



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 06:41 am GMT

PDB ID : 2FRV  
Title : CRYSTAL STRUCTURE OF THE OXIDIZED FORM OF NI-FE HYDRO-  
GENASE  
Authors : Volbeda, A.; Frey, M.; Fontecilla-Camps, J.C.  
Deposited on : 1997-06-10  
Resolution : 2.54 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

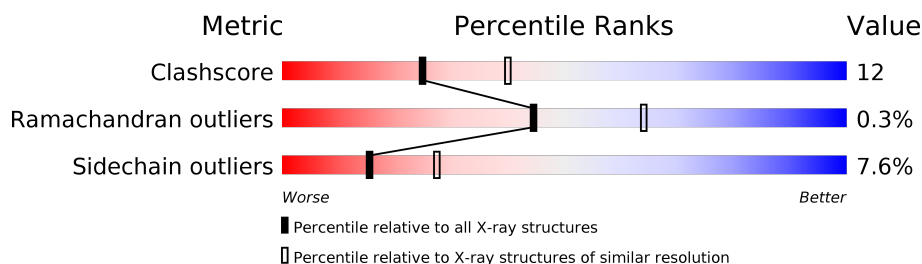
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.54 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))
Clashscore	112137	5755 (2.58-2.50)
Ramachandran outliers	110173	5652 (2.58-2.50)
Sidechain outliers	110143	5654 (2.58-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$ . 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	264	
1	C	264	
1	E	264	
1	G	264	
1	I	264	
1	S	264	
2	B	536	

*Continued on next page...*

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Mol	Chain	Length	Quality of chain
2	D	536	 63% 30% 5% ..
2	F	536	 62% 31% 5% ..
2	H	536	 63% 30% 5% ..
2	J	536	 63% 30% 5% ..
2	L	536	 63% 30% 5% ..

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
7	FCO	B	537	-	-	X	-
7	FCO	D	537	-	-	X	-
7	FCO	F	537	-	-	X	-
7	FCO	H	537	-	-	X	-
7	FCO	J	537	-	-	X	-
7	FCO	L	537	-	-	X	-

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 38040 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 PERIPLASMIC HYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	S	261	Total	C	N	O	S	0	0	0
			1964	1249	329	367	19			
1	A	261	Total	C	N	O	S	0	0	0
			1964	1249	329	367	19			
1	C	261	Total	C	N	O	S	0	0	0
			1964	1249	329	367	19			
1	E	261	Total	C	N	O	S	0	0	0
			1964	1249	329	367	19			
1	G	261	Total	C	N	O	S	0	0	0
			1964	1249	329	367	19			
1	I	261	Total	C	N	O	S	0	0	0
			1964	1249	329	367	19			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	24	VAL	LEU	CONFLICT	UNP P12943
S	89	GLY	ARG	CONFLICT	UNP P12943
A	24	VAL	LEU	CONFLICT	UNP P12943
A	89	GLY	ARG	CONFLICT	UNP P12943
C	24	VAL	LEU	CONFLICT	UNP P12943
C	89	GLY	ARG	CONFLICT	UNP P12943
E	24	VAL	LEU	CONFLICT	UNP P12943
E	89	GLY	ARG	CONFLICT	UNP P12943
G	24	VAL	LEU	CONFLICT	UNP P12943
G	89	GLY	ARG	CONFLICT	UNP P12943
I	24	VAL	LEU	CONFLICT	UNP P12943
I	89	GLY	ARG	CONFLICT	UNP P12943

- Molecule 2 is a protein called PERIPLASMIC HYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	530	Total 4152	C 2653	N 725	O 757	S 17	0	0	0
2	B	530	Total 4152	C 2653	N 725	O 757	S 17	0	0	0
2	D	530	Total 4152	C 2653	N 725	O 757	S 17	0	0	0
2	F	530	Total 4152	C 2653	N 725	O 757	S 17	0	0	0
2	H	530	Total 4152	C 2653	N 725	O 757	S 17	0	0	0
2	J	530	Total 4152	C 2653	N 725	O 757	S 17	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	144	LYS	ARG	CONFLICT	UNP P12944
L	332	GLY	ASP	CONFLICT	UNP P12944
L	482	LEU	HIS	CONFLICT	UNP P12944
L	497	GLY	ARG	CONFLICT	UNP P12944
B	144	LYS	ARG	CONFLICT	UNP P12944
B	332	GLY	ASP	CONFLICT	UNP P12944
B	482	LEU	HIS	CONFLICT	UNP P12944
B	497	GLY	ARG	CONFLICT	UNP P12944
D	144	LYS	ARG	CONFLICT	UNP P12944
D	332	GLY	ASP	CONFLICT	UNP P12944
D	482	LEU	HIS	CONFLICT	UNP P12944
D	497	GLY	ARG	CONFLICT	UNP P12944
F	144	LYS	ARG	CONFLICT	UNP P12944
F	332	GLY	ASP	CONFLICT	UNP P12944
F	482	LEU	HIS	CONFLICT	UNP P12944
F	497	GLY	ARG	CONFLICT	UNP P12944
H	144	LYS	ARG	CONFLICT	UNP P12944
H	332	GLY	ASP	CONFLICT	UNP P12944
H	482	LEU	HIS	CONFLICT	UNP P12944
H	497	GLY	ARG	CONFLICT	UNP P12944
J	144	LYS	ARG	CONFLICT	UNP P12944
J	332	GLY	ASP	CONFLICT	UNP P12944
J	482	LEU	HIS	CONFLICT	UNP P12944
J	497	GLY	ARG	CONFLICT	UNP P12944

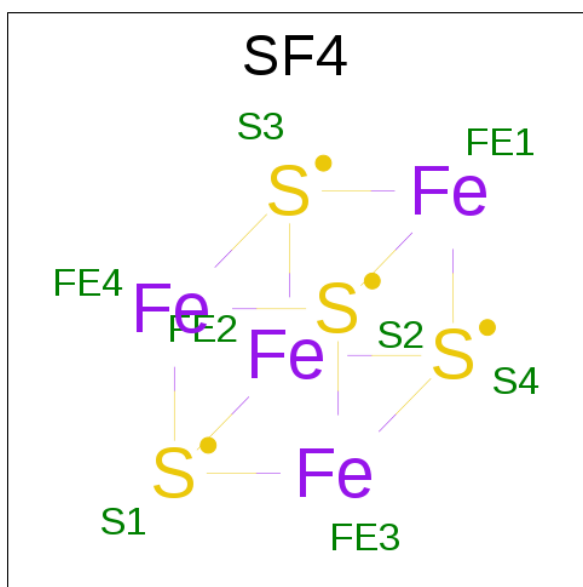
- Molecule 3 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	J	1	Total Ni 1 1	0	0
3	D	1	Total Ni 1 1	0	0
3	H	1	Total Ni 1 1	0	0
3	B	1	Total Ni 1 1	0	0
3	L	1	Total Ni 1 1	0	0
3	F	1	Total Ni 1 1	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

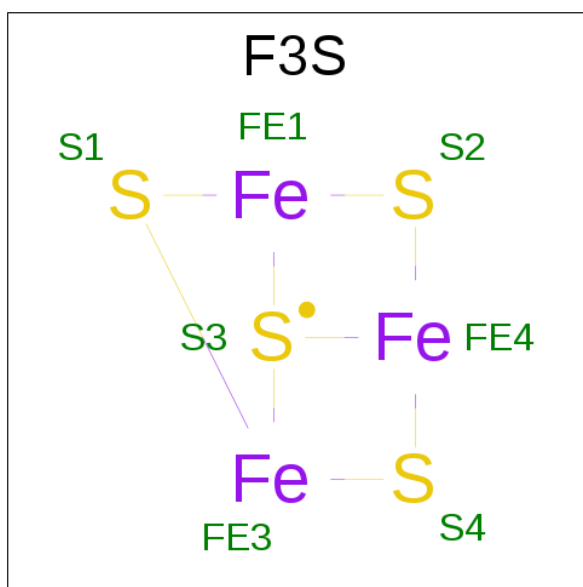
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	J	1	Total Mg 1 1	0	0
4	D	1	Total Mg 1 1	0	0
4	H	1	Total Mg 1 1	0	0
4	B	1	Total Mg 1 1	0	0
4	L	1	Total Mg 1 1	0	0
4	F	1	Total Mg 1 1	0	0

- Molecule 5 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	S	1	Total	Fe	S	0	0
			8	4	4		
5	S	1	Total	Fe	S	0	0
			8	4	4		
5	A	1	Total	Fe	S	0	0
			8	4	4		
5	A	1	Total	Fe	S	0	0
			8	4	4		
5	C	1	Total	Fe	S	0	0
			8	4	4		
5	C	1	Total	Fe	S	0	0
			8	4	4		
5	E	1	Total	Fe	S	0	0
			8	4	4		
5	E	1	Total	Fe	S	0	0
			8	4	4		
5	G	1	Total	Fe	S	0	0
			8	4	4		
5	G	1	Total	Fe	S	0	0
			8	4	4		
5	I	1	Total	Fe	S	0	0
			8	4	4		
5	I	1	Total	Fe	S	0	0
			8	4	4		

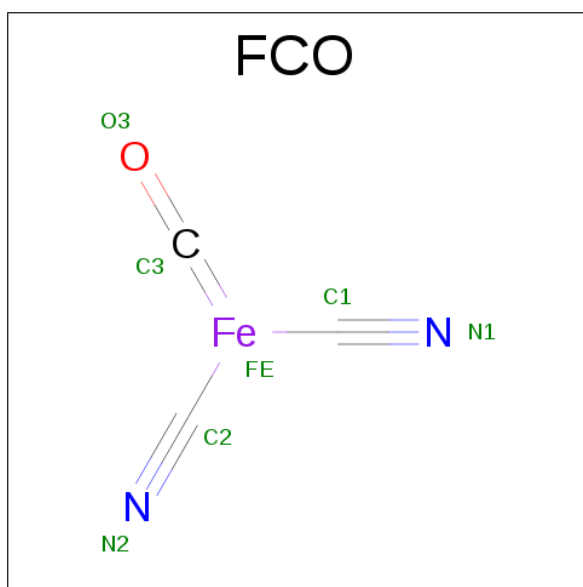
- Molecule 6 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe<sub>3</sub>S<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	S	1	Total	Fe	S	0	0
			7	3	4		
6	A	1	Total	Fe	S	0	0
			7	3	4		
6	C	1	Total	Fe	S	0	0
			7	3	4		
6	E	1	Total	Fe	S	0	0
			7	3	4		
6	G	1	Total	Fe	S	0	0
			7	3	4		
6	I	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 7 is CARBONMONOXIDE-(DICYANO) IRON (three-letter code: FCO) (formula:  $C_3FeN_2O$ ).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	L	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		
7	B	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		
7	D	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		
7	F	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		
7	H	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		
7	J	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		

- Molecule 8 is OXYGEN ATOM (three-letter code: O) (formula: O).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	J	1	Total	O	0	0
			1	1		
8	D	1	Total	O	0	0
			1	1		
8	H	1	Total	O	0	0
			1	1		
8	B	1	Total	O	0	0
			1	1		
8	L	1	Total	O	0	0
			1	1		
8	F	1	Total	O	0	0
			1	1		

- Molecule 9 is water.

