44
1:M:583:GLY:HA3	1:S:586:VAL:O	2.17	0.44
1:S:98:ARG:HG3	1:S:180:PHE:CZ	2.52	0.44
3:U:129:GLU:HG2	3:U:172:TYR:HE1	1.82	0.44
1:A:101:LEU:HD22	2:B:498:LEU:HB2	1.99	0.44
2:B:285:LYS:HE3	2:B:477:ALA:HB3	1.99	0.44
1:G:95:LEU:HD22	1:G:155:VAL:CG2	2.43	0.44
2:H:192:ARG:CZ	2:H:231:ILE:HG12	2.47	0.44
3:I:6:ALA:HB3	5:K:142:ASP:HB3	1.98	0.44
2:N:123:HIS:HD2	2:N:126:LEU:HA	1.83	0.44
6:R:22:ARG:HD2	6:R:148:LYS:HZ3	1.81	0.44
1:S:34:PRO:HB3	1:S:117:LEU:HD22	1.99	0.44
1:S:282:ARG:NH2	1:S:543:GLU:OE2	2.50	0.44
2:T:37:PHE:C	2:T:40:PRO:HD2	2.38	0.44
1:A:318:SER:HB2	1:A:495:PHE:O	2.18	0.44
2:B:4:VAL:CG2	2:B:84:VAL:HG22	2.44	0.44
2:B:110:ARG:HB2	2:B:129:MET:HE2	1.99	0.44
2:B:268:LEU:O	2:B:272:GLU:HB2	2.18	0.44
2:B:288:TYR:CZ	2:B:469:LYS:HE3	2.53	0.44
2:B:414:GLY:HA2	2:B:451:VAL:HG21	1.98	0.44
2:H:220:LEU:HD13	2:H:567:ILE:HD13	1.99	0.44
2:T:25:THR:HG22	2:T:26:LYS:N	2.32	0.44
3:U:294:SER:HB3	3:U:298:ASP:HB2	1.99	0.44



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Atom-1	Atom-2	distance (\AA)	overlap (Å)
4:V:94:GLN:O	4:V:100:PRO:HB3	2.18	0.44
1:A:464:LEU:HD23	1:A:464:LEU:HA	1.79	0.44
2:B:176:HIS:CE1	6:F:113:LEU:HD12	2.52	0.44
1:G:514:LYS:HB2	1:G:514:LYS:HE2	1.58	0.44
2:H:38:LEU:HD23	2:H:96:PRO:HD2	1.99	0.44
1:M:55:TRP:NE1	1:M:57:ASP:HB2	2.33	0.44
4:P:191:GLU:HA	4:P:195:GLY:H	1.83	0.44
6:R:27:TRP:HE1	6:R:56:ILE:HD12	1.83	0.44
1:S:32:ASP:OD2	1:S:121:TYR:OH	2.26	0.44
2:T:123:HIS:HD2	2:T:126:LEU:HA	1.83	0.44
1:A:36:PHE:HB2	1:A:48:CYS:SG	2.57	0.44
3:C:196:ARG:HD3	3:C:198:HIS:NE2	2.32	0.44
2:H:123:HIS:CD2	2:H:126:LEU:HA	2.52	0.44
2:H:553:TYR:O	2:H:556:SER:OG	2.36	0.44
4:J:125:LEU:HD13	6:L:102:SER:HB3	2.00	0.44
1:M:132:ALA:HB3	4:P:69:ASP:HB3	2.00	0.44
4:P:31:LEU:HD23	4:P:31:LEU:HA	1.84	0.44
1:S:99:HIS:CD2	1:S:100:PRO:HD2	2.53	0.44
2:T:411:VAL:HA	2:T:448:ARG:HD3	1.99	0.44
5:W:159:TYR:O	5:W:160:THR:HB	2.17	0.44
2:B:411:VAL:HA	2:B:448:ARG:HD3	1.98	0.44
6:F:117:ASP:HA	6:F:120:ILE:O	2.18	0.44
1:G:34:PRO:HB3	1:G:117:LEU:HD22	2.00	0.44
1:G:318:SER:HB2	1:G:495:PHE:O	2.17	0.44
1:M:52:VAL:HG11	3:O:390:THR:HG22	1.99	0.44
2:N:127:ARG:HD2	2:N:133:GLU:OE1	2.18	0.44
2:T:4:VAL:HG13	2:T:84:VAL:HG22	1.98	0.44
4:V:153:TYR:CE1	6:X:146:LYS:HB2	2.53	0.44
4:D:134:VAL:HG21	4:D:144:MET:HG2	2.00	0.44
1:G:6:LYS:HE2	1:G:8:TYR:OH	2.18	0.44
1:G:102:ASP:OD2	1:G:153:ARG:NH1	2.51	0.44
1:G:426:LEU:HD23	1:G:455:ILE:HB	1.98	0.44
1:G:485:GLU:HA	1:G:514:LYS:HD2	1.99	0.44
2:H:401:ASP:OD2	2:H:560:LYS:NZ	2.50	0.44
2:H:411:VAL:HA	2:H:448:ARG:HD3	2.00	0.44
1:M:246:GLY:HA3	1:M:253:LYS:O	2.18	0.44
2:N:25:THR:HG22	2:N:26:LYS:N	2.32	0.44
2:N:328:LYS:HG3	4:P:193:LEU:HD11	1.99	0.44
2:N:396:VAL:HG22	2:N:444:ASP:HB3	1.99	0.44
4:P:78:MET:HE2	4:P:115:LYS:HB3	2.00	0.44
6:L:26:LEU:HD23	6:L:26:LEU:HA	1.86	0.44



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Atom-1	Atom-2	distance (Å)	overlap (Å)
1:S:456:PRO:O	1:S:458:PRO:HD3	2.17	0.44
1:A:112:CYS:HB3	1:A:115:GLN:HB3	1.98	0.43
3:C:287:LYS:HD3	3:C:328:GLU:OE1	2.17	0.43
4:J:40:THR:HG21	6:L:49:ASP:HB2	2.00	0.43
4:J:55:ARG:HB3	4:J:144:MET:HE3	2.00	0.43
2:N:164:ARG:HB3	4:P:156:ARG:HH21	1.83	0.43
2:N:418:PRO:HB3	2:N:439:VAL:HG21	2.00	0.43
3:O:25:LYS:HA	3:O:25:LYS:HD3	1.83	0.43
5:Q:119:LYS:HD2	5:Q:119:LYS:HA	1.69	0.43
5:W:92:HIS:HA	5:W:96:THR:HB	2.00	0.43
1:A:171:ARG:NH1	10:A:804:HOH:O	2.45	0.43
2:B:115:MET:HB3	2:B:140:LEU:HB2	1.99	0.43
2:H:300:ASN:HB2	2:H:329:ILE:HG21	1.99	0.43
4:J:47:LYS:HG2	4:J:48:LEU:N	2.32	0.43
1:S:236:PRO:O	1:S:550:THR:HB	2.18	0.43
2:T:5:ASN:HD21	2:T:8:THR:HG23	1.82	0.43
6:X:85:TRP:HA	6:X:88:MET:HE3	2.00	0.43
2:B:123:HIS:HD2	2:B:126:LEU:HA	1.84	0.43
2:B:321:TYR:OH	4:D:34:LEU:HG	2.19	0.43
1:G:36:PHE:CE2	1:G:50:MET:HE3	2.52	0.43
2:H:57:MET:HA	2:H:72:VAL:O	2.18	0.43
1:S:94:ALA:O	3:U:355:VAL:HG11	2.18	0.43
1:S:497:GLU:HB2	1:S:606:TRP:CG	2.53	0.43
2:T:522:ALA:HB1	2:T:529:GLU:HG3	2.00	0.43
2:B:474:PRO:C	2:B:476:ASP:H	2.22	0.43
1:G:339:TYR:CD1	1:G:587:VAL:HG22	2.53	0.43
2:H:571:ILE:HD12	2:H:571:ILE:H	1.83	0.43
1:M:36:PHE:CE2	1:M:50:MET:HE3	2.54	0.43
1:M:97:THR:O	1:M:135:LYS:HE2	2.18	0.43
2:N:261:ILE:HG22	2:N:301:SER:HA	2.00	0.43
3:O:363:LEU:HD13	3:O:380:PHE:HA	2.01	0.43
1:S:98:ARG:HG3	1:S:180:PHE:HZ	1.82	0.43
1:S:155:VAL:O	1:S:155:VAL:CG1	2.66	0.43
2:T:213:THR:HB	2:T:581:VAL:HG11	2.00	0.43
3:U:314:LEU:HD22	3:U:314:LEU:H	1.83	0.43
5:W:88:SER:HB3	8:W:201:FES:S2	2.58	0.43
3:C:2:ARG:HD3	3:C:2:ARG:O	2.18	0.43
1:M:164:CYS:SG	1:M:170:THR:HG23	2.58	0.43
2:H:385:ARG:HD3	2:H:388:LEU:HD12	1.99	0.43
3:I:83:ASN:O	3:I:87:ARG:NH1	2.52	0.43
2:N:186:GLU:HB3	2:N:190:LYS:NZ	2.34	0.43



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:N:442:VAL:N	2:N:447:ASP:OD2	2.49	0.43
5:Q:93:LEU:HD12	5:Q:93:LEU:HA	1.80	0.43
1:S:41:ARG:HG2	1:S:265:LEU:HD22	2.00	0.43
1:S:433:ASN:O	1:S:433:ASN:ND2	2.49	0.43
2:T:65:HIS:CG	2:T:66:PRO:HD2	2.54	0.43
6:X:56:ILE:HG22	6:X:58:ARG:HG3	2.00	0.43
2:B:435:PHE:CG	2:B:462:ILE:HD11	2.53	0.43
2:B:555:LEU:HD23	2:B:555:LEU:HA	1.80	0.43
3:C:294:SER:HB3	3:C:298:ASP:HB2	2.01	0.43
2:H:407:LEU:HD11	2:H:557:ILE:HD12	1.99	0.43
4:J:52:LYS:HE3	4:J:176:ARG:O	2.19	0.43
4:J:75:GLU:HG2	4:J:80:TYR:CE1	2.53	0.43
1:M:7:ILE:HD13	1:M:69:VAL:HG22	1.99	0.43
1:M:602:TYR:CD2	1:M:617:LEU:HB3	2.52	0.43
2:N:497:ASP:HB2	2:N:499:GLU:OE1	2.18	0.43
4:P:42:GLU:HG3	4:P:44:PRO:HD3	2.00	0.43
1:S:511:LEU:HD23	1:S:511:LEU:HA	1.80	0.43
2:T:304:LEU:HD22	2:T:326:ARG:NH1	2.34	0.43
2:B:123:HIS:CG	2:B:123:HIS:O	2.72	0.43
2:B:139:PRO:HA	2:B:144:PHE:CD2	2.54	0.43
4:D:142:LEU:HD12	4:D:142:LEU:HA	1.89	0.43
4:D:171:ASP:OD2	4:D:175:ARG:NH1	2.52	0.43
3:I:192:LEU:HA	3:I:192:LEU:HD12	1.73	0.43
3:I:314:LEU:HD22	3:I:314:LEU:H	1.83	0.43
2:N:140:LEU:HD23	2:N:140:LEU:HA	1.62	0.43
1:S:178:ARG:HD3	5:W:69:PHE:CE1	2.54	0.43
1:S:464:LEU:HD23	1:S:464:LEU:HA	1.74	0.43
2:T:273:THR:OG1	2:T:521:PHE:HB3	2.19	0.43
1:A:417:GLN:O	1:A:450:LYS:NZ	2.41	0.43
2:H:139:PRO:HA	2:H:144:PHE:CD2	2.53	0.43
2:H:416:GLY:HA2	2:H:439:VAL:HG13	2.00	0.43
5:K:139:VAL:HG12	5:K:140:ASN:H	1.83	0.43
2:N:421:LEU:HB2	2:N:524:GLU:HG2	2.01	0.43
2:T:57:MET:HA	2:T:72:VAL:O	2.19	0.43
4:V:21:ILE:O	4:V:25:LYS:HG2	2.19	0.43
1:A:170:THR:HG21	7:A:704:SF4:S3	2.59	0.43
2:B:26:LYS:HB3	2:B:27:HIS:CE1	2.54	0.43
2:B:164:ARG:HH11	4:D:156:ARG:HD2	1.84	0.43
2:B:215:TRP:HB3	2:B:231:ILE:O	2.19	0.43
1:G:339:TYR:CE1	1:G:587:VAL:HG22	2.54	0.43
4:J:184:TRP:CD2	4:J:190:ARG:HG3	2.54	0.43



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
6:L:29:VAL:HG21	6:L:61:PRO:HA	2.01	0.43
2:N:52:LEU:H	2:N:52:LEU:HG	1.62	0.43
2:N:221:GLU:HG3	2:N:226:VAL:HG21	2.01	0.43
3:O:271:THR:OG1	3:O:274:GLU:HG3	2.18	0.43
4:V:14:ILE:HG22	4:V:14:ILE:O	2.19	0.43
5:W:81:TYR:CE2	5:W:159:TYR:HB3	2.54	0.43
1:A:99:HIS:CE1	1:A:153:ARG:O	2.71	0.42
4:D:55:ARG:HG2	4:D:144:MET:HE2	2.00	0.42
2:H:154:LEU:HD12	2:H:154:LEU:HA	1.77	0.42
2:H:359:THR:HA	4:J:183:ILE:HD12	2.00	0.42
6:L:146:LYS:HE2	6:L:150:GLN:HE22	1.85	0.42
2:N:54:PHE:HB2	2:N:102:TRP:CD1	2.54	0.42
2:T:2:LYS:O	2:T:82:GLU:HA	2.19	0.42
6:X:93:TRP:CE2	6:X:147:ILE:HG12	2.54	0.42
6:F:72:THR:HB	6:F:100:CYS:HB3	2.01	0.42
2:N:201:LEU:HB3	2:N:218:PHE:HB2	2.01	0.42
2:N:210:THR:HG23	2:N:211:HIS:H	1.84	0.42
3:0:94:ASP:0	3:O:135:ARG:HD2	2.19	0.42
1:S:49:ARG:HH21	1:S:63:ILE:HD13	1.84	0.42
2:T:304:LEU:HD22	2:T:326:ARG:HH12	1.84	0.42
3:U:94:ASP:O	3:U:135:ARG:HB3	2.20	0.42
2:B:288:TYR:CE1	2:B:469:LYS:HG2	2.53	0.42
6:L:65:ASP:O	6:L:92:LYS:HA	2.19	0.42
2:N:407:LEU:HD11	2:N:557:ILE:HD12	2.01	0.42
3:O:160:LYS:HE2	10:O:611:HOH:O	2.19	0.42
4:P:21:ILE:O	4:P:25:LYS:HG2	2.20	0.42
6:R:117:ASP:HB3	6:R:122:VAL:HG13	2.00	0.42
3:U:257:LYS:HA	3:U:284:LEU:HD12	2.01	0.42
1:A:373:VAL:HG11	1:A:416:LEU:HD21	2.00	0.42
1:A:579:LYS:HA	1:A:579:LYS:HD3	1.75	0.42
6:F:64:ALA:O	6:F:89:PRO:HD2	2.19	0.42
3:O:245:ASP:HB2	3:O:246:TYR:CD2	2.55	0.42
2:T:94:LYS:HG2	2:T:119:VAL:HG22	2.02	0.42
3:U:98:PRO:HA	5:W:127:CYS:SG	2.60	0.42
1:A:481:MET:HG3	1:A:503:TYR:CZ	2.54	0.42
2:B:255:THR:O	2:B:258:MET:HG3	2.19	0.42
2:H:300:ASN:ND2	2:H:329:ILE:HB	2.34	0.42
2:T:343:SER:O	4:V:55:ARG:NH1	2.34	0.42
2:T:383:ARG:HH12	4:V:24:LEU:HD12	1.84	0.42
2:T:402:VAL:HA	2:T:407:LEU:HD12	2.01	0.42
6:X:27:TRP:CD1	6:X:56:ILE:HD12	2.54	0.42



	1	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:52:VAL:HG11	3:C:390:THR:CG2	2.50	0.42
2:B:57:MET:HA	2:B:72:VAL:O	2.19	0.42
2:H:57:MET:HG3	2:H:108:ALA:HB1	2.02	0.42
3:I:331:ILE:HD13	3:I:331:ILE:HA	1.92	0.42
4:J:124:LEU:HD11	4:J:160:LEU:HD11	2.02	0.42
6:L:62:ARG:HE	6:L:62:ARG:HB2	1.72	0.42
1:S:61:LEU:HD23	1:S:61:LEU:HA	1.90	0.42
1:S:479:ALA:HB2	1:S:589:SER:HB3	2.01	0.42
2:T:210:THR:HG23	2:T:211:HIS:H	1.84	0.42
1:A:236:PRO:HG3	1:A:458:PRO:O	2.18	0.42
2:H:94:LYS:HD2	2:H:121:GLU:CG	2.50	0.42
4:J:133:CYS:HB2	4:J:142:LEU:HD23	2.01	0.42
4:J:161:ARG:HE	4:J:161:ARG:HB3	1.66	0.42
1:M:178:ARG:NH2	3:O:178:GLY:O	2.52	0.42
4:P:13:ASN:HB3	4:P:15:LEU:H	1.85	0.42
1:S:579:LYS:HA	1:S:579:LYS:HD3	1.78	0.42
2:T:182:LEU:HD21	6:X:83:LEU:HB2	2.02	0.42
1:A:150:TYR:HB3	1:A:153:ARG:HG3	2.02	0.42
1:A:246:GLY:HA3	1:A:253:LYS:O	2.20	0.42
1:G:337:GLN:HA	1:G:583:GLY:O	2.20	0.42
4:J:125:LEU:HD23	4:J:125:LEU:HA	1.91	0.42
1:M:485:GLU:HA	1:M:514:LYS:HD2	2.01	0.42
4:P:30:THR:O	4:P:34:LEU:N	2.52	0.42
1:S:396:LYS:NZ	1:S:403:ASP:OD2	2.52	0.42
2:T:154:LEU:HA	2:T:154:LEU:HD12	1.74	0.42
4:V:78:MET:CE	4:V:115:LYS:HB3	2.50	0.42
5:W:130:ALA:HB3	5:W:136:VAL:HG21	2.02	0.42
1:A:388:TYR:O	1:A:391:LYS:HE2	2.20	0.42
3:C:142:TYR:CD1	3:C:175:ARG:HG3	2.54	0.42
2:H:12:VAL:HG12	2:H:20:VAL:HG21	2.01	0.42
2:H:196:LYS:HD3	2:H:226:VAL:CG1	2.50	0.42
2:N:267:GLU:O	2:N:271:VAL:HB	2.20	0.42
2:N:527:ARG:HD3	2:N:578:ASP:O	2.19	0.42
4:P:71:LEU:HD11	4:P:86:ARG:HB3	2.02	0.42
5:Q:109:ILE:HD13	5:Q:115:THR:HG23	2.01	0.42
1:S:155:VAL:O	1:S:156:VAL:C	2.58	0.42
2:T:270:TYR:HB2	2:T:532:PHE:CZ	2.55	0.42
3:U:383:VAL:O	3:U:387:ILE:HG13	2.20	0.42
1:A:156:VAL:O	1:A:156:VAL:HG22	2.20	0.42
1:A:302:LEU:HD11	1:A:536:ILE:HD11	2.02	0.42
1:A:396:LYS:HG3	1:A:397:ILE:N	2.34	0.42