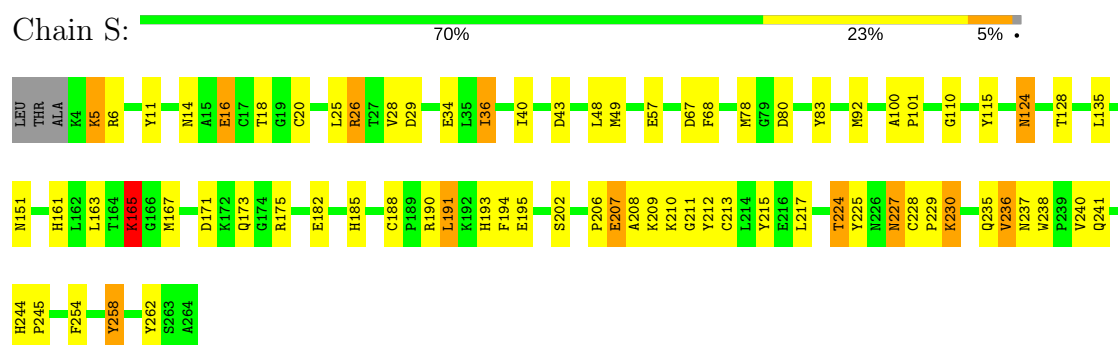
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	78	Total O 78 78	0	0
9	B	114	Total O 114 114	0	0
9	C	76	Total O 76 76	0	0
9	D	114	Total O 114 114	0	0
9	E	81	Total O 81 81	0	0
9	F	115	Total O 115 115	0	0
9	G	76	Total O 76 76	0	0
9	H	112	Total O 112 112	0	0
9	I	80	Total O 80 80	0	0
9	J	113	Total O 113 113	0	0
9	L	110	Total O 110 110	0	0
9	S	77	Total O 77 77	0	0

### 3 Residue-property plots

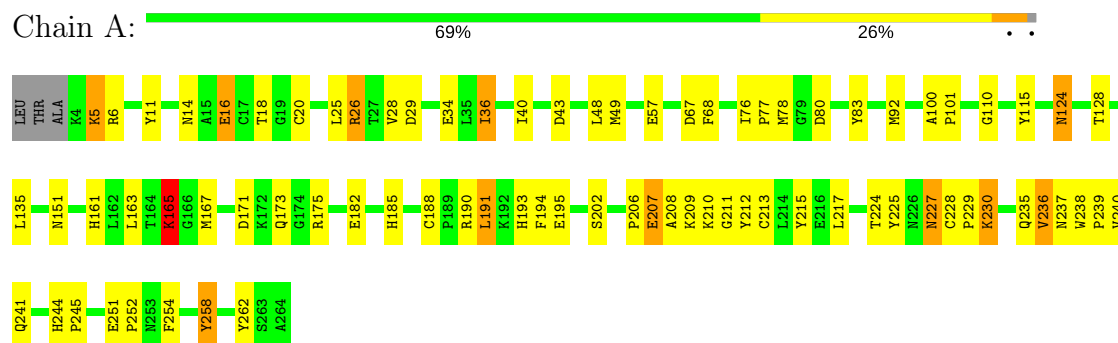
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

Note EDS was not executed.

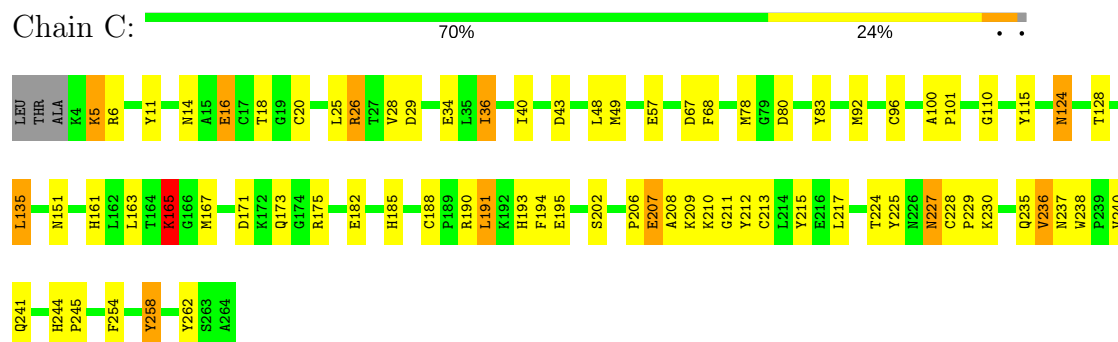
#### • Molecule 1: PERIPLASMIC HYDROGENASE



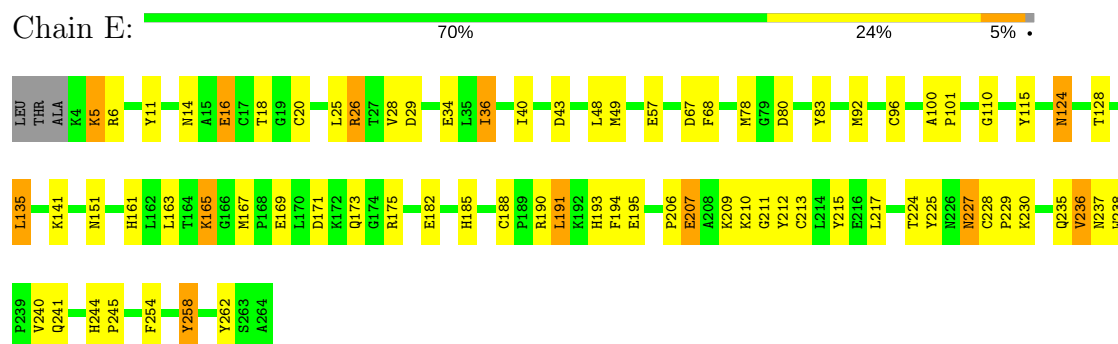
#### • Molecule 1: PERIPLASMIC HYDROGENASE



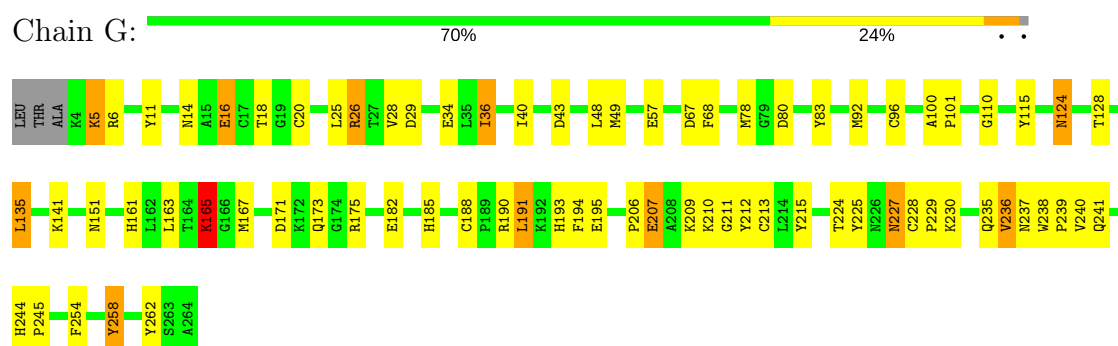
#### • Molecule 1: PERIPLASMIC HYDROGENASE