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:G:374:PHE:HB2	1:G:396:LYS:HE3	2.02	0.42
2:H:25:THR:HG22	2:H:26:LYS:H	1.85	0.42
3:I:196:ARG:HD3	3:I:198:HIS:NE2	2.35	0.42
4:J:42:GLU:OE2	6:L:52:ARG:HD2	2.20	0.42
1:M:6:LYS:HE2	1:M:8:TYR:OH	2.20	0.42
1:M:218:TYR:CG	4:P:115:LYS:HB2	2.55	0.42
1:M:346:VAL:HG11	1:M:502:PHE:CE1	2.55	0.42
2:N:445:VAL:HA	2:N:448:ARG:NH1	2.35	0.42
2:N:474:PRO:C	2:N:476:ASP:H	2.23	0.42
5:Q:128:LEU:HD13	5:Q:138:MET:HG3	2.01	0.42
6:R:85:TRP:HA	6:R:88:MET:HE3	2.02	0.42
2:T:3:TRP:CZ2	2:T:28:THR:HG22	2.55	0.42
2:T:434:GLU:O	2:T:465:GLN:NE2	2.37	0.42
5:W:128:LEU:HD13	5:W:138:MET:HG3	2.01	0.42
2:B:110:ARG:HD2	2:B:129:MET:HE2	2.02	0.41
3:C:31:ILE:HD12	3:C:112:HIS:CE1	2.55	0.41
6:F:72:THR:HA	6:F:100:CYS:HB3	2.02	0.41
1:G:374:PHE:CE1	1:G:426:LEU:HD12	2.55	0.41
4:J:67:GLU:HG3	4:J:86:ARG:NE	2.34	0.41
2:N:217:LEU:O	2:N:228:SER:HA	2.20	0.41
2:N:503:LYS:HB3	2:N:503:LYS:HE2	1.79	0.41
2:T:100:ASP:OD1	2:T:100:ASP:N	2.49	0.41
2:T:213:THR:OG1	2:T:581:VAL:HG21	2.20	0.41
2:H:293:PHE:HE1	2:H:355:LEU:HD21	1.86	0.41
5:K:138:MET:CG	5:K:143:GLU:HG3	2.49	0.41
2:N:304:LEU:HD22	2:N:326:ARG:NH1	2.35	0.41
6:R:89:PRO:HB2	6:R:91:PRO:HD2	2.01	0.41
1:S:374:PHE:CE1	1:S:426:LEU:HD12	2.55	0.41
1:S:396:LYS:HG3	1:S:397:ILE:N	2.34	0.41
2:T:367:ILE:HG23	2:T:460:VAL:HG13	2.02	0.41
3:U:153:LYS:HE3	3:U:170:GLU:OE2	2.20	0.41
5:W:44:ILE:HD12	5:W:73:PHE:HB3	2.02	0.41
2:B:179:LEU:HD21	6:F:113:LEU:HD13	2.02	0.41
2:H:516:PRO:HA	2:H:536:SER:O	2.21	0.41
3:I:245:ASP:HB2	3:I:246:TYR:CE2	2.55	0.41
4:J:42:GLU:HB3	4:J:45:LYS:O	2.20	0.41
4:J:78:MET:HE2	4:J:115:LYS:HB3	2.01	0.41
2:N:468:GLN:H	2:N:468:GLN:HG2	1.64	0.41
1:S:76:ARG:NH1	1:S:80:THR:HG21	2.35	0.41
2:T:267:GLU:O	2:T:271:VAL:HB	2.20	0.41
1:A:233:ASN:H	1:A:541:MET:HE2	1.84	0.41



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
6:F:133:PRO:O	6:F:137:ILE:HG13	2.21	0.41
2:H:320:LEU:HD23	2:H:320:LEU:HA	1.87	0.41
4:J:20:PHE:CE2	4:J:24:LEU:HD22	2.56	0.41
4:J:45:LYS:HZ1	6:L:52:ARG:HH22	1.67	0.41
2:N:304:LEU:HD22	2:N:326:ARG:HH12	1.86	0.41
2:T:157:LEU:O	2:T:161:LEU:HD23	2.20	0.41
2:T:421:LEU:HB2	2:T:524:GLU:HG2	2.02	0.41
3:U:7:ILE:HA	3:U:8:PRO:HD3	1.91	0.41
4:V:184:TRP:NE1	4:V:190:ARG:HG3	2.35	0.41
2:B:347:ARG:NH1	4:D:135:ASP:OD2	2.53	0.41
3:C:257:LYS:HA	3:C:284:LEU:HD12	2.00	0.41
5:K:100:LEU:HD22	5:K:111:PRO:HG3	2.03	0.41
4:P:30:THR:O	4:P:34:LEU:HB2	2.20	0.41
1:S:49:ARG:NH2	10:S:806:HOH:O	2.49	0.41
1:S:57:ASP:OD2	1:S:73:MET:HA	2.19	0.41
1:G:322:PRO:HB3	1:G:546:GLY:HA3	2.02	0.41
1:M:36:PHE:HE2	1:M:50:MET:HE3	1.86	0.41
1:M:99:HIS:CE1	1:M:153:ARG:O	2.74	0.41
2:N:164:ARG:HB3	4:P:156:ARG:NH2	2.36	0.41
2:N:202:ASN:ND2	2:N:204:GLY:O	2.53	0.41
2:N:268:LEU:HD23	2:N:268:LEU:HA	1.79	0.41
3:O:115:ILE:O	3:O:119:ILE:HG13	2.20	0.41
2:T:203:TRP:HA	2:T:203:TRP:CE3	2.55	0.41
2:H:168:PRO:HA	4:J:156:ARG:NH1	2.35	0.41
5:K:23:PHE:CE2	5:K:32:LEU:HD12	2.52	0.41
1:M:443:LEU:HA	1:M:443:LEU:HD23	1.85	0.41
1:M:497:GLU:HB2	1:M:606:TRP:CG	2.56	0.41
2:N:8:THR:HG22	2:N:49:GLU:OE2	2.20	0.41
3:O:87:ARG:HG2	3:O:215:PRO:HB2	2.03	0.41
1:S:283:LEU:HB2	1:S:525:GLU:HG3	2.03	0.41
3:U:2:ARG:O	3:U:2:ARG:HD3	2.21	0.41
3:U:359:GLU:OE2	3:U:359:GLU:HA	2.19	0.41
1:A:348:LEU:HD12	1:A:429:PRO:HG2	2.01	0.41
2:B:235:LEU:HD12	2:B:235:LEU:HA	1.85	0.41
1:G:176:GLU:CG	1:G:176:GLU:O	2.69	0.41
1:G:236:PRO:HG3	1:G:458:PRO:O	2.21	0.41
1:M:101:LEU:HA	2:N:501:MET:HE2	2.02	0.41
2:N:580:VAL:HG12	2:N:582:GLY:H	1.85	0.41
4:P:57:ALA:HB2	4:P:150:LEU:HD11	2.02	0.41
4:P:133:CYS:HB2	4:P:142:LEU:HD23	2.01	0.41
4:P:142:LEU:HD12	4:P:142:LEU:HA	1.91	0.41



	• • • • • •	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:T:369:ASP:O	2:T:373:ARG:HG3	2.20	0.41
2:T:390:ARG:HH22	2:T:568:ALA:HB1	1.85	0.41
2:B:195:LYS:HD2	2:B:195:LYS:HA	1.93	0.41
2:B:255:THR:HA	2:B:258:MET:HG3	2.02	0.41
2:B:503:LYS:HE2	2:B:503:LYS:HB3	1.80	0.41
4:D:55:ARG:HB3	4:D:144:MET:HE3	2.02	0.41
4:D:75:GLU:HG2	4:D:80:TYR:CE1	2.56	0.41
4:D:176:ARG:NH2	4:D:185:PRO:HG3	2.36	0.41
1:G:212:ILE:HD13	1:G:212:ILE:HA	1.75	0.41
1:G:345:SER:HA	1:G:349:PHE:HB2	2.02	0.41
2:H:151:GLU:OE1	2:H:178:LYS:HB2	2.20	0.41
4:J:31:LEU:HD23	4:J:31:LEU:HA	1.82	0.41
4:J:133:CYS:HB2	4:J:142:LEU:CD2	2.50	0.41
1:M:433:ASN:OD1	1:M:433:ASN:N	2.53	0.41
1:M:476:ASP:OD2	1:M:588:LYS:HD2	2.21	0.41
2:N:100:ASP:OD1	2:N:100:ASP:N	2.54	0.41
2:N:143:ASP:OD1	2:N:143:ASP:N	2.42	0.41
3:O:36:LYS:HE3	3:O:36:LYS:HB3	1.77	0.41
1:S:451:GLY:N	10:S:801:HOH:O	2.25	0.41
2:T:324:ARG:HH11	2:T:373:ARG:NH2	2.15	0.41
2:T:495:PHE:HB3	4:V:68:PRO:HB2	2.01	0.41
6:X:50:LEU:HD11	6:X:57:PHE:CE2	2.55	0.41
1:A:432:LEU:HA	1:A:432:LEU:HD23	1.88	0.41
2:B:367:ILE:HG23	2:B:460:VAL:HG13	2.03	0.41
3:C:415:GLU:HG3	3:C:418:ARG:HD3	2.02	0.41
5:E:83:ILE:HA	5:E:138:MET:O	2.21	0.41
3:I:31:ILE:HD12	3:I:112:HIS:CE1	2.56	0.41
2:N:467:VAL:O	2:N:471:GLU:HG3	2.21	0.41
5:Q:99:LEU:HD13	5:Q:146:PHE:HB2	2.04	0.41
6:X:30:THR:HB	6:X:57:PHE:HE1	1.86	0.41
3:C:177:ALA:O	5:E:70:TYR:HB3	2.21	0.40
3:C:356:GLY:HA3	3:C:387:ILE:HG12	2.03	0.40
4:D:47:LYS:HE2	4:D:148:PHE:CZ	2.56	0.40
5:E:38:GLN:HB2	5:E:44:ILE:HG13	2.02	0.40
3:I:337:LYS:HA	3:I:337:LYS:HD3	1.79	0.40
5:K:48:SER:C	5:K:51:PRO:HD2	2.40	0.40
4:P:15:LEU:O	4:P:18:ILE:HG13	2.21	0.40
1:S:133:LEU:HA	1:S:133:LEU:HD23	1.85	0.40
2:T:388:LEU:HD23	2:T:388:LEU:HA	1.84	0.40
3:U:115:ILE:O	3:U:119:ILE:HG13	2.21	0.40
4:J:78:MET:CE	4:J:115:LYS:HB3	2.51	0.40



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
6:L:72:THR:CA	6:L:100:CYS:HB3	2.51	0.40
1:M:368:LYS:O	1:M:422:ASN:ND2	2.53	0.40
1:M:547:THR:HA	1:M:556:LYS:HA	2.03	0.40
2:N:232:LEU:HD13	2:N:584:THR:HB	2.02	0.40
3:O:12:ALA:HB3	3:O:24:LYS:HA	2.04	0.40
3:O:331:ILE:HD13	3:O:331:ILE:HA	1.93	0.40
4:P:163:GLU:O	4:P:167:LYS:HG3	2.21	0.40
1:S:322:PRO:HB3	1:S:546:GLY:HA3	2.04	0.40
2:T:268:LEU:O	2:T:272:GLU:HB2	2.21	0.40
2:T:503:LYS:HE2	2:T:503:LYS:HB3	1.85	0.40
3:U:255:SER:HB2	5:W:90:VAL:HG11	2.02	0.40
1:A:99:HIS:HB3	2:B:498:LEU:CD2	2.50	0.40
2:B:260:TYR:CB	6:F:35:CYS:HB3	2.51	0.40
5:E:44:ILE:HD12	5:E:73:PHE:HB3	2.02	0.40
1:G:355:LEU:HD23	1:G:358:TYR:HB3	2.03	0.40
2:H:8:THR:HG22	2:H:49:GLU:OE2	2.21	0.40
4:J:58:HIS:H	4:J:58:HIS:CD2	2.39	0.40
1:M:212:ILE:HD13	1:M:212:ILE:HA	1.83	0.40
1:M:396:LYS:HD3	1:M:400:SER:CB	2.51	0.40
1:M:423:VAL:HB	1:M:452:PHE:CD1	2.57	0.40
2:T:195:LYS:HD2	2:T:195:LYS:HA	1.91	0.40
2:T:468:GLN:H	2:T:468:GLN:HG2	1.75	0.40
4:V:97:CYS:HA	4:V:98:PRO:HD3	1.99	0.40
1:A:374:PHE:HB2	1:A:396:LYS:HE3	2.02	0.40
2:B:197:ALA:HB3	2:B:219:ASP:OD1	2.22	0.40
2:H:140:LEU:HD23	2:H:140:LEU:HA	1.85	0.40
4:V:75:GLU:HG2	4:V:80:TYR:CE1	2.56	0.40
5:W:109:ILE:HD13	5:W:115:THR:HG23	2.03	0.40
1:A:231:VAL:HG23	1:A:557:GLY:HA2	2.03	0.40
2:B:65:HIS:HE1	2:B:67:ASN:OD1	2.03	0.40
2:N:278:LEU:HB2	2:N:280:VAL:HG23	2.03	0.40
6:R:27:TRP:CD1	6:R:56:ILE:HD12	2.57	0.40
1:S:458:PRO:HG3	1:S:464:LEU:HG	2.03	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	ntiles
1	А	624/632~(99%)	592~(95%)	29~(5%)	3~(0%)	29	54
1	G	624/632~(99%)	593~(95%)	29~(5%)	2~(0%)	41	66
1	М	624/632~(99%)	589 (94%)	33~(5%)	2 (0%)	41	66
1	S	624/632~(99%)	595~(95%)	25 (4%)	4 (1%)	25	50
2	В	583/586~(100%)	556 (95%)	26 (4%)	1 (0%)	47	73
2	Н	583/586~(100%)	554 (95%)	28 (5%)	1 (0%)	47	73
2	Ν	583/586~(100%)	557 (96%)	25~(4%)	1 (0%)	47	73
2	Т	583/586~(100%)	556~(95%)	26 (4%)	1 (0%)	47	73
3	С	417/426 (98%)	405 (97%)	12 (3%)	0	100	100
3	Ι	417/426 (98%)	407 (98%)	10 (2%)	0	100	100
3	Ο	417/426 (98%)	404 (97%)	13 (3%)	0	100	100
3	U	417/426 (98%)	406 (97%)	11 (3%)	0	100	100
4	D	195/201~(97%)	187 (96%)	7 (4%)	1 (0%)	29	54
4	J	195/201~(97%)	183 (94%)	11 (6%)	1 (0%)	29	54
4	Р	195/201~(97%)	183 (94%)	11 (6%)	1 (0%)	29	54
4	V	195/201~(97%)	182 (93%)	11 (6%)	2 (1%)	15	37
5	Е	153/160~(96%)	146 (95%)	7(5%)	0	100	100
5	Κ	153/160~(96%)	146 (95%)	6 (4%)	1 (1%)	22	46
5	Q	153/160~(96%)	147 (96%)	6 (4%)	0	100	100
5	W	153/160~(96%)	147 (96%)	6 (4%)	0	100	100
6	F	133/179~(74%)	122 (92%)	11 (8%)	0	100	100
6	L	133/179~(74%)	120 (90%)	13 (10%)	0	100	100
6	R	133/179 (74%)	119 (90%)	14 (10%)	0	100	100
6	Х	133/179 (74%)	121 (91%)	12 (9%)	0	100	100
All	All	8420/8736~(96%)	8017 (95%)	382 (4%)	21 (0%)	47	73



Mol	Chain	Res	Type
1	А	156	VAL
1	А	177	ASP
1	G	156	VAL
1	М	156	VAL
4	Р	13	ASN
1	S	156	VAL
4	V	13	ASN
2	В	428	ALA
2	Н	428	ALA
1	М	177	ASP
2	Ν	428	ALA
1	S	177	ASP
2	Т	428	ALA
1	А	178	ARG
1	G	177	ASP
1	S	178	ARG
1	S	433	ASN
4	D	46	GLU
4	J	46	GLU
5	K	140	ASN
4	V	12	LEU

All (21) 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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
1	А	559/565~(99%)	540~(97%)	19 (3%)	37	66
1	G	559/565~(99%)	529~(95%)	30 (5%)	22	47
1	М	559/565~(99%)	530~(95%)	29~(5%)	23	49
1	S	559/565~(99%)	531 (95%)	28~(5%)	24	51
2	В	513/514~(100%)	486 (95%)	27~(5%)	22	48
2	Н	513/514~(100%)	488 (95%)	25~(5%)	25	52
2	Ν	513/514~(100%)	488 (95%)	25~(5%)	25	52



Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
2	Т	513/514~(100%)	487~(95%)	26~(5%)	24	50
3	С	345/351~(98%)	338~(98%)	7 (2%)	55	81
3	Ι	345/351~(98%)	341 (99%)	4 (1%)	71	88
3	О	345/351~(98%)	337~(98%)	8 (2%)	50	78
3	U	345/351~(98%)	337~(98%)	8 (2%)	50	78
4	D	178/181~(98%)	167~(94%)	11 (6%)	18	40
4	J	178/181 (98%)	166 (93%)	12 (7%)	16	37
4	Р	178/181~(98%)	165~(93%)	13 (7%)	14	33
4	V	178/181~(98%)	166~(93%)	12 (7%)	16	37
5	Ε	141/146~(97%)	139~(99%)	2(1%)	67	86
5	Κ	141/146~(97%)	140 (99%)	1 (1%)	84	94
5	Q	141/146~(97%)	141 (100%)	0	100	100
5	W	141/146~(97%)	140 (99%)	1 (1%)	84	94
6	F	112/152~(74%)	104~(93%)	8 (7%)	14	34
6	L	112/152~(74%)	106~(95%)	6 (5%)	22	47
6	R	112/152~(74%)	105 (94%)	7 (6%)	18	40
6	Х	112/152~(74%)	106 (95%)	6 (5%)	22	47
All	All	$\overline{7392}/\overline{7636}~(97\%)$	7077~(96%)	315 (4%)	29	57

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All (315) residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
1	А	48	CYS
1	А	49	ARG
1	А	79	ARG
1	А	101	LEU
1	А	135	LYS
1	А	156	VAL
1	А	164	CYS
1	А	212	ILE
1	А	235	CYS
1	А	357	GLU
1	А	396	LYS
1	А	400	SER
1	А	402	ARG
1	А	462	ASN



1 A 469 VAL 1 A 498 ASP 1 A 522 SER 1 A 587 VAL 1 A 626 VAL	
1 A 498 ASP 1 A 522 SER 1 A 587 VAL 1 A 626 VAL	
1 A 522 SER 1 A 587 VAL 1 A 626 VAL	
1 A 587 VAL 1 A 626 VAL	
1 A 626 VAL	
2 B 4 VAL	
2 B 52 LEU	
2 B 68 ARG	
2 B 98 VAL	
2 B 154 LEU	
2 B 175 VAL	
2 B 177 THR	
2 B 188 THR	
2 B 192 ARG	
2 B 210 THR	
2 B 213 THR	
2 B 260 TYR	
2 B 268 LEU	
2 B 271 VAL	
2 B 277 LEU	
2 B 297 GLN	
2 B 325 GLU	
2 B 339 TYR	
2 B 352 HIS	
2 B 375 LYS	
2 B 425 GLN	
2 B 431 ASP	
2 B 461 ARG	
2 B 480 LEU	
2 B 506 ARG	
2 B 566 THR	
2 B 567 ILE	
3 C 37 ASP	
3 C 82 GLN	
3 C 208 GLN	
3 C 346 THR	
3 C 364 LEU	
3 C 388 GLN	
3 C 412 GLU	
4 D 6 LEU	
4 D 10 ASP	
4 D 11 TYR	



Mol	Chain	Res	Type
4	D	15	LEU
4	D	16	GLU
4	D	19	LEU
4	D	34	LEU
4	D	39	ILE
4	D	48	LEU
4	D	62	VAL
4	D	104	ARG
5	Е	11	GLU
5	Е	88	SER
6	F	20	TRP
6	F	35	CYS
6	F	50	LEU
6	F	57	PHE
6	F	72	THR
6	F	81	LEU
6	F	122	VAL
6	F	141	LEU
1	G	6	LYS
1	G	44	ILE
1	G	49	ARG
1	G	69	VAL
1	G	70	GLN
1	G	79	ARG
1	G	97	THR
1	G	101	LEU
1	G	135	LYS
1	G	155	VAL
1	G	156	VAL
1	G	161	THR
1	G	164	CYS
1	G	170	THR
1	G	177	ASP
1	G	178	ARG
1	G	235	CYS
1	G	265	LEU
1	G	357	GLU
1	G	396	LYS
1	G	402	ARG
1	G	449	GLU
1	G	450	LYS
1	G	462	ASN



Mol	Chain	Res	Type
1	G	468	GLU
1	G	498	ASP
1	G	547	THR
1	G	587	VAL
1	G	589	SER
1	G	626	VAL
2	Н	4	VAL
2	Н	52	LEU
2	Н	57	MET
2	Н	68	ARG
2	Н	98	VAL
2	Н	188	THR
2	Н	192	ARG
2	Н	210	THR
2	Н	213	THR
2	Н	260	TYR
2	Н	268	LEU
2	Н	271	VAL
2	Н	277	LEU
2	Н	297	GLN
2	Н	325	GLU
2	Н	339	TYR
2	Н	353	TYR
2	Н	393	ASP
2	Н	396	VAL
2	Н	425	GLN
2	Н	461	ARG
2	Н	506	ARG
2	Н	512	GLU
2	Н	565	ARG
2	Н	567	ILE
3	Ι	208	GLN
3	Ι	346	THR
3	Ι	364	LEU
3	Ι	412	GLU
4	J	10	ASP
4	J	11	TYR
4	J	16	GLU
4	J	34	LEU
4	J	39	ILE
4	J	45	LYS
4	J	48	LEU