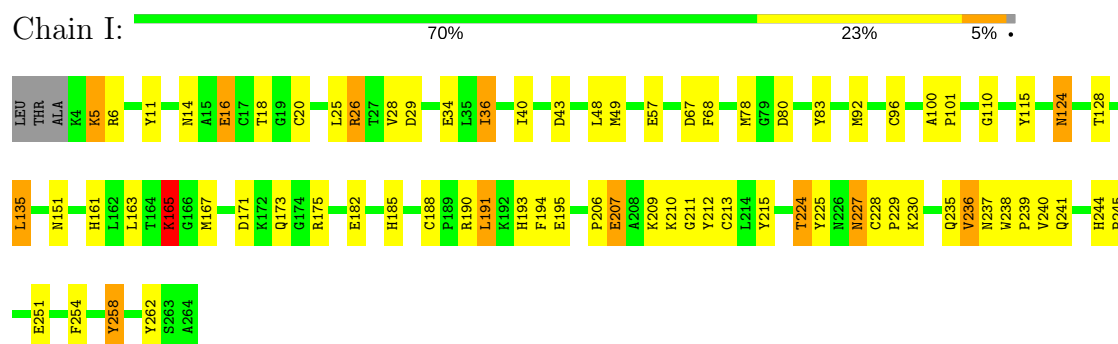
• Molecule 1: PERIPLASMIC HYDROGENASE



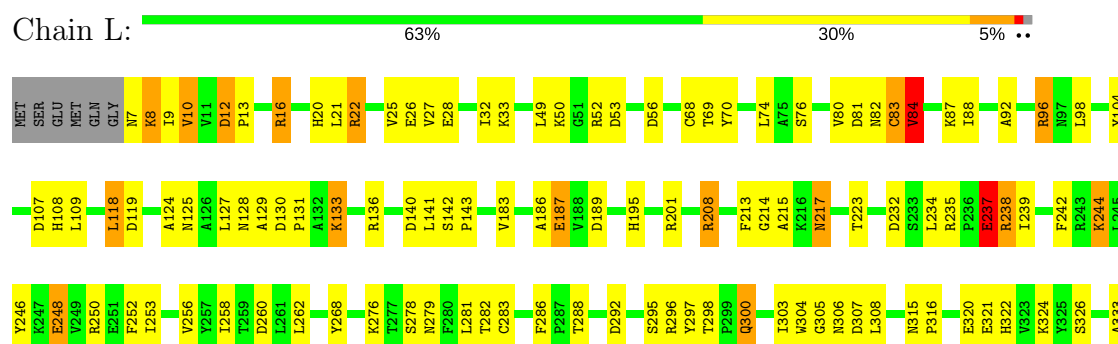
• Molecule 1: PERIPLASMIC HYDROGENASE

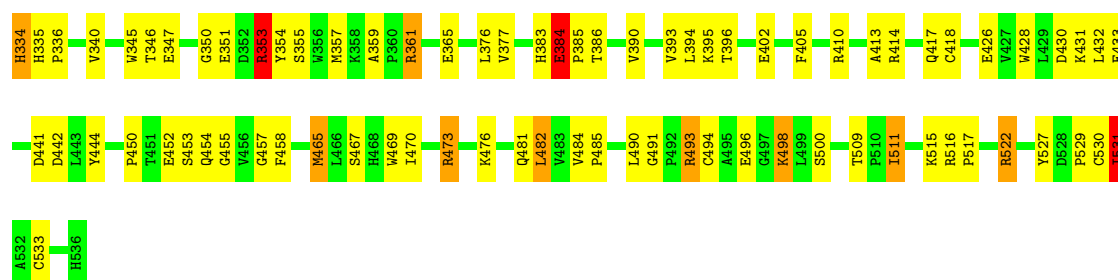


• Molecule 1: PERIPLASMIC HYDROGENASE



• Molecule 2: PERIPLASMIC HYDROGENASE





# Chain F:

Item	Category
Y527	62%
D528	62%
P529	62%
C530	62%
I531	62%
A532	62%
C533	62%
H536	62%
L432	62%
E433	62%
D441	62%
D442	62%
L443	62%
Y444	62%
Q448	62%
Y449	62%
F450	62%
T451	62%
E452	62%
S453	62%
Q454	62%
A455	62%
V456	62%
G457	62%
F458	62%
M465	62%
L466	62%
S467	62%
G468	62%
W469	62%
L470	62%
R473	62%
K476	62%
L477	62%
Q481	62%
L482	62%
V483	62%
Y484	62%
F485	62%
L490	62%
G491	62%
P492	62%
R493	62%
C494	62%
A495	62%
E496	62%
G497	62%
V498	62%
L499	62%
S500	62%
T509	62%
P510	62%
I511	62%
K515	62%
R516	62%
P517	62%
R522	62%
H334	62%
H335	62%
P336	62%
V340	62%
W345	62%
T346	62%
E347	62%
G350	62%
E351	62%
D352	62%
R353	62%
Y354	62%
S355	62%
W356	62%
K357	62%
K358	62%
A359	62%
P360	62%
R361	62%
E365	62%
L376	62%
V377	62%
H383	62%
E384	62%
P385	62%
T386	62%
V390	62%
V393	62%
L394	62%
K395	62%
T396	62%
E402	62%
F405	62%
L408	62%
G409	62%
R410	62%
A413	62%
R414	62%
Q417	62%
C418	62%
E426	62%
V427	62%
W428	62%
L429	62%
D430	62%
R431	62%
E243	62%
K244	62%
L245	62%
Y246	62%
E248	62%
V249	62%
R250	62%
E251	62%
F252	62%
T253	62%
V256	62%
T257	62%
Y258	62%
T259	62%
D260	62%
L261	62%
L262	62%
Y268	62%
K276	62%
T277	62%
S278	62%
M279	62%
F280	62%
L281	62%
T282	62%
C283	62%
F286	62%
P287	62%
T288	62%
D292	62%
S295	62%
R296	62%
Y297	62%
T298	62%
P299	62%
Q300	62%
L303	62%
W304	62%
G305	62%
N306	62%
D307	62%
L308	62%
E320	62%
E321	62%
H322	62%
V323	62%
K324	62%
V325	62%
W326	62%
L327	62%
E328	62%
R208	31%
F213	31%
G214	31%
A215	31%
K216	31%
N217	31%
T223	31%
D232	31%
S233	31%
L234	31%
R235	31%
E236	31%
E237	31%
L238	31%
L239	31%
F242	31%
R201	31%
H195	31%
A186	31%
E187	31%
V188	31%
D189	31%
H183	31%
A132	31%
K133	31%
R136	31%
D140	31%
L141	31%
S142	31%
P143	31%
V149	31%
K501	31%
G51	31%
R52	31%
D53	31%
D56	31%
C68	31%
T69	31%
Y70	31%
L74	31%
A75	31%
S76	31%
V80	

# Chain H:

63%

30%

C550	L432	Y825	F242	MET
A532	E433	S526	R96	SER
C533	D441	A333	K244	GLU
	D442	H334	L245	MET
	L443	H335	Y247	GLN
H536	Y444	P336	E248	GLY
	P450	V340	Y249	N7
	T451	G350	E256	K8
	E452	T351	Y257	I9
	S453	D352	T258	V10
	Q454	R353	D260	V11
	G455	Y354	L261	D12
		S355	L262	P13
	M465	M356	Y268	
	L466	B357	K276	R16
	H468	K358	T277	H20
	V469	P359	N279	L21
	L470	R360	F280	R22
	R473	R361	T282	V25
	K476	E365	C283	E26
	Q481	L376	F286	V27
	L482	V377	E287	E28
	V484	H383	T288	I32
	P485	P385	D292	K33
		T386	S295	N34
	L490	V390	Y297	A35
	G491	V393	T298	L49
	P492	K394	P299	K50
	R493	K395	Q300	G51
	C494	T396	I303	R52
	A495	E402	G304	D53
	E496	R410	W305	D56
	G497	A413	D307	Q62
	K498	R414	L308	C68
	S500	Q417	N315	T69
	T509	C418	P316	Y70
	P510	E426	E320	V71
	L511	V427	E321	H72
	K515	W428	H322	A73
	R516	L429	D430	L74
	P517	D522	V431	A75
		Y527		S76
		O528		V80
				D81
				N82
				C83
				V84
				K87
				I88
				A90

Chain J:

Y527	D430	A333	F242	L98
D528	K431	H334	R243	Y104
P529	L432	H335	K244	M105
C530	E433	P336	L245	H106
	D441	V340	Y246	D107
A531	D442	W345	E247	H108
A532	L443	W346	E248	H109
C533	Y444	E347	R249	L118
			R250	D119
H536	Q448		F251	
	Y449	G350	F252	A124
	P450	E351	I253	N125
	T451	D352	V256	A126
	S453	R353	V257	L127
	Q454	Y354	I258	N128
	G455	S355	T259	A129
	Y456	W356	D260	
	Y457	M357	L261	K133
	F458	K358	L262	
		A359		R136
	Y465	P360	Y268	
	L466	R361		D140
	S467		K276	L141
	H468	E365	T277	S142
	Y469		S278	P143
	L470	L376	N279	K144
		S377	F280	
	R473		L281	Y183
		H383	T282	
	K476	E384	C283	A186
		P385		E187
Q481		T386	F286	L188
L482			P287	D189
Y483		V390	T288	
Y484				H195
P485		V393	D292	
		L394		E198
L490		K395	S295	
Q491		T396	R296	R201
F492			Y297	
R493		E402	T298	R208
C494		F405	P299	
A495			Q300	F213
E496		L408	I303	G214
G497		G409	W304	A215
K498		R410	G305	K216
L499			N306	N217
S500		A413	D307	
		R414	L308	T223
		Q417	E320	D232
		C418	E321	S233
			H322	L234
		E426	R325	R236
		Y427	V323	E237
		F428	K324	P238
		L429	Y325	R238
			S326	T239

## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	112.78Å 113.16Å 133.91Å 90.03° 90.02° 119.99°	Depositor
Resolution (Å)	8.00 – 2.54	Depositor
% Data completeness (in resolution range)	92.5 (8.00-2.54)	Depositor
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, $R_{free}$	0.201 , 0.219	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	38040	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	9.0	wwPDB-VP



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NI, MG, SF4, O, F3S, FCO

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	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	1.02	0/2017	1.83	44/2742 (1.6%)
1	C	1.02	0/2017	1.83	44/2742 (1.6%)
1	E	1.01	0/2017	1.83	43/2742 (1.6%)
1	G	1.02	0/2017	1.83	44/2742 (1.6%)
1	I	1.02	0/2017	1.83	45/2742 (1.6%)
1	S	1.01	0/2017	1.83	44/2742 (1.6%)
2	B	0.96	0/4257	1.90	81/5786 (1.4%)
2	D	0.96	0/4257	1.90	81/5786 (1.4%)
2	F	0.96	0/4257	1.90	81/5786 (1.4%)
2	H	0.96	0/4257	1.90	81/5786 (1.4%)
2	J	0.96	0/4257	1.90	80/5786 (1.4%)
2	L	0.96	0/4257	1.90	81/5786 (1.4%)
All	All	0.98	0/37644	1.88	749/51168 (1.5%)

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
2	B	0	1
2	D	0	1
2	F	0	1
2	H	0	1
2	J	0	1
2	L	0	1
All	All	0	6

There are no bond length outliers.