Mol	Chain	Res	Type
4	J	62	VAL
4	J	71	LEU
4	J	104	ARG
4	J	117	VAL
4	J	165	LEU
5	K	88	SER
6	L	35	CYS
6	L	50	LEU
6	L	57	PHE
6	L	72	THR
6	L	81	LEU
6	L	141	LEU
1	М	6	LYS
1	М	49	ARG
1	М	70	GLN
1	М	79	ARG
1	М	101	LEU
1	М	135	LYS
1	М	155	VAL
1	М	156	VAL
1	М	161	THR
1	М	170	THR
1	М	177	ASP
1	М	178	ARG
1	М	212	ILE
1	М	235	CYS
1	М	265	LEU
1	М	347	ASP
1	М	357	GLU
1	М	396	LYS
1	М	400	SER
1	М	402	ARG
1	М	420	GLU
1	М	446	LEU
1	М	449	GLU
1	М	469	VAL
1	М	498	ASP
1	М	522	SER
1	М	587	VAL
1	М	589	SER
1	М	626	VAL
2	Ν	4	VAL



Mol	Chain	Res	Type
2	Ν	52	LEU
2	Ν	57	MET
2	Ν	68	ARG
2	Ν	98	VAL
2	Ν	177	THR
2	Ν	188	THR
2	Ν	192	ARG
2	Ν	210	THR
2	N	213	THR
2	Ν	260	TYR
2	Ν	268	LEU
2	N	277	LEU
2	N	297	GLN
2	Ν	325	GLU
2	Ν	339	TYR
2	N	353	TYR
2	Ν	375	LYS
2	N	393	ASP
2	N	398	THR
2	N	425	GLN
2	N	461	ARG
2	N	497	ASP
2	N	506	ARG
2	N	567	ILE
3	0	37	ASP
3	0	150	GLU
3	0	208	GLN
3	0	245	ASP
3	0	364	LEU
3	0	388	GLN
3	0	412	GLU
3	0	419	LYS
4	Р	10	ASP
4	Р	11	TYR
4	Р	16	GLU
4	Р	19	LEU
4	Р	39	ILE
4	Р	48	LEU
4	Р	62	VAL
4	Р	71	LEU
4	Р	102	LEU
4	Р	104	ARG



Mol	Chain	Res	Type
4	Р	117	VAL
4	Р	139	VAL
4	Р	165	LEU
6	R	30	THR
6	R	35	CYS
6	R	57	PHE
6	R	72	THR
6	R	81	LEU
6	R	122	VAL
6	R	141	LEU
1	S	6	LYS
1	S	48	CYS
1	S	49	ARG
1	S	69	VAL
1	S	70	GLN
1	S	79	ARG
1	S	80	THR
1	S	135	LYS
1	S	155	VAL
1	S	164	CYS
1	S	212	ILE
1	S	235	CYS
1	S	265	LEU
1	S	301	LEU
1	S	357	GLU
1	S	396	LYS
1	S	400	SER
1	S	402	ARG
1	S	420	GLU
1	S	433	ASN
1	S	446	LEU
1	S	449	GLU
1	S	468	GLU
1	S	492	LEU
1	S	498	ASP
1	S	522	SER
1	S	587	VAL
1	S	626	VAL
2	Т	4	VAL
2	Т	13	LYS
2	Т	52	LEU
2	Т	68	ARG



Mol	Chain	Res	Type
2	Т	98	VAL
2	Т	133	GLU
2	Т	177	THR
2	Т	188	THR
2	Т	192	ARG
2	Т	210	THR
2	Т	213	THR
2	Т	260	TYR
2	Т	268	LEU
2	Т	271	VAL
2	Т	277	LEU
2	Т	325	GLU
2	Т	339	TYR
2	Т	375	LYS
2	Т	398	THR
2	Т	425	GLN
2	Т	449	TYR
2	Т	461	ARG
2	Т	497	ASP
2	Т	506	ARG
2	Т	566	THR
2	Т	567	ILE
3	U	37	ASP
3	U	82	GLN
3	U	208	GLN
3	U	214	LYS
3	U	245	ASP
3	U	364	LEU
3	U	388	GLN
3	U	412	GLU
4	V	10	ASP
4	V	11	TYR
4	V	16	GLU
4	V	19	LEU
4	V	34	LEU
4	V	39	ILE
4	V	62	VAL
4	V	71	LEU
4	V	104	ARG
4	V	117	VAL
4	V	139	VAL
4	V	165	LEU



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Mol	Chain	Res	Type
5	W	88	SER
6	Х	35	CYS
6	Х	50	LEU
6	Х	57	PHE
6	Х	72	THR
6	Х	81	LEU
6	Х	141	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	433	ASN
3	Ι	208	GLN
4	J	58	HIS
4	Р	58	HIS
1	S	88	GLN

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)

44 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).



$\begin{array}{ c c c c c c c c c c c c c c c c c c c$	N <i>T</i> - 1	— ———————————————————————————————————	Cluit	D	T	Bond lengths		Bond angles			
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	IVIOI	Type	Chain	Res	Link	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	7	SF4	М	701	1	$0,\!12,\!12$	-	-	-		
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	7	SF4	G	702	1	$0,\!12,\!12$	-	-	-		
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	8	FES	G	705	1	0,4,4	-	-	-		
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	9	FMN	С	501	-	33,33,33	1.04	2 (6%)	48,50,50	1.34	9 (18%)
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	7	SF4	V	302	4	0,12,12	-	-	-		
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	9	FMN	Ι	501	-	33,33,33	1.12	2 (6%)	48,50,50	1.46	8 (16%)
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	7	SF4	Р	301	4	0,12,12	-	-	-		
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	7	SF4	Ι	502	3	0,12,12	-	-	-		
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	7	SF4	S	704	1	0,12,12	-	-	-		
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	7	SF4	Х	701	6	0,12,12	-	-	-		
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	9	FMN	Ο	501	-	33,33,33	0.99	1 (3%)	48,50,50	1.35	8 (16%)
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	7	SF4	F	701	6	0,12,12	-	-	-		
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	7	SF4	М	703	1	0,12,12	-	-	-		
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	7	SF4	М	704	1	0,12,12	-	-	-		
$ \begin{array}{ c c c c c c c c c c c c c c c c c c c$	7	SF4	А	702	1	0,12,12	-	-	-		
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	7	SF4	А	704	1	$0,\!12,\!12$	-	-	-		
$ \begin{array}{ c c c c c c c c c c c c c c c c c c c$	7	SF4	S	702	1	0,12,12	-	-	-		
8 FES A 705 1 0,4,4 -	7	SF4	С	502	3	0,12,12	-	-	-		
8 FES S 705 1 0,4,4 - - -	8	FES	А	705	1	0,4,4	-	-	-		
	8	FES	S	705	1	0,4,4	-	-	-		
8 FES E 201 5 0,4,4	8	FES	E	201	5	0,4,4	-	-	-		
$\begin{array}{ c c c c c c c c c c c c c c c c c c c$	7	SF4	М	702	1	0,12,12	-	-	-		
9 FMN U 501 - 33,33,33 1.07 2 (6%) 48,50,50 1.34 7 (14%)	9	FMN	U	501	-	33,33,33	1.07	2(6%)	48,50,50	1.34	7 (14%)
7 SF4 P 302 4 0,12,12	7	SF4	Р	302	4	0,12,12	-	-	-		
7 SF4 S 701 1 0,12,12	7	SF4	S	701	1	0,12,12	-	-	-		
8 FES W 201 5 0,4,4	8	FES	W	201	5	0,4,4	-	-	-		
$\begin{array}{ c c c c c c c c c c c c c c c c c c c$	7	SF4	A	701	1	0,12,12	-	-	-		
$\begin{array}{ c c c c c c c c c c c c c c c c c c c$	7	SF4	V	301	4	0,12,12	-	-	-		
$\begin{array}{ c c c c c c c c c c c c c c c c c c c$	7	SF4	G	703	1	0,12,12	-	-	-		
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	7	SF4	D	301	4	0,12,12	-	-	-		
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	7	SF4	L	701	6	0,12,12	-	-	-		
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$		SF4 SF4	J	301	4	0,12,12	-	-	-		
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$		SF4 SF4	R C	701	0	0,12,12	-	-	-		
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$				703	1	0,12,12 0.12.12	-	-	-		
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	7	SF4 SF4	G A	704	1	0,12,12 0.12.12	-	-	-		
I DI H A 100 I 0,12,12 - <t< td=""><td>8</td><td>FES</td><td>л К</td><td>201</td><td>5</td><td>$\begin{array}{c} 0,12,12 \\ 0.4 \end{array}$</td><td></td><td></td><td></td><td></td><td></td></t<>	8	FES	л К	201	5	$\begin{array}{c} 0,12,12 \\ 0.4 \end{array}$					
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	7	SF4	D	302		$0, \pm, \pm$ 0 12 12					
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	7	SF4 SF4	0	502	3	0,12,12 0,12,12					
8 FES Q 201 5 044	8	FES	0	201	5	0.4.4	_	_	_		
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	7	SF4	J	302	4	0.12.12	_	_	_		
8 FES M 705 1 0,4,4	8	FES	M	705	1	0,4.4	_	_	_		



Mal	Turne	Chain	Dec	Link Bond lengths			Bond angles		
	туре	Chain	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ # Z > 2
7	SF4	U	502	3	$0,\!12,\!12$	-	-	-	
7	SF4	G	701	1	0,12,12	-	-	-	