All (749) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	96	ARG	NE-CZ-NH1	22.41	131.51	120.30
2	H	96	ARG	NE-CZ-NH1	22.36	131.48	120.30
2	F	96	ARG	NE-CZ-NH1	22.35	131.47	120.30
2	L	96	ARG	NE-CZ-NH1	22.33	131.46	120.30
2	D	96	ARG	NE-CZ-NH1	22.32	131.46	120.30
2	J	96	ARG	NE-CZ-NH1	22.21	131.40	120.30
2	H	353	ARG	NE-CZ-NH1	17.38	128.99	120.30
2	J	353	ARG	NE-CZ-NH1	17.30	128.95	120.30
2	D	353	ARG	NE-CZ-NH1	17.27	128.93	120.30
2	F	353	ARG	NE-CZ-NH1	17.24	128.92	120.30
2	L	353	ARG	NE-CZ-NH1	17.22	128.91	120.30
2	B	353	ARG	NE-CZ-NH1	17.19	128.90	120.30
2	L	353	ARG	CD-NE-CZ	17.10	147.54	123.60
2	F	353	ARG	CD-NE-CZ	17.10	147.54	123.60
2	D	353	ARG	CD-NE-CZ	17.09	147.52	123.60
2	B	353	ARG	CD-NE-CZ	17.07	147.50	123.60
2	J	353	ARG	CD-NE-CZ	17.07	147.50	123.60
2	H	353	ARG	CD-NE-CZ	17.05	147.47	123.60
2	H	52	ARG	NE-CZ-NH2	14.95	127.78	120.30
2	L	52	ARG	NE-CZ-NH2	14.84	127.72	120.30
2	B	52	ARG	NE-CZ-NH2	14.84	127.72	120.30
2	D	52	ARG	NE-CZ-NH2	14.82	127.71	120.30
2	J	52	ARG	NE-CZ-NH2	14.81	127.71	120.30
2	F	52	ARG	NE-CZ-NH2	14.80	127.70	120.30
2	B	16	ARG	NE-CZ-NH1	-14.78	112.91	120.30
2	J	16	ARG	NE-CZ-NH1	-14.77	112.92	120.30
2	H	16	ARG	NE-CZ-NH1	-14.73	112.93	120.30
2	F	16	ARG	NE-CZ-NH1	-14.72	112.94	120.30
2	L	16	ARG	NE-CZ-NH1	-14.70	112.95	120.30
2	D	16	ARG	NE-CZ-NH1	-14.67	112.97	120.30
2	B	12	ASP	CB-CG-OD2	14.53	131.37	118.30
2	L	12	ASP	CB-CG-OD2	14.47	131.32	118.30
2	D	12	ASP	CB-CG-OD2	14.46	131.31	118.30
2	F	12	ASP	CB-CG-OD2	14.45	131.30	118.30
2	J	12	ASP	CB-CG-OD2	14.43	131.29	118.30
2	H	12	ASP	CB-CG-OD2	14.43	131.28	118.30
2	F	16	ARG	NE-CZ-NH2	13.72	127.16	120.30
2	J	16	ARG	NE-CZ-NH2	13.68	127.14	120.30
2	B	16	ARG	NE-CZ-NH2	13.68	127.14	120.30
2	L	16	ARG	NE-CZ-NH2	13.64	127.12	120.30
2	D	16	ARG	NE-CZ-NH2	13.61	127.10	120.30
2	H	16	ARG	NE-CZ-NH2	13.60	127.10	120.30
2	B	516	ARG	NE-CZ-NH2	-12.15	114.23	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	516	ARG	NE-CZ-NH2	-12.06	114.27	120.30
2	D	516	ARG	NE-CZ-NH2	-12.03	114.28	120.30
2	H	516	ARG	NE-CZ-NH2	-12.02	114.29	120.30
2	F	516	ARG	NE-CZ-NH2	-12.01	114.30	120.30
2	J	516	ARG	NE-CZ-NH2	-12.00	114.30	120.30
2	B	22	ARG	NE-CZ-NH1	11.59	126.09	120.30
2	F	22	ARG	NE-CZ-NH1	11.53	126.06	120.30
2	L	22	ARG	NE-CZ-NH1	11.52	126.06	120.30
2	H	22	ARG	NE-CZ-NH1	11.49	126.05	120.30
2	D	22	ARG	NE-CZ-NH1	11.48	126.04	120.30
2	J	22	ARG	NE-CZ-NH1	11.47	126.03	120.30
2	D	104	TYR	CB-CG-CD2	-11.32	114.20	121.00
2	B	104	TYR	CB-CG-CD2	-11.30	114.22	121.00
2	H	104	TYR	CB-CG-CD2	-11.29	114.23	121.00
2	J	104	TYR	CB-CG-CD2	-11.26	114.25	121.00
2	L	104	TYR	CB-CG-CD2	-11.24	114.26	121.00
2	F	104	TYR	CB-CG-CD2	-11.20	114.28	121.00
2	B	522	ARG	NE-CZ-NH2	-11.16	114.72	120.30
2	H	522	ARG	NE-CZ-NH2	-11.14	114.73	120.30
2	L	522	ARG	NE-CZ-NH2	-11.10	114.75	120.30
2	J	522	ARG	NE-CZ-NH2	-11.08	114.76	120.30
2	D	522	ARG	NE-CZ-NH2	-11.05	114.77	120.30
2	F	522	ARG	NE-CZ-NH2	-11.05	114.78	120.30
2	F	361	ARG	NE-CZ-NH1	10.94	125.77	120.30
2	L	361	ARG	NE-CZ-NH1	10.92	125.76	120.30
2	J	361	ARG	NE-CZ-NH1	10.92	125.76	120.30
2	B	361	ARG	NE-CZ-NH1	10.89	125.75	120.30
2	H	361	ARG	NE-CZ-NH1	10.86	125.73	120.30
2	D	361	ARG	NE-CZ-NH1	10.80	125.70	120.30
2	B	22	ARG	NE-CZ-NH2	-10.70	114.95	120.30
2	F	22	ARG	NE-CZ-NH2	-10.69	114.96	120.30
2	H	22	ARG	NE-CZ-NH2	-10.64	114.98	120.30
2	J	22	ARG	NE-CZ-NH2	-10.63	114.98	120.30
2	L	22	ARG	NE-CZ-NH2	-10.63	114.98	120.30
2	D	22	ARG	NE-CZ-NH2	-10.62	114.99	120.30
1	G	190	ARG	NE-CZ-NH2	10.52	125.56	120.30
1	C	190	ARG	NE-CZ-NH2	10.47	125.53	120.30
1	S	190	ARG	NE-CZ-NH2	10.47	125.53	120.30
1	I	190	ARG	NE-CZ-NH2	10.47	125.53	120.30
1	E	190	ARG	NE-CZ-NH2	10.45	125.52	120.30
1	A	190	ARG	NE-CZ-NH2	10.42	125.51	120.30
2	J	81	ASP	CB-CG-OD2	10.30	127.57	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	81	ASP	CB-CG-OD2	10.27	127.54	118.30
2	L	81	ASP	CB-CG-OD2	10.26	127.54	118.30
2	F	81	ASP	CB-CG-OD2	10.23	127.51	118.30
2	B	81	ASP	CB-CG-OD2	10.22	127.50	118.30
2	D	81	ASP	CB-CG-OD2	10.22	127.50	118.30
1	I	190	ARG	NE-CZ-NH1	10.13	125.36	120.30
1	S	190	ARG	NE-CZ-NH1	10.05	125.33	120.30
1	C	190	ARG	NE-CZ-NH1	10.05	125.32	120.30
1	A	190	ARG	NE-CZ-NH1	10.04	125.32	120.30
1	E	190	ARG	NE-CZ-NH1	10.01	125.31	120.30
1	G	190	ARG	NE-CZ-NH1	9.97	125.28	120.30
2	H	104	TYR	CB-CG-CD1	9.82	126.89	121.00
2	F	104	TYR	CB-CG-CD1	9.80	126.88	121.00
2	J	104	TYR	CB-CG-CD1	9.80	126.88	121.00
2	L	104	TYR	CB-CG-CD1	9.79	126.87	121.00
2	D	104	TYR	CB-CG-CD1	9.77	126.86	121.00
2	B	104	TYR	CB-CG-CD1	9.75	126.85	121.00
2	B	296	ARG	NE-CZ-NH1	9.59	125.10	120.30
2	H	296	ARG	NE-CZ-NH1	9.59	125.09	120.30
2	L	296	ARG	NE-CZ-NH1	9.54	125.07	120.30
2	J	296	ARG	NE-CZ-NH1	9.54	125.07	120.30
2	F	410	ARG	NE-CZ-NH2	-9.54	115.53	120.30
2	L	410	ARG	NE-CZ-NH2	-9.50	115.55	120.30
2	F	296	ARG	NE-CZ-NH1	9.50	125.05	120.30
2	J	410	ARG	NE-CZ-NH2	-9.48	115.56	120.30
2	B	410	ARG	NE-CZ-NH2	-9.46	115.57	120.30
2	B	296	ARG	NE-CZ-NH2	-9.45	115.58	120.30
2	F	296	ARG	NE-CZ-NH2	-9.45	115.58	120.30
2	J	296	ARG	NE-CZ-NH2	-9.45	115.58	120.30
2	D	296	ARG	NE-CZ-NH1	9.44	125.02	120.30
2	D	410	ARG	NE-CZ-NH2	-9.43	115.58	120.30
2	H	296	ARG	NE-CZ-NH2	-9.42	115.59	120.30
2	H	410	ARG	NE-CZ-NH2	-9.40	115.60	120.30
2	L	296	ARG	NE-CZ-NH2	-9.39	115.61	120.30
1	I	190	ARG	NH1-CZ-NH2	-9.37	109.10	119.40
2	D	296	ARG	NE-CZ-NH2	-9.35	115.62	120.30
1	C	190	ARG	NH1-CZ-NH2	-9.33	109.14	119.40
1	S	190	ARG	NH1-CZ-NH2	-9.33	109.14	119.40
1	G	190	ARG	NH1-CZ-NH2	-9.32	109.15	119.40
1	A	190	ARG	NH1-CZ-NH2	-9.31	109.16	119.40
1	E	190	ARG	NH1-CZ-NH2	-9.31	109.16	119.40
1	A	262	TYR	CB-CG-CD2	-9.29	115.42	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	262	TYR	CB-CG-CD2	-9.26	115.45	121.00
1	G	262	TYR	CB-CG-CD2	-9.25	115.45	121.00
1	I	262	TYR	CB-CG-CD2	-9.25	115.45	121.00
1	S	262	TYR	CB-CG-CD2	-9.22	115.47	121.00
1	E	262	TYR	CB-CG-CD2	-9.22	115.47	121.00
1	S	49	MET	CA-CB-CG	-9.10	97.84	113.30
1	G	49	MET	CA-CB-CG	-9.09	97.84	113.30
1	A	49	MET	CA-CB-CG	-9.09	97.85	113.30
1	I	49	MET	CA-CB-CG	-9.09	97.85	113.30
1	E	49	MET	CA-CB-CG	-9.08	97.87	113.30
1	C	49	MET	CA-CB-CG	-9.07	97.88	113.30
1	C	175	ARG	NE-CZ-NH2	-8.91	115.84	120.30
1	S	175	ARG	NE-CZ-NH2	-8.88	115.86	120.30
1	A	175	ARG	NE-CZ-NH2	-8.87	115.87	120.30
1	G	175	ARG	NE-CZ-NH2	-8.87	115.87	120.30
1	E	6	ARG	NE-CZ-NH2	8.83	124.72	120.30
1	G	6	ARG	NE-CZ-NH2	8.83	124.71	120.30
1	E	175	ARG	NE-CZ-NH2	-8.81	115.89	120.30
1	I	175	ARG	NE-CZ-NH2	-8.80	115.90	120.30
1	S	6	ARG	NE-CZ-NH2	8.76	124.68	120.30
2	F	56	ASP	CB-CG-OD1	8.76	126.18	118.30
1	C	6	ARG	NE-CZ-NH2	8.76	124.68	120.30
2	H	56	ASP	CB-CG-OD1	8.75	126.18	118.30
2	D	56	ASP	CB-CG-OD1	8.74	126.17	118.30
1	I	6	ARG	NE-CZ-NH2	8.73	124.67	120.30
2	L	56	ASP	CB-CG-OD1	8.72	126.15	118.30
2	J	56	ASP	CB-CG-OD1	8.72	126.15	118.30
1	A	6	ARG	NE-CZ-NH2	8.72	124.66	120.30
2	B	56	ASP	CB-CG-OD1	8.72	126.15	118.30
2	H	53	ASP	CB-CG-OD2	-8.47	110.67	118.30
2	B	53	ASP	CB-CG-OD2	-8.45	110.69	118.30
2	D	53	ASP	CB-CG-OD2	-8.45	110.70	118.30
2	L	53	ASP	CB-CG-OD2	-8.44	110.70	118.30
2	F	53	ASP	CB-CG-OD2	-8.43	110.71	118.30
2	J	53	ASP	CB-CG-OD2	-8.41	110.73	118.30
2	J	223	THR	CA-CB-CG2	8.39	124.15	112.40
2	D	223	THR	CA-CB-CG2	8.39	124.14	112.40
2	B	223	THR	CA-CB-CG2	8.38	124.12	112.40
2	L	223	THR	CA-CB-CG2	8.36	124.11	112.40
2	F	223	THR	CA-CB-CG2	8.36	124.11	112.40
1	G	175	ARG	NE-CZ-NH1	8.35	124.48	120.30
2	B	414	ARG	NE-CZ-NH2	-8.34	116.13	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	223	THR	CA-CB-CG2	8.33	124.06	112.40
2	L	414	ARG	NE-CZ-NH2	-8.32	116.14	120.30
2	J	414	ARG	NE-CZ-NH2	-8.32	116.14	120.30
2	F	107	ASP	CB-CG-OD2	8.30	125.77	118.30
1	S	175	ARG	NE-CZ-NH1	8.29	124.44	120.30
2	F	414	ARG	NE-CZ-NH2	-8.28	116.16	120.30
2	J	107	ASP	CB-CG-OD2	8.28	125.75	118.30
2	H	414	ARG	NE-CZ-NH2	-8.27	116.17	120.30
2	L	107	ASP	CB-CG-OD2	8.26	125.74	118.30
1	C	175	ARG	NE-CZ-NH1	8.24	124.42	120.30
1	A	175	ARG	NE-CZ-NH1	8.24	124.42	120.30
1	E	175	ARG	NE-CZ-NH1	8.23	124.42	120.30
2	D	414	ARG	NE-CZ-NH2	-8.23	116.18	120.30
2	H	107	ASP	CB-CG-OD2	8.23	125.71	118.30
2	D	107	ASP	CB-CG-OD2	8.22	125.70	118.30
2	B	107	ASP	CB-CG-OD2	8.22	125.70	118.30
1	I	175	ARG	NE-CZ-NH1	8.19	124.39	120.30
1	S	225	TYR	CB-CG-CD1	-8.14	116.12	121.00
1	G	225	TYR	CB-CG-CD1	-8.14	116.12	121.00
1	C	225	TYR	CB-CG-CD1	-8.12	116.12	121.00
1	A	225	TYR	CB-CG-CD1	-8.09	116.14	121.00
1	I	225	TYR	CB-CG-CD1	-8.08	116.15	121.00
1	E	225	TYR	CB-CG-CD1	-8.06	116.17	121.00
1	I	57	GLU	OE1-CD-OE2	-7.99	113.71	123.30
2	B	96	ARG	NE-CZ-NH2	-7.97	116.32	120.30
2	H	26	GLU	CA-CB-CG	7.97	130.93	113.40
2	J	26	GLU	CA-CB-CG	7.96	130.91	113.40
2	J	493	ARG	NE-CZ-NH1	7.96	124.28	120.30
2	L	26	GLU	CA-CB-CG	7.95	130.90	113.40
2	F	26	GLU	CA-CB-CG	7.95	130.90	113.40
1	S	57	GLU	OE1-CD-OE2	-7.95	113.76	123.30
2	D	493	ARG	NE-CZ-NH1	7.95	124.28	120.30
1	G	57	GLU	OE1-CD-OE2	-7.95	113.77	123.30
2	D	26	GLU	CA-CB-CG	7.94	130.87	113.40
1	A	57	GLU	OE1-CD-OE2	-7.94	113.77	123.30
1	E	57	GLU	OE1-CD-OE2	-7.94	113.77	123.30
2	B	26	GLU	CA-CB-CG	7.94	130.86	113.40
1	C	57	GLU	OE1-CD-OE2	-7.94	113.78	123.30
2	F	493	ARG	NE-CZ-NH1	7.92	124.26	120.30
2	H	96	ARG	NE-CZ-NH2	-7.92	116.34	120.30
2	L	493	ARG	NE-CZ-NH1	7.90	124.25	120.30
2	B	493	ARG	NE-CZ-NH1	7.89	124.25	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	96	ARG	NE-CZ-NH2	-7.89	116.36	120.30
2	L	96	ARG	NE-CZ-NH2	-7.87	116.36	120.30
2	D	96	ARG	NE-CZ-NH2	-7.87	116.37	120.30
2	L	522	ARG	NE-CZ-NH1	7.84	124.22	120.30
2	D	522	ARG	NE-CZ-NH1	7.84	124.22	120.30
2	F	522	ARG	NE-CZ-NH1	7.83	124.21	120.30
2	B	522	ARG	NE-CZ-NH1	7.83	124.21	120.30
2	J	522	ARG	NE-CZ-NH1	7.82	124.21	120.30
2	H	493	ARG	NE-CZ-NH1	7.81	124.20	120.30
2	H	522	ARG	NE-CZ-NH1	7.79	124.20	120.30
2	J	96	ARG	NE-CZ-NH2	-7.79	116.41	120.30
1	G	43	ASP	CB-CG-OD1	7.77	125.29	118.30
1	A	11	TYR	CB-CG-CD1	-7.74	116.36	121.00
1	E	43	ASP	CB-CG-OD1	7.73	125.26	118.30
1	C	43	ASP	CB-CG-OD1	7.71	125.24	118.30
1	A	43	ASP	CB-CG-OD1	7.71	125.24	118.30
1	S	43	ASP	CB-CG-OD1	7.70	125.23	118.30
1	C	11	TYR	CB-CG-CD1	-7.70	116.38	121.00
1	G	11	TYR	CB-CG-CD1	-7.70	116.38	121.00
1	I	43	ASP	CB-CG-OD1	7.70	125.23	118.30
1	S	11	TYR	CB-CG-CD1	-7.68	116.39	121.00
1	A	26	ARG	NE-CZ-NH1	7.64	124.12	120.30
2	B	208	ARG	NE-CZ-NH1	-7.64	116.48	120.30
2	B	201	ARG	NE-CZ-NH2	-7.63	116.48	120.30
1	I	11	TYR	CB-CG-CD1	-7.63	116.42	121.00
1	E	11	TYR	CB-CG-CD1	-7.62	116.43	121.00
2	H	208	ARG	NE-CZ-NH1	-7.62	116.49	120.30
2	D	201	ARG	NE-CZ-NH2	-7.61	116.50	120.30
1	E	26	ARG	NE-CZ-NH1	7.60	124.10	120.30
1	S	26	ARG	NE-CZ-NH1	7.59	124.10	120.30
2	L	208	ARG	NE-CZ-NH1	-7.59	116.50	120.30
2	H	53	ASP	CB-CG-OD1	7.58	125.13	118.30
1	I	26	ARG	NE-CZ-NH1	7.58	124.09	120.30
2	L	201	ARG	NE-CZ-NH2	-7.58	116.51	120.30
2	J	201	ARG	NE-CZ-NH2	-7.58	116.51	120.30
1	C	26	ARG	NE-CZ-NH1	7.57	124.08	120.30
2	J	208	ARG	NE-CZ-NH1	-7.57	116.52	120.30
2	F	201	ARG	NE-CZ-NH2	-7.57	116.52	120.30
2	F	208	ARG	NE-CZ-NH1	-7.57	116.52	120.30
2	L	53	ASP	CB-CG-OD1	7.56	125.10	118.30
2	D	53	ASP	CB-CG-OD1	7.56	125.10	118.30
2	D	208	ARG	NE-CZ-NH1	-7.55	116.52	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	53	ASP	CB-CG-OD1	7.55	125.09	118.30
2	B	53	ASP	CB-CG-OD1	7.54	125.08	118.30
1	G	26	ARG	NE-CZ-NH1	7.54	124.07	120.30