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	\mathbf{Res}	Link	Chirals	Torsions	Rings
7	SF4	М	701	1	-	-	0/6/5/5
7	SF4	G	702	1	-	-	0/6/5/5
9	FMN	С	501	-	-	2/18/18/18	0/3/3/3
9	FMN	Ι	501	-	-	2/18/18/18	0/3/3/3
7	SF4	V	302	4	-	-	0/6/5/5
8	FES	G	705	1	-	-	0/1/1/1
7	SF4	Р	301	4	-	-	0/6/5/5
7	SF4	Ι	502	3	-	-	0/6/5/5
7	SF4	S	704	1	-	-	0/6/5/5
7	SF4	Х	701	6	-	-	0/6/5/5
9	FMN	0	501	-	-	2/18/18/18	0/3/3/3
7	SF4	F	701	6	-	-	0/6/5/5
7	SF4	М	703	1	-	-	0/6/5/5
7	SF4	М	704	1	-	-	0/6/5/5
7	SF4	А	702	1	-	-	0/6/5/5
7	SF4	А	704	1	-	-	0/6/5/5
7	SF4	S	702	1	-	-	0/6/5/5
7	SF4	С	502	3	-	-	0/6/5/5
8	FES	А	705	1	-	-	0/1/1/1
8	FES	S	705	1	-	-	0/1/1/1
8	FES	Е	201	5	-	-	0/1/1/1
7	SF4	М	702	1	-	-	0/6/5/5
9	FMN	U	501	-	-	2/18/18/18	0/3/3/3
7	SF4	Р	302	4	-	-	0/6/5/5
7	SF4	S	701	1	_	-	0/6/5/5
8	FES	W	201	5	_	-	0/1/1/1
7	SF4	А	701	1	-	-	0/6/5/5
7	SF4	V	301	4	-	-	0/6/5/5
7	SF4	G	703	1	-	-	0/6/5/5
7	SF4	D	301	4	-	-	0/6/5/5
7	SF4	L	701	6	-	-	0/6/5/5
7	SF4	J	301	4	-	-	0/6/5/5
7	SF4	R	701	6	-	-	0/6/5/5



7Q5Y	7
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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	SF4	S	703	1	-	-	0/6/5/5
7	SF4	G	704	1	-	-	0/6/5/5
7	SF4	А	703	1	-	-	0/6/5/5
8	FES	K	201	5	-	-	0/1/1/1
7	SF4	D	302	4	-	-	0/6/5/5
7	SF4	0	502	3	-	-	0/6/5/5
8	FES	Q	201	5	-	-	0/1/1/1
7	SF4	J	302	4	-	-	0/6/5/5
8	FES	М	705	1	-	-	0/1/1/1
7	SF4	U	502	3	-	-	0/6/5/5
7	SF4	G	701	1	-	-	0/6/5/5

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
9	U	501	FMN	C4A-N5	3.98	1.38	1.30
9	Ι	501	FMN	C4A-N5	3.87	1.38	1.30
9	0	501	FMN	C4A-N5	3.31	1.37	1.30
9	С	501	FMN	C4A-N5	3.04	1.36	1.30
9	С	501	FMN	C10-N1	2.46	1.38	1.33
9	U	501	FMN	C10-N1	2.26	1.37	1.33
9	Ι	501	FMN	C10-N1	2.15	1.37	1.33

	All ((32)	bond	angle	outliers	are	listed	below:
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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
9	0	501	FMN	C5'-C4'-C3'	-3.46	105.52	112.20
9	U	501	FMN	C4-N3-C2	-3.39	119.38	125.64
9	Ι	501	FMN	C5'-C4'-C3'	-3.31	105.82	112.20
9	0	501	FMN	C4-N3-C2	-3.10	119.91	125.64
9	U	501	FMN	C4A-C10-N10	3.07	120.97	116.48
9	С	501	FMN	C4-C4A-C10	3.02	121.87	116.79
9	U	501	FMN	O2-C2-N1	-3.01	116.84	121.83
9	0	501	FMN	C4A-C10-N10	2.82	120.61	116.48
9	U	501	FMN	O4-C4-C4A	-2.73	119.36	126.60
9	Ι	501	FMN	C4A-C10-N10	2.69	120.42	116.48
9	С	501	FMN	O4-C4-C4A	-2.65	119.58	126.60
9	С	501	FMN	C4-N3-C2	-2.60	120.83	125.64
9	0	501	FMN	O4-C4-C4A	-2.59	119.73	126.60
9	U	501	FMN	C4A-C4-N3	2.51	119.58	113.19
9	С	501	FMN	O2'-C2'-C1'	-2.50	103.75	109.80
9	Ι	501	FMN	O4'-C4'-C5'	2.50	115.53	109.92



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
9	0	501	FMN	C4-C4A-C10	2.47	120.94	116.79
9	Ι	501	FMN	C10-C4A-N5	-2.43	119.71	124.86
9	Ι	501	FMN	C4-N3-C2	-2.43	121.16	125.64
9	U	501	FMN	C10-C4A-N5	-2.39	119.79	124.86
9	Ι	501	FMN	C9A-C5A-N5	-2.34	119.89	122.43
9	С	501	FMN	C6-C5A-C9A	2.34	122.24	118.94
9	С	501	FMN	C4A-C10-N10	2.27	119.80	116.48
9	С	501	FMN	C10-C4A-N5	-2.16	120.28	124.86
9	С	501	FMN	C9A-C5A-N5	-2.15	120.10	122.43
9	0	501	FMN	C10-C4A-N5	-2.15	120.30	124.86
9	0	501	FMN	C9A-C5A-N5	-2.14	120.11	122.43
9	0	501	FMN	C4A-C4-N3	2.14	118.62	113.19
9	С	501	FMN	C4A-C10-N1	-2.13	119.80	124.73
9	Ι	501	FMN	P-O5'-C5'	2.12	124.14	118.30
9	Ι	501	FMN	C4A-C4-N3	2.11	118.54	113.19
9	U	501	FMN	O2'-C2'-C1'	-2.03	104.89	109.80

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	С	501	FMN	N10-C1'-C2'-O2'
9	С	501	FMN	C4'-C5'-O5'-P
9	0	501	FMN	C4'-C5'-O5'-P
9	Ι	501	FMN	C4'-C5'-O5'-P
9	U	501	FMN	C4'-C5'-O5'-P
9	U	501	FMN	N10-C1'-C2'-O2'
9	Ι	501	FMN	N10-C1'-C2'-O2'
9	0	501	FMN	N10-C1'-C2'-O2'

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	S	704	SF4	1	0
7	А	704	SF4	1	0
8	S	705	FES	1	0
8	W	201	FES	1	0
7	G	704	SF4	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 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	$OWAB(Å^2)$	Q<0.9
1	А	626/632~(99%)	-0.33	3 (0%) 91 92	37, 53, 90, 132	0
1	G	626/632~(99%)	-0.31	3 (0%) 91 92	38, 60, 93, 150	0
1	М	626/632~(99%)	-0.37	0 100 100	42,60,93,148	0
1	S	626/632~(99%)	-0.24	10 (1%) 72 74	50,69,99,138	0
2	В	585/586~(99%)	0.37	52 (8%) 9 7	51, 104, 155, 231	0
2	Н	585/586~(99%)	0.73	90~(15%) 2 1	58, 130, 188, 250	0
2	Ν	585/586~(99%)	0.42	59 (10%) 7 5	57, 108, 164, 237	0
2	Т	585/586~(99%)	0.44	58 (9%) 7 5	73, 115, 165, 236	0
3	С	419/426~(98%)	-0.25	1 (0%) 95 96	41, 62, 94, 127	0
3	Ι	419/426~(98%)	-0.30	1 (0%) 95 96	35, 52, 85, 129	0
3	Ο	419/426~(98%)	-0.18	3 (0%) 87 89	48, 74, 105, 172	0
3	U	419/426~(98%)	-0.08	6 (1%) 75 77	59, 80, 114, 165	0
4	D	197/201~(98%)	0.46	28 (14%) 2 1	48, 79, 198, 217	0
4	J	197/201~(98%)	0.68	35 (17%) 1 1	62, 105, 223, 267	0
4	Р	197/201~(98%)	0.59	32~(16%) 1 1	59, 94, 206, 254	0
4	V	197/201~(98%)	0.76	35 (17%) 1 1	76, 111, 204, 224	0
5	Е	155/160~(96%)	-0.48	0 100 100	35, 59, 83, 116	0
5	K	155/160~(96%)	-0.48	0 100 100	40, 59, 90, 119	0
5	Q	155/160~(96%)	-0.26	0 100 100	50, 80, 110, 145	0
5	W	155/160~(96%)	0.19	10 (6%) 18 17	61, 90, 127, 152	0
6	F	135/179~(75%)	0.35	9 (6%) 17 16	68, 95, 159, 180	0
6	L	135/179~(75%)	1.20	27~(20%) 1 0	99, 135, 191, 241	0
6	R	135/179~(75%)	1.10	$26\ (19\%)$ 1 0	76, 113, 181, 245	0
6	X	135/179~(75%)	0.80	23~(17%) 1 1	90, 123, 183, 238	0



Mol	Chain	Analysed	<RSRZ $>$	# RS	RZ>	2	$OWAB(Å^2)$	Q<0.9
All	All	8468/8736~(96%)	0.10	511 (6%)	21	20	35, 80, 159, 267	0

All (511) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	R	153	THR	13.3
6	R	152	ILE	10.2
4	J	19	LEU	9.7
3	0	1	MET	9.7
4	J	18	ILE	9.7
6	L	152	ILE	9.1
4	D	19	LEU	8.9
4	J	23	PHE	8.6
4	Р	44	PRO	8.5
2	Н	194	LYS	8.4
2	Н	585	ASP	8.4
4	V	23	PHE	8.3
4	Р	23	PHE	7.6
6	Х	153	THR	7.4
2	В	584	THR	7.4
6	L	153	THR	7.1
2	В	585	ASP	6.9
2	Т	585	ASP	6.9
6	R	154	LYS	6.8
4	D	23	PHE	6.8
6	Х	154	LYS	6.7
2	Н	199	LEU	6.7
2	В	196	LYS	6.6
2	Н	195	LYS	6.6
4	V	19	LEU	6.5
4	D	201	GLY	6.4
4	Р	19	LEU	6.4
4	D	12	LEU	6.2
6	Х	152	ILE	6.2
4	V	45	LYS	6.1
6	L	154	LYS	6.1
4	J	201	GLY	6.0
3	U	1	MET	6.0
4	Р	18	ILE	6.0
2	Ν	386	ILE	5.9
2	Н	389	ARG	5.8
4	J	20	PHE	5.8