2	J	53	ASP	CB-CG-OD1	7.51	125.06	118.30
2	H	201	ARG	NE-CZ-NH2	-7.51	116.55	120.30
2	L	527	TYR	CB-CG-CD1	7.50	125.50	121.00
2	F	527	TYR	CB-CG-CD1	7.50	125.50	121.00
2	J	527	TYR	CB-CG-CD1	7.50	125.50	121.00
2	B	527	TYR	CB-CG-CD1	7.47	125.48	121.00
2	H	527	TYR	CB-CG-CD1	7.46	125.48	121.00
2	D	527	TYR	CB-CG-CD1	7.43	125.46	121.00
1	G	36	ILE	CA-CB-CG2	7.35	125.61	110.90
1	S	36	ILE	CA-CB-CG2	7.35	125.60	110.90
1	E	36	ILE	CA-CB-CG2	7.35	125.61	110.90
1	I	36	ILE	CA-CB-CG2	7.35	125.60	110.90
1	A	36	ILE	CA-CB-CG2	7.35	125.60	110.90
1	C	36	ILE	CA-CB-CG2	7.34	125.58	110.90
2	B	441	ASP	CB-CG-OD1	7.31	124.88	118.30
2	F	441	ASP	CB-CG-OD1	7.30	124.87	118.30
2	H	441	ASP	CB-CG-OD1	7.30	124.87	118.30
2	L	441	ASP	CB-CG-OD1	7.30	124.87	118.30
2	J	441	ASP	CB-CG-OD1	7.30	124.87	118.30
2	D	441	ASP	CB-CG-OD1	7.26	124.84	118.30
2	B	22	ARG	CD-NE-CZ	-7.22	113.49	123.60
2	F	22	ARG	CD-NE-CZ	-7.21	113.51	123.60
2	H	22	ARG	CD-NE-CZ	-7.20	113.52	123.60
2	L	22	ARG	CD-NE-CZ	-7.19	113.53	123.60
2	H	353	ARG	NE-CZ-NH2	-7.18	116.71	120.30
2	D	22	ARG	CD-NE-CZ	-7.17	113.56	123.60
2	J	22	ARG	CD-NE-CZ	-7.17	113.56	123.60
2	F	353	ARG	NE-CZ-NH2	-7.17	116.72	120.30
2	B	353	ARG	NE-CZ-NH2	-7.14	116.73	120.30
2	D	353	ARG	NE-CZ-NH2	-7.10	116.75	120.30
2	L	353	ARG	NE-CZ-NH2	-7.09	116.76	120.30
1	A	262	TYR	CB-CG-CD1	7.06	125.24	121.00
1	C	11	TYR	CB-CG-CD2	7.06	125.23	121.00
1	E	11	TYR	CB-CG-CD2	7.05	125.23	121.00
2	J	353	ARG	NE-CZ-NH2	-7.05	116.77	120.30
1	G	11	TYR	CB-CG-CD2	7.04	125.23	121.00
1	I	262	TYR	CB-CG-CD1	7.04	125.23	121.00
1	S	11	TYR	CB-CG-CD2	7.02	125.21	121.00
1	A	11	TYR	CB-CG-CD2	7.01	125.21	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	81	ASP	OD1-CG-OD2	-6.99	110.02	123.30
2	D	248	GLU	CG-CD-OE1	6.97	132.24	118.30
1	S	262	TYR	CB-CG-CD1	6.97	125.18	121.00
1	G	262	TYR	CB-CG-CD1	6.96	125.17	121.00
2	L	248	GLU	CG-CD-OE1	6.95	132.21	118.30
2	L	81	ASP	OD1-CG-OD2	-6.95	110.09	123.30
2	F	248	GLU	CG-CD-OE1	6.95	132.20	118.30
2	H	248	GLU	CG-CD-OE1	6.95	132.19	118.30
2	B	248	GLU	CG-CD-OE1	6.94	132.19	118.30
2	H	81	ASP	OD1-CG-OD2	-6.93	110.12	123.30
2	J	248	GLU	CG-CD-OE1	6.93	132.17	118.30
2	D	81	ASP	OD1-CG-OD2	-6.93	110.13	123.30
1	I	11	TYR	CB-CG-CD2	6.93	125.16	121.00
2	F	81	ASP	OD1-CG-OD2	-6.92	110.14	123.30
1	E	262	TYR	CB-CG-CD1	6.92	125.15	121.00
2	B	81	ASP	OD1-CG-OD2	-6.92	110.16	123.30
1	C	262	TYR	CB-CG-CD1	6.91	125.14	121.00
2	L	133	LYS	CB-CA-C	6.89	124.17	110.40
2	F	133	LYS	CB-CA-C	6.88	124.17	110.40
2	H	133	LYS	CB-CA-C	6.88	124.16	110.40
2	J	136	ARG	NE-CZ-NH2	-6.88	116.86	120.30
2	D	133	LYS	CB-CA-C	6.88	124.15	110.40
2	D	296	ARG	CD-NE-CZ	6.87	133.22	123.60
2	J	133	LYS	CB-CA-C	6.87	124.14	110.40
2	B	133	LYS	CB-CA-C	6.87	124.13	110.40
2	B	136	ARG	NE-CZ-NH2	-6.86	116.87	120.30
2	H	296	ARG	CD-NE-CZ	6.86	133.21	123.60
2	L	361	ARG	NH1-CZ-NH2	-6.86	111.85	119.40
2	F	361	ARG	NH1-CZ-NH2	-6.86	111.86	119.40
2	L	296	ARG	CD-NE-CZ	6.84	133.18	123.60
2	F	296	ARG	CD-NE-CZ	6.83	133.17	123.60
2	B	296	ARG	CD-NE-CZ	6.83	133.17	123.60
2	D	136	ARG	NE-CZ-NH2	-6.83	116.88	120.30
2	L	136	ARG	NE-CZ-NH2	-6.83	116.89	120.30
2	J	361	ARG	NH1-CZ-NH2	-6.83	111.89	119.40
2	H	361	ARG	NH1-CZ-NH2	-6.82	111.89	119.40
2	F	136	ARG	NE-CZ-NH2	-6.82	116.89	120.30
2	B	361	ARG	NH1-CZ-NH2	-6.82	111.90	119.40
2	J	296	ARG	CD-NE-CZ	6.82	133.15	123.60
2	D	361	ARG	NH1-CZ-NH2	-6.82	111.90	119.40
2	J	213	PHE	CB-CG-CD1	-6.82	116.03	120.80
2	D	213	PHE	CB-CG-CD1	-6.81	116.03	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	213	PHE	CB-CG-CD1	-6.81	116.03	120.80
1	E	43	ASP	CB-CG-OD2	-6.81	112.17	118.30
2	H	213	PHE	CB-CG-CD1	-6.80	116.04	120.80
2	H	136	ARG	NE-CZ-NH2	-6.79	116.90	120.30
2	L	213	PHE	CB-CG-CD1	-6.79	116.05	120.80
2	F	213	PHE	CB-CG-CD1	-6.79	116.05	120.80
1	S	43	ASP	CB-CG-OD2	-6.78	112.19	118.30
1	I	43	ASP	CB-CG-OD2	-6.78	112.19	118.30
1	A	43	ASP	CB-CG-OD2	-6.78	112.20	118.30
1	C	43	ASP	CB-CG-OD2	-6.77	112.21	118.30
1	G	43	ASP	CB-CG-OD2	-6.77	112.21	118.30
2	D	248	GLU	OE1-CD-OE2	-6.75	115.20	123.30
2	L	248	GLU	OE1-CD-OE2	-6.74	115.21	123.30
2	B	248	GLU	OE1-CD-OE2	-6.74	115.21	123.30
2	H	248	GLU	OE1-CD-OE2	-6.71	115.25	123.30
2	J	248	GLU	OE1-CD-OE2	-6.71	115.25	123.30
2	L	527	TYR	CB-CG-CD2	-6.70	116.98	121.00
2	F	248	GLU	OE1-CD-OE2	-6.70	115.26	123.30
2	D	527	TYR	CB-CG-CD2	-6.69	116.98	121.00
1	E	78	MET	CA-CB-CG	-6.69	101.92	113.30
2	J	527	TYR	CB-CG-CD2	-6.69	116.99	121.00
2	B	527	TYR	CB-CG-CD2	-6.68	116.99	121.00
2	H	527	TYR	CB-CG-CD2	-6.68	116.99	121.00
1	I	78	MET	CA-CB-CG	-6.68	101.94	113.30
1	S	78	MET	CA-CB-CG	-6.67	101.95	113.30
1	A	78	MET	CA-CB-CG	-6.67	101.96	113.30
2	F	527	TYR	CB-CG-CD2	-6.67	117.00	121.00
1	C	78	MET	CA-CB-CG	-6.66	101.97	113.30
1	G	78	MET	CA-CB-CG	-6.66	101.98	113.30
2	F	96	ARG	NH1-CZ-NH2	-6.64	112.10	119.40
2	L	96	ARG	NH1-CZ-NH2	-6.64	112.10	119.40
2	D	96	ARG	NH1-CZ-NH2	-6.63	112.10	119.40
2	B	96	ARG	NH1-CZ-NH2	-6.63	112.11	119.40
2	H	96	ARG	NH1-CZ-NH2	-6.63	112.11	119.40
2	J	96	ARG	NH1-CZ-NH2	-6.62	112.12	119.40
1	C	34	GLU	OE1-CD-OE2	-6.58	115.41	123.30
1	S	34	GLU	OE1-CD-OE2	-6.57	115.41	123.30
1	I	34	GLU	OE1-CD-OE2	-6.57	115.41	123.30
1	A	34	GLU	OE1-CD-OE2	-6.56	115.43	123.30
1	G	34	GLU	OE1-CD-OE2	-6.55	115.44	123.30
2	D	482	LEU	CA-CB-CG	6.54	130.35	115.30
2	B	482	LEU	CA-CB-CG	6.54	130.34	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	482	LEU	CA-CB-CG	6.54	130.34	115.30
1	E	34	GLU	OE1-CD-OE2	-6.54	115.45	123.30
2	J	482	LEU	CA-CB-CG	6.54	130.34	115.30
1	E	40	ILE	O-C-N	6.54	133.16	122.70
1	A	40	ILE	O-C-N	6.53	133.15	122.70
2	F	482	LEU	CA-CB-CG	6.53	130.32	115.30
1	G	40	ILE	O-C-N	6.52	133.14	122.70
1	C	40	ILE	O-C-N	6.52	133.14	122.70
1	S	40	ILE	O-C-N	6.52	133.13	122.70
2	H	482	LEU	CA-CB-CG	6.51	130.28	115.30
1	I	40	ILE	O-C-N	6.50	133.11	122.70
2	B	52	ARG	NE-CZ-NH1	-6.50	117.05	120.30
2	D	300	GLN	CA-CB-CG	6.46	127.61	113.40
2	J	300	GLN	CA-CB-CG	6.46	127.61	113.40
2	B	300	GLN	CA-CB-CG	6.46	127.61	113.40
2	F	300	GLN	CA-CB-CG	6.45	127.58	113.40
2	L	300	GLN	CA-CB-CG	6.45	127.58	113.40
2	H	52	ARG	NE-CZ-NH1	-6.45	117.08	120.30
2	H	300	GLN	CA-CB-CG	6.45	127.58	113.40
2	J	238	ARG	CD-NE-CZ	-6.44	114.59	123.60
2	D	238	ARG	CD-NE-CZ	-6.43	114.60	123.60
2	L	52	ARG	NE-CZ-NH1	-6.42	117.09	120.30
2	J	52	ARG	NE-CZ-NH1	-6.42	117.09	120.30
2	L	238	ARG	CD-NE-CZ	-6.41	114.62	123.60
1	C	115	TYR	CA-C-N	6.41	129.03	116.20
2	B	238	ARG	CD-NE-CZ	-6.41	114.62	123.60
1	S	115	TYR	CA-C-N	6.41	129.02	116.20
1	I	115	TYR	CA-C-N	6.41	129.02	116.20
1	A	115	TYR	CA-C-N	6.41	129.01	116.20
1	G	115	TYR	CA-C-N	6.41	129.01	116.20
1	E	115	TYR	CA-C-N	6.40	129.00	116.20
2	H	238	ARG	CD-NE-CZ	-6.40	114.64	123.60
2	D	52	ARG	NE-CZ-NH1	-6.40	117.10	120.30
2	F	52	ARG	NE-CZ-NH1	-6.40	117.10	120.30
2	F	238	ARG	CD-NE-CZ	-6.39	114.65	123.60
2	H	250	ARG	NE-CZ-NH1	6.29	123.44	120.30
2	F	248	GLU	CA-CB-CG	6.27	127.19	113.40
2	D	183	VAL	CA-C-N	6.26	130.98	117.20
2	B	183	VAL	CA-C-N	6.26	130.98	117.20
2	L	248	GLU	CA-CB-CG	6.26	127.17	113.40
2	J	248	GLU	CA-CB-CG	6.26	127.17	113.40
2	J	183	VAL	CA-C-N	6.26	130.97	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	183	VAL	CA-C-N	6.25	130.96	117.20
2	F	183	VAL	CA-C-N	6.25	130.96	117.20
2	H	248	GLU	CA-CB-CG	6.25	127.16	113.40
2	D	248	GLU	CA-CB-CG	6.25	127.14	113.40
2	B	248	GLU	CA-CB-CG	6.24	127.13	113.40
2	L	250	ARG	NE-CZ-NH1	6.24	123.42	120.30
2	F	250	ARG	NE-CZ-NH1	6.24	123.42	120.30
2	H	183	VAL	CA-C-N	6.24	130.92	117.20
2	H	81	ASP	CA-CB-CG	6.23	127.11	113.40
2	F	81	ASP	CA-CB-CG	6.23	127.11	113.40
1	I	34	GLU	CG-CD-OE2	6.23	130.76	118.30
1	C	34	GLU	CG-CD-OE2	6.23	130.75	118.30
2	D	250	ARG	NE-CZ-NH1	6.23	123.41	120.30
2	J	81	ASP	CA-CB-CG	6.23	127.10	113.40
2	L	81	ASP	CA-CB-CG	6.22	127.09	113.40
1	G	34	GLU	CG-CD-OE2	6.22	130.74	118.30
1	S	34	GLU	CG-CD-OE2	6.22	130.74	118.30
2	B	81	ASP	CA-CB-CG	6.22	127.08	113.40
2	D	81	ASP	CA-CB-CG	6.21	127.07	113.40
1	A	34	GLU	CG-CD-OE2	6.20	130.70	118.30
1	E	34	GLU	CG-CD-OE2	6.19	130.69	118.30
1	A	29	ASP	CB-CG-OD1	-6.19	112.73	118.30
2	B	250	ARG	NE-CZ-NH1	6.18	123.39	120.30
2	J	250	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	A	16	GLU	OE1-CD-OE2	-6.16	115.91	123.30
1	G	29	ASP	CB-CG-OD1	-6.15	112.76	118.30
1	S	29	ASP	CB-CG-OD1	-6.15	112.77	118.30
1	C	29	ASP	CB-CG-OD1	-6.15	112.76	118.30
1	C	16	GLU	OE1-CD-OE2	-6.15	115.92	123.30
1	S	16	GLU	OE1-CD-OE2	-6.14	115.94	123.30
1	I	16	GLU	OE1-CD-OE2	-6.14	115.94	123.30
1	I	29	ASP	CB-CG-OD1	-6.12	112.79	118.30
2	B	238	ARG	NE-CZ-NH2	6.10	123.35	120.30
1	C	16	GLU	CA-CB-CG	6.10	126.82	113.40
1	E	16	GLU	CA-CB-CG	6.10	126.81	113.40
1	S	16	GLU	CA-CB-CG	6.10	126.81	113.40
2	H	238	ARG	NE-CZ-NH2	6.09	123.35	120.30
1	I	16	GLU	CA-CB-CG	6.09	126.81	113.40
1	E	29	ASP	CB-CG-OD1	-6.09	112.82	118.30
1	G	16	GLU	CA-CB-CG	6.09	126.79	113.40
1	A	16	GLU	CA-CB-CG	6.08	126.78	113.40
1	E	16	GLU	OE1-CD-OE2	-6.08	116.00	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	16	GLU	OE1-CD-OE2	-6.08	116.00	123.30
2	F	238	ARG	NE-CZ-NH2	6.08	123.34	120.30
2	J	493	ARG	NE-CZ-NH2	-6.06	117.27	120.30
2	B	493	ARG	NE-CZ-NH2	-6.06	117.27	120.30
2	F	531	ILE	CB-CG1-CD1	6.06	130.86	113.90
2	B	531	ILE	CB-CG1-CD1	6.05	130.85	113.90
2	J	531	ILE	CB-CG1-CD1	6.05	130.85	113.90
2	L	531	ILE	CB-CG1-CD1	6.04	130.82	113.90
2	H	531	ILE	CB-CG1-CD1	6.04	130.81	113.90
2	D	531	ILE	CB-CG1-CD1	6.04	130.81	113.90
2	F	493	ARG	NE-CZ-NH2	-6.04	117.28	120.30
2	L	238	ARG	NE-CZ-NH2	6.03	123.32	120.30
2	L	493	ARG	NE-CZ-NH2	-6.00	117.30	120.30
2	D	493	ARG	NE-CZ-NH2	-5.99	117.30	120.30
2	L	27	VAL	CB-CA-C	5.99	122.77	111.40
2	D	27	VAL	CB-CA-C	5.99	122.77	111.40
2	J	27	VAL	CB-CA-C	5.99	122.77	111.40
2	D	238	ARG	NE-CZ-NH2	5.98	123.29	120.30
2	F	27	VAL	CB-CA-C	5.98	122.77	111.40
1	E	167	MET	CA-CB-CG	-5.97	103.14	113.30
2	H	27	VAL	CB-CA-C	5.96	122.73	111.40
2	B	27	VAL	CB-CA-C	5.96	122.73	111.40
2	J	238	ARG	NE-CZ-NH2	5.96	123.28	120.30
1	G	167	MET	CA-CB-CG	-5.96	103.17	113.30
2	J	353	ARG	NH1-CZ-NH2	-5.96	112.85	119.40
1	S	167	MET	CA-CB-CG	-5.95	103.19	113.30
1	C	167	MET	CA-CB-CG	-5.95	103.19	113.30
1	A	167	MET	CA-CB-CG	-5.94	103.19	113.30
1	G	182	GLU	CA-CB-CG	5.94	126.47	113.40
2	H	353	ARG	NH1-CZ-NH2	-5.94	112.87	119.40
1	A	182	GLU	CA-CB-CG	5.94	126.46	113.40
2	D	353	ARG	NH1-CZ-NH2	-5.94	112.87	119.40
1	S	182	GLU	CA-CB-CG	5.93	126.45	113.40
2	F	473	ARG	CA-CB-CG	5.92	126.43	113.40
1	I	167	MET	CA-CB-CG	-5.92	103.23	113.30
1	E	182	GLU	CA-CB-CG	5.92	126.43	113.40
2	B	473	ARG	CA-CB-CG	5.92	126.43	113.40
1	C	182	GLU	CA-CB-CG	5.92	126.43	113.40
1	I	182	GLU	CA-CB-CG	5.92	126.43	113.40
2	L	353	ARG	NH1-CZ-NH2	-5.92	112.89	119.40
2	D	473	ARG	CA-CB-CG	5.92	126.42	113.40
2	H	493	ARG	NE-CZ-NH2	-5.92	117.34	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	473	ARG	CA-CB-CG	5.91	126.41	113.40
2	F	353	ARG	NH1-CZ-NH2	-5.90	112.91	119.40
2	H	473	ARG	CA-CB-CG	5.90	126.38	113.40
1	I	236	VAL	N-CA-CB	-5.90	98.53	111.50
1	G	236	VAL	N-CA-CB	-5.89	98.53	111.50
2	B	353	ARG	NH1-CZ-NH2	-5.89	112.92	119.40
1	C	236	VAL	N-CA-CB	-5.89	98.55	111.50
1	E	236	VAL	N-CA-CB	-5.89	98.55	111.50
1	S	236	VAL	N-CA-CB	-5.88	98.55	111.50
2	J	473	ARG	CA-CB-CG	5.88	126.35	113.40
2	J	96	ARG	CD-NE-CZ	5.88	131.83	123.60
1	A	236	VAL	N-CA-CB	-5.87	98.58	111.50
2	F	96	ARG	CD-NE-CZ	5.87	131.82	123.60