7Q5Y

Mol	Chain	Res	Type	RSRZ
6	L	151	GLY	5.8
4	D	18	ILE	5.7
4	J	29	VAL	5.7
4	J	22	ASP	5.7
2	Ν	585	ASP	5.7
2	В	199	LEU	5.6
2	Ν	584	THR	5.6
2	Т	394	VAL	5.5
2	Т	582	GLY	5.4
2	В	389	ARG	5.4
4	D	17	SER	5.4
4	Р	5	LYS	5.3
2	Н	584	THR	5.3
6	R	150	GLN	5.2
2	N	196	LYS	5.2
2	Н	390	ARG	5.2
2	Ν	389	ARG	5.1
2	Т	263	ALA	5.0
4	V	12	LEU	5.0
2	Н	196	LYS	4.9
4	D	20	PHE	4.9
2	В	194	LYS	4.9
4	V	32	LYS	4.8
4	V	18	ILE	4.8
4	J	24	LEU	4.8
2	Т	260	TYR	4.7
2	Т	386	ILE	4.7
2	Ν	262	SER	4.7
4	V	21	ILE	4.7
4	Р	11	TYR	4.6
4	Р	16	GLU	4.6
4	D	13	ASN	4.6
4	Р	6	LEU	4.6
3	С	1	MET	4.6
2	Ν	259	ASP	4.5
2	Т	584	THR	4.5
4	D	14	ILE	4.5
6	L	63	GLN	4.4
2	Ν	200	VAL	4.4
4	Р	17	SER	4.4
2	Т	210	THR	4.4
4	J	21	ILE	4.4



7Q5Y

Mol	Chain	Res	Type	RSRZ
2	Ν	258	MET	4.4
4	D	11	TYR	4.4
2	В	263	ALA	4.4
2	В	387	TRP	4.4
4	J	28	SER	4.3
4	Р	22	ASP	4.3
4	V	201	GLY	4.3
4	D	21	ILE	4.3
2	Н	258	MET	4.3
2	В	582	GLY	4.3
4	V	5	LYS	4.2
6	L	23	ARG	4.2
2	Н	263	ALA	4.2
2	Н	582	GLY	4.2
2	В	198	GLU	4.2
2	В	386	ILE	4.2
2	Н	526	PRO	4.2
2	В	475	LYS	4.2
2	Т	258	MET	4.2
4	D	30	THR	4.2
2	Т	392	LYS	4.1
2	Т	383	ARG	4.1
4	Р	12	LEU	4.1
2	В	383	ARG	4.1
4	V	20	PHE	4.1
5	W	6	PHE	4.1
6	R	35	CYS	4.0
4	D	28	SER	4.0
4	V	17	SER	4.0
2	Т	197	ALA	4.0
2	Н	387	TRP	4.0
2	Ν	341	LEU	3.9
4	V	24	LEU	3.9
6	F	53	LEU	3.9
4	J	17	SER	3.9
2	Т	198	GLU	3.9
2	В	388	LEU	3.9
6	L	53	LEU	3.9
6	Х	23	ARG	3.9
4	J	32	LYS	3.9
6	L	146	LYS	3.9
4	J	10	ASP	3.9



7Q5Y

Mol	Chain	Res	Type	RSRZ
2	В	210	THR	3.8
2	В	258	MET	3.8
2	Ν	210	THR	3.8
2	Н	262	SER	3.8
6	F	23	ARG	3.8
4	V	196	LYS	3.8
2	Н	580	VAL	3.8
2	Ν	16	PHE	3.8
2	Н	386	ILE	3.7
6	L	50	LEU	3.7
4	J	16	GLU	3.7
4	D	29	VAL	3.7
2	Т	390	ARG	3.7
2	Т	262	SER	3.7
6	R	34	ALA	3.7
2	Ν	580	VAL	3.7
2	Н	383	ARG	3.7
4	Р	196	LYS	3.7
6	R	23	ARG	3.7
2	Н	221	GLU	3.7
4	Р	13	ASN	3.7
4	D	8	ARG	3.6
6	R	93	TRP	3.6
6	R	151	GLY	3.6
2	В	219	ASP	3.6
2	Ν	383	ARG	3.6
2	Т	199	LEU	3.6
2	Т	580	VAL	3.6
4	Р	10	ASP	3.6
2	N	194	LYS	3.6
2	Н	197	ALA	3.6
2	Н	393	ASP	3.6
2	Н	450	LEU	3.6
4	Р	21	ILE	3.6
1	G	629	GLU	3.6
2	Т	220	LEU	3.6
6	R	130	PRO	3.6
6	L	56	ILE	3.6
4	Р	32	LYS	3.6
2	В	220	LEU	3.6
4	J	27	LEU	3.6
2	Т	84	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
2	Ν	221	GLU	3.5
2	Т	464	GLU	3.5
2	В	579	PRO	3.5
2	В	262	SER	3.5
6	R	129	CYS	3.5
2	Т	196	LYS	3.5
4	J	11	TYR	3.5
3	Ι	1	MET	3.5
2	Ν	263	ALA	3.5
4	D	22	ASP	3.5
2	Н	260	TYR	3.5
2	Н	193	LEU	3.5
4	D	6	LEU	3.5
4	J	13	ASN	3.4
6	L	26	LEU	3.4
6	R	36	CYS	3.4
4	V	11	TYR	3.4
6	R	26	LEU	3.4
4	D	24	LEU	3.4
4	J	14	ILE	3.4
6	R	56	ILE	3.4
2	В	197	ALA	3.4
2	В	259	ASP	3.4
2	Ν	195	LYS	3.4
4	V	8	ARG	3.4
2	В	227	GLN	3.4
2	Н	210	THR	3.3
6	R	57	PHE	3.3
2	Н	569	ASP	3.3
6	R	71	GLY	3.3
2	Н	224	LYS	3.3
3	0	2	ARG	3.3
2	N	199	LEU	3.3
2	N	265	CYS	3.3
4	D	26	GLY	3.3
2	Т	579	PRO	3.3
4	V	29	VAL	3.3
6	L	150	GLN	3.3
6	X	34	ALA	3.3
6	F	26	LEU	3.3
2	Н	259	ASP	3.3
4	J	12	LEU	3.3



7Q5Y

Mol	Chain	Res	Type	RSRZ
2	В	390	ARG	3.3
2	Н	342	THR	3.3
2	Н	391	THR	3.2
2	В	581	VAL	3.2
2	Ν	212	GLY	3.2
4	V	28	SER	3.2
6	L	35	CYS	3.2
4	J	5	LYS	3.2
4	D	5	LYS	3.2
2	Н	95	LEU	3.2
4	D	7	SER	3.2
2	Т	379	THR	3.2
2	Т	391	THR	3.2
4	V	47	LYS	3.2
4	Р	28	SER	3.2
2	Ν	582	GLY	3.2
2	Ν	390	ARG	3.2
2	В	382	THR	3.1
2	В	580	VAL	3.1
4	J	9	LYS	3.1
4	D	15	LEU	3.1
2	Н	382	THR	3.1
2	Н	385	ARG	3.1
2	Т	389	ARG	3.1
2	N	583	GLU	3.1
6	Х	93	TRP	3.1
2	Н	161	LEU	3.1
2	Т	527	ARG	3.1
2	Т	342	THR	3.1
2	Ν	163	GLY	3.1
4	V	25	LYS	3.1
2	В	392	LYS	3.1
6	R	41	MET	3.1
2	В	193	LEU	3.1
4	V	34	LEU	3.1
4	J	36	ARG	3.1
4	J	25	LYS	3.0
6	Х	148	LYS	3.0
2	N	527	ARG	3.0
4	Р	20	PHE	3.0
2	Т	581	VAL	3.0
2	N	260	TYR	3.0

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7Q5Y

Mol	Chain	Res	Type	RSRZ
2	Ν	266	ASN	3.0
6	Х	36	CYS	3.0
2	Н	218	PHE	3.0
4	J	8	ARG	3.0
4	D	25	LYS	2.9
2	Ν	382	THR	2.9
6	Х	150	GLN	2.9
2	Н	198	GLU	2.9
6	R	88	MET	2.9
2	Т	583	GLU	2.9
2	В	222	GLY	2.9
2	Т	256	ASP	2.9
1	А	629	GLU	2.9
2	Н	261	ILE	2.9
6	X	35	CYS	2.9
4	V	173	LYS	2.9
2	Т	174	LEU	2.9
1	S	5	VAL	2.9
6	L	37	ALA	2.9
2	Н	163	GLY	2.8
2	Н	440	GLY	2.8
2	Н	379	THR	2.8
2	Ν	308	THR	2.8
4	V	9	LYS	2.8
6	L	62	ARG	2.8
2	Т	255	THR	2.8
4	J	30	THR	2.8
2	Ν	394	VAL	2.8
2	Н	564	GLY	2.8
2	В	472	LYS	2.8
6	X	56	ILE	2.8
2	Ν	301	SER	2.8
2	Т	211	HIS	2.8
2	В	342	THR	2.8
2	Н	570	ALA	2.8
4	D	32	LYS	2.8
2	В	16	PHE	2.8
2	Н	256	ASP	2.8
2	Т	393	ASP	2.8
2	Т	367	ILE	2.8
4	J	6	LEU	2.8
2	Ν	197	ALA	2.8



7Q5Y

Mol	Chain	Res	Type	RSRZ
4	V	16	GLU	2.8
4	D	31	LEU	2.8
5	W	107	LEU	2.8
5	W	152	LEU	2.8
2	Н	528	GLY	2.8
2	Т	265	CYS	2.8
4	Р	29	VAL	2.7
4	V	22	ASP	2.7
2	В	260	TYR	2.7
2	Н	381	LEU	2.7
2	Н	200	VAL	2.7
2	N	220	LEU	2.7
1	S	17	GLU	2.7
6	L	34	ALA	2.7
2	В	195	LYS	2.7
2	Н	178	LYS	2.7
6	Х	129	CYS	2.7
4	V	6	LEU	2.7
6	F	27	TRP	2.7
2	Н	265	CYS	2.7
6	L	149	GLU	2.7
2	Т	259	ASP	2.7
2	Т	301	SER	2.7
4	Р	15	LEU	2.7
4	V	14	ILE	2.7
2	Ν	198	GLU	2.7
2	Т	223	GLU	2.7
4	V	13	ASN	2.7
6	Х	65	ASP	2.7
6	L	80	MET	2.7
4	J	33	ASN	2.7
2	Н	219	ASP	2.7
4	Р	27	LEU	2.6
6	R	148	LYS	2.6
5	W	41	TYR	2.6
4	Р	201	GLY	2.6
2	N	579	PRO	2.6
6	F	35	CYS	2.6
6	R	37	ALA	2.6
4	J	15	LEU	2.6
2	Н	321	TYR	2.6
4	Р	9	LYS	2.6



7Q5Y

Mol	Chain	Res	Type	RSRZ
2	Н	388	LEU	2.6
2	В	256	ASP	2.6
2	Н	255	THR	2.6
2	Н	583	GLU	2.6
2	Ν	165	THR	2.6
2	Т	253	PRO	2.6
2	Т	417	VAL	2.6
6	Х	72	THR	2.6
1	S	22	VAL	2.6
2	Н	75	LEU	2.6
2	Ν	342	THR	2.5
2	Н	215	TRP	2.5
2	Т	221	GLU	2.5
2	В	226	VAL	2.5
2	Н	20	VAL	2.5
2	Н	220	LEU	2.5
2	В	399	ARG	2.5
4	Р	33	ASN	2.5
4	V	44	PRO	2.5
4	V	10	ASP	2.5
2	Н	581	VAL	2.5
2	Ν	321	TYR	2.5
6	R	63	GLN	2.5
6	L	93	TRP	2.5
2	Н	216	PHE	2.5
2	Н	579	PRO	2.5
1	S	16	ALA	2.5
2	Ν	211	HIS	2.5
6	R	58	ARG	2.5
4	V	199	TRP	2.5
2	Ν	160	VAL	2.5
2	Ν	255	THR	2.5
6	F	152	ILE	2.5
6	X	27	TRP	2.5
4	J	45	LYS	2.5
2	H	578	ASP	2.5
1	G	16	ALA	2.5
2	Ν	472	LYS	2.5
2	Н	301	SER	2.5
2	Т	193	LEU	2.4
2	Т	528	GLY	2.4
2	Т	194	LYS	2.4

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7Q5Y

Mol	Chain	Res	Type	RSRZ
2	Т	475	LYS	2.4
2	В	211	HIS	2.4
4	J	37	ARG	2.4
4	Р	8	ARG	2.4
4	Р	36	ARG	2.4
6	Х	53	LEU	2.4
4	V	81	GLU	2.4
2	Н	468	GLN	2.4
4	D	10	ASP	2.4
1	S	624	ILE	2.4
1	S	69	VAL	2.4
2	Н	525	ASN	2.4
2	N	446	TYR	2.4
2	Т	381	LEU	2.4
2	Т	551	ALA	2.4
4	J	7	SER	2.4
6	F	63	GLN	2.4
6	L	25	SER	2.4
4	Р	128	LEU	2.4
2	Н	475	LYS	2.4
2	Т	257	ARG	2.4
2	В	301	SER	2.4
2	Т	344	CYS	2.4
5	W	120	PHE	2.4
6	Х	151	GLY	2.3
1	S	15	GLU	2.3
2	Н	223	GLU	2.3
6	Х	21	GLY	2.3
2	Н	300	ASN	2.3
2	В	118	VAL	2.3
4	D	16	GLU	2.3
5	W	8	PHE	2.3
2	Н	185	LEU	2.3
4	J	182	ARG	2.3
2	N	393	ASP	2.3
2	Н	188	THR	2.3
1	A	71	GLU	2.3
2	Н	226	VAL	2.3
4	V	63	TRP	2.3
6	L	98	GLY	2.3
4	J	34	LEU	2.3
4	Р	24	LEU	2.3



7Q5Y

Mol	Chain	Res	Type	RSRZ
5	W	155	ILE	2.3
4	J	26	GLY	2.3
1	G	433	ASN	2.3
2	Н	157	LEU	2.3
2	Н	266	ASN	2.3
2	Т	235	LEU	2.3
6	L	72	THR	2.3
2	Н	472	LYS	2.3
2	Ν	395	GLY	2.2
6	Х	71	GLY	2.2
2	Ν	313	LEU	2.2
4	D	27	LEU	2.2
6	Х	41	MET	2.2
2	N	340	ARG	2.2
3	0	416	LYS	2.2
2	H	394	VAL	2.2
5	W	11	GLU	2.2
6	F	34	ALA	2.2
2	Н	16	PHE	2.2
2	Н	442	VAL	2.2
2	Ν	344	CYS	2.2
2	Н	392	LYS	2.2
5	W	156	LEU	2.2
2	Ν	391	THR	2.2
4	V	26	GLY	2.2
2	Т	266	ASN	2.2
2	Н	527	ARG	2.2
2	N	261	ILE	2.2
4	V	27	LEU	2.2
2	Н	222	GLY	2.2
2	Т	446	TYR	2.2
2	Н	211	HIS	2.2
2	В	265	CYS	2.2
2	В	583	GLU	2.2
2	N	223	GLU	2.2
3	U	347	CYS	2.2
6	F	149	GLU	2.2
6	L	144	GLN	2.2
3	U	348	GLY	2.2
1	S	626	VAL	2.2
2	H	341	LEU	2.2
2	Н	59	CYS	2.2



Mol	Chain	Res	Type	RSRZ
3	U	346	THR	2.2
4	Р	186	ASN	2.1
6	L	24	ASN	2.1
2	Н	118	VAL	2.1
3	U	327	GLU	2.1
4	V	46	GLU	2.1
6	Х	66	VAL	2.1
4	Р	37	ARG	2.1
2	В	266	ASN	2.1
1	А	5	VAL	2.1
2	Н	60	ILE	2.1
2	Т	227	GLN	2.1
2	Н	174	LEU	2.1
2	Ν	253	PRO	2.1
6	R	53	LEU	2.1
2	Н	473	LEU	2.1
2	Т	385	ARG	2.1
6	Х	37	ALA	2.1
2	Ν	525	ASN	2.1
6	L	129	CYS	2.1
2	В	52	LEU	2.1
2	В	378	HIS	2.1
2	Н	43	LYS	2.1
2	Н	48	ARG	2.1
4	Р	43	TYR	2.1
6	L	148	LYS	2.1
2	Т	212	GLY	2.1
2	В	47	GLU	2.1
4	J	188	GLU	2.1
2	В	213	THR	2.1
6	R	146	LYS	2.1
2	В	91	LYS	2.1
2	N	475	LYS	2.1
6	Х	146	LYS	2.1
2	Т	300	ASN	2.1
4	Р	7	SER	2.1
6	R	65	ASP	2.1
5	W	118	GLY	2.1
2	Ν	256	ASP	2.0
1	S	7	ILE	2.0
1	S	14	ILE	2.0
6	L	75	ASN	2.0



Mol	Chain	Res	Type	RSRZ
2	Т	549	SER	2.0
2	Н	378	HIS	2.0
2	Н	180	PRO	2.0
2	В	43	LYS	2.0
2	В	391	THR	2.0
3	U	377	TRP	2.0
2	Н	237	ARG	2.0
2	Ν	201	LEU	2.0
2	N	217	LEU	2.0
6	R	50	LEU	2.0
2	N	302	HIS	2.0
2	В	96	PRO	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, 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	$B-factors(A^2)$	Q<0.9
7	SF4	G	704	8/8	0.94	0.12	99,123,183,232	8
7	SF4	М	704	8/8	0.94	0.11	100,154,218,234	8
7	SF4	S	704	8/8	0.94	0.12	84,136,176,213	8
7	SF4	А	704	8/8	0.95	0.13	78,96,170,191	8
9	FMN	С	501	31/31	0.98	0.21	41,55,65,67	0
9	FMN	0	501	31/31	0.98	0.20	48,54,65,78	0
9	FMN	U	501	31/31	0.98	0.25	61,69,74,82	0
7	SF4	А	702	8/8	0.99	0.19	39,41,46,49	0
7	SF4	J	301	8/8	0.99	0.18	77,81,83,83	0
7	SF4	J	302	8/8	0.99	0.14	69,74,78,79	0
7	SF4	L	701	8/8	0.99	0.23	99,106,113,122	0



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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	SF4	D	301	8/8	0.99	0.17	60.62.65.67	0
7	SF4	Р	301	8/8	0.99	0.17	66,71,74,74	0
7	SF4	Р	302	8/8	0.99	0.15	58.65.69.72	0
7	SF4	R	701	8/8	0.99	0.23	78,83,92,97	0
7	SF4	S	703	8/8	0.99	0.18	51,54,57,59	0
7	SF4	D	302	8/8	0.99	0.16	54,57,59,60	0
7	SF4	U	502	8/8	0.99	0.20	62,65,69,70	0
7	SF4	V	301	8/8	0.99	0.17	85,87,89,90	0
7	SF4	Х	701	8/8	0.99	0.22	96,99,101,101	0
8	FES	Е	201	4/4	0.99	0.19	$53,\!56,\!57,\!59$	0
8	FES	Κ	201	4/4	0.99	0.17	52,52,53,53	0
8	FES	Q	201	4/4	0.99	0.19	66,72,77,79	0
8	FES	W	201	4/4	0.99	0.17	74,78,81,91	0
7	SF4	F	701	8/8	0.99	0.20	70,72,74,75	0
9	FMN	Ι	501	31/31	0.99	0.19	32,44,54,60	0
7	SF4	G	701	8/8	0.99	0.15	46,54,57,57	0
7	SF4	G	703	8/8	0.99	0.19	42,44,46,46	0
7	SF4	М	702	8/8	1.00	0.18	47,51,53,55	0
7	SF4	М	703	8/8	1.00	0.18	48,50,54,67	0
7	SF4	V	302	8/8	1.00	0.12	80,82,85,90	0
7	SF4	С	502	8/8	1.00	0.19	45,50,52,52	0
8	FES	А	705	4/4	1.00	0.18	51,52,54,57	0
7	SF4	0	502	8/8	1.00	0.19	52,55,58,60	0
8	FES	G	705	4/4	1.00	0.18	$50,\!50,\!52,\!52$	0
7	SF4	Ι	502	8/8	1.00	0.22	$43,\!47,\!49,\!53$	0
8	FES	М	705	4/4	1.00	0.17	52,53,54,54	0
7	SF4	А	703	8/8	1.00	0.18	$37,\!42,\!46,\!47$	0
8	FES	S	705	4/4	1.00	0.15	$6\overline{5},\!66,\!69,\!71$	0
7	SF4	G	702	8/8	1.00	0.19	44,47,50,50	0
7	SF4	S	701	8/8	1.00	0.15	67,69,74,79	0
7	SF4	S	702	8/8	1.00	0.18	58,62,65,66	0
7	SF4	А	701	8/8	1.00	0.17	45,50,53,53	0
7	SF4	М	701	8/8	1.00	0.15	$5\overline{0,}54,\!56,\!58$	0

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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.