2	D	96	ARG	CD-NE-CZ	5.86	131.81	123.60
2	L	96	ARG	CD-NE-CZ	5.85	131.79	123.60
2	J	10	VAL	CA-CB-CG1	5.85	119.67	110.90
2	H	96	ARG	CD-NE-CZ	5.84	131.78	123.60
2	F	10	VAL	CA-CB-CG1	5.83	119.64	110.90
2	B	96	ARG	CD-NE-CZ	5.81	131.74	123.60
2	L	10	VAL	CA-CB-CG1	5.81	119.62	110.90
2	H	10	VAL	CA-CB-CG1	5.80	119.61	110.90
2	D	10	VAL	CA-CB-CG1	5.79	119.59	110.90
2	B	10	VAL	CA-CB-CG1	5.79	119.58	110.90
2	B	357	MET	CG-SD-CE	5.72	109.36	100.20
2	D	357	MET	CG-SD-CE	5.70	109.32	100.20
2	F	357	MET	CG-SD-CE	5.70	109.32	100.20
2	H	357	MET	CG-SD-CE	5.70	109.31	100.20
2	L	357	MET	CG-SD-CE	5.69	109.31	100.20
2	J	357	MET	CG-SD-CE	5.68	109.28	100.20
1	S	258	TYR	CB-CG-CD2	5.63	124.38	121.00
1	G	258	TYR	CB-CG-CD2	5.63	124.38	121.00
1	E	258	TYR	CB-CG-CD2	5.62	124.37	121.00
1	A	258	TYR	CB-CG-CD2	5.61	124.36	121.00
2	H	268	TYR	CB-CG-CD2	5.61	124.36	121.00
2	B	384	GLU	CG-CD-OE2	-5.60	107.11	118.30
2	D	384	GLU	CG-CD-OE2	-5.60	107.11	118.30
2	B	12	ASP	OD1-CG-OD2	-5.59	112.68	123.30
1	I	258	TYR	CB-CG-CD2	5.59	124.35	121.00
2	H	384	GLU	CG-CD-OE2	-5.58	107.13	118.30
2	J	384	GLU	CG-CD-OE2	-5.58	107.14	118.30
1	E	215	TYR	CA-CB-CG	-5.58	102.80	113.40
2	L	384	GLU	CG-CD-OE2	-5.58	107.15	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	215	TYR	CA-CB-CG	-5.57	102.81	113.40
2	F	384	GLU	CG-CD-OE2	-5.57	107.15	118.30
2	L	12	ASP	OD1-CG-OD2	-5.57	112.72	123.30
2	J	12	ASP	OD1-CG-OD2	-5.57	112.72	123.30
2	H	12	ASP	OD1-CG-OD2	-5.57	112.72	123.30
2	L	268	TYR	CB-CG-CD2	5.57	124.34	121.00
2	D	12	ASP	OD1-CG-OD2	-5.57	112.73	123.30
2	F	268	TYR	CB-CG-CD2	5.57	124.34	121.00
1	G	215	TYR	CA-CB-CG	-5.57	102.83	113.40
2	J	268	TYR	CB-CG-CD2	5.57	124.34	121.00
1	S	215	TYR	CA-CB-CG	-5.56	102.84	113.40
2	F	12	ASP	OD1-CG-OD2	-5.56	112.74	123.30
2	J	413	ALA	O-C-N	-5.56	113.80	122.70
2	B	268	TYR	CB-CG-CD2	5.56	124.33	121.00
1	I	215	TYR	CA-CB-CG	-5.55	102.85	113.40
1	A	215	TYR	CA-CB-CG	-5.55	102.85	113.40
2	B	413	ALA	O-C-N	-5.55	113.82	122.70
2	L	413	ALA	O-C-N	-5.55	113.82	122.70
1	C	258	TYR	CB-CG-CD2	5.54	124.33	121.00
2	D	268	TYR	CB-CG-CD2	5.54	124.32	121.00
2	H	98	LEU	CB-CG-CD2	-5.53	101.59	111.00
2	F	413	ALA	O-C-N	-5.53	113.85	122.70
2	D	413	ALA	O-C-N	-5.53	113.86	122.70
2	F	98	LEU	CB-CG-CD2	-5.53	101.61	111.00
2	H	413	ALA	O-C-N	-5.52	113.86	122.70
2	L	98	LEU	CB-CG-CD2	-5.52	101.62	111.00
2	B	98	LEU	CB-CG-CD2	-5.52	101.62	111.00
2	D	189	ASP	CB-CG-OD2	5.52	123.27	118.30
2	B	292	ASP	CB-CG-OD1	5.51	123.26	118.30
2	D	98	LEU	CB-CG-CD2	-5.51	101.64	111.00
2	J	98	LEU	CB-CG-CD2	-5.50	101.66	111.00
2	J	189	ASP	CB-CG-OD2	5.49	123.25	118.30
2	H	292	ASP	CB-CG-OD1	5.49	123.24	118.30
1	I	258	TYR	CB-CG-CD1	-5.48	117.71	121.00
2	F	292	ASP	CB-CG-OD1	5.48	123.23	118.30
2	L	292	ASP	CB-CG-OD1	5.47	123.22	118.30
2	J	292	ASP	CB-CG-OD1	5.47	123.22	118.30
2	D	292	ASP	CB-CG-OD1	5.46	123.21	118.30
2	F	189	ASP	CB-CG-OD2	5.46	123.21	118.30
2	B	189	ASP	CB-CG-OD2	5.45	123.20	118.30
1	E	258	TYR	CB-CG-CD1	-5.45	117.73	121.00
2	L	189	ASP	CB-CG-OD2	5.44	123.20	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	258	TYR	CB-CG-CD1	-5.44	117.74	121.00
2	J	444	TYR	CB-CG-CD1	-5.44	117.74	121.00
1	G	258	TYR	CB-CG-CD1	-5.43	117.74	121.00
2	B	444	TYR	CB-CG-CD1	-5.43	117.74	121.00
2	H	444	TYR	CB-CG-CD1	-5.43	117.74	121.00
1	I	78	MET	N-CA-CB	-5.41	100.86	110.60
2	H	189	ASP	CB-CG-OD2	5.41	123.17	118.30
2	L	444	TYR	CB-CG-CD1	-5.41	117.76	121.00
1	A	258	TYR	CB-CG-CD1	-5.40	117.76	121.00
2	D	444	TYR	CB-CG-CD1	-5.40	117.76	121.00
1	E	78	MET	N-CA-CB	-5.40	100.89	110.60
1	S	16	GLU	CG-CD-OE1	5.39	129.09	118.30
1	I	241	GLN	CG-CD-NE2	5.39	129.65	116.70
1	E	241	GLN	CG-CD-NE2	5.39	129.64	116.70
1	G	241	GLN	CG-CD-NE2	5.39	129.64	116.70
1	A	16	GLU	CG-CD-OE1	5.39	129.08	118.30
1	C	241	GLN	CG-CD-NE2	5.39	129.64	116.70
1	C	16	GLU	CG-CD-OE1	5.39	129.08	118.30
1	S	241	GLN	CG-CD-NE2	5.39	129.63	116.70
1	A	78	MET	N-CA-CB	-5.39	100.90	110.60
1	A	241	GLN	CG-CD-NE2	5.38	129.62	116.70
1	E	16	GLU	CG-CD-OE1	5.38	129.07	118.30
1	G	16	GLU	CG-CD-OE1	5.38	129.06	118.30
1	G	78	MET	N-CA-CB	-5.38	100.91	110.60
1	S	78	MET	N-CA-CB	-5.38	100.92	110.60
1	C	151	ASN	N-CA-CB	-5.38	100.92	110.60
1	I	16	GLU	CG-CD-OE1	5.38	129.06	118.30
1	C	258	TYR	CB-CG-CD1	-5.38	117.78	121.00
1	C	78	MET	N-CA-CB	-5.37	100.94	110.60
1	S	151	ASN	N-CA-CB	-5.35	100.97	110.60
1	G	151	ASN	N-CA-CB	-5.35	100.97	110.60
2	J	334	HIS	CB-CA-C	-5.35	99.70	110.40
1	E	151	ASN	N-CA-CB	-5.35	100.97	110.60
1	A	57	GLU	CG-CD-OE1	5.34	128.99	118.30
2	B	334	HIS	CB-CA-C	-5.34	99.73	110.40
2	H	334	HIS	CB-CA-C	-5.34	99.73	110.40
1	I	151	ASN	N-CA-CB	-5.34	101.00	110.60
2	D	334	HIS	CB-CA-C	-5.33	99.73	110.40
2	F	334	HIS	CB-CA-C	-5.33	99.73	110.40
2	L	334	HIS	CB-CA-C	-5.33	99.74	110.40
1	A	151	ASN	N-CA-CB	-5.33	101.01	110.60
1	G	57	GLU	CG-CD-OE1	5.33	128.96	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	57	GLU	CG-CD-OE1	5.33	128.95	118.30
1	A	135	LEU	N-CA-CB	-5.33	99.75	110.40
2	H	345	TRP	CA-CB-CG	5.33	123.82	113.70
1	I	57	GLU	CG-CD-OE1	5.33	128.95	118.30
1	S	135	LEU	N-CA-CB	-5.32	99.75	110.40
1	G	135	LEU	N-CA-CB	-5.32	99.76	110.40
2	J	345	TRP	CA-CB-CG	5.32	123.81	113.70
1	E	57	GLU	CG-CD-OE1	5.32	128.94	118.30
2	F	444	TYR	CB-CG-CD1	-5.32	117.81	121.00
1	C	135	LEU	N-CA-CB	-5.32	99.77	110.40
1	E	135	LEU	N-CA-CB	-5.32	99.77	110.40
2	F	345	TRP	CA-CB-CG	5.31	123.79	113.70
1	I	135	LEU	N-CA-CB	-5.31	99.79	110.40
2	B	345	TRP	CA-CB-CG	5.31	123.78	113.70
2	L	345	TRP	CA-CB-CG	5.30	123.77	113.70
1	C	57	GLU	CG-CD-OE1	5.30	128.90	118.30
2	D	345	TRP	CA-CB-CG	5.30	123.77	113.70
1	C	224	THR	O-C-N	5.28	131.15	122.70
1	S	224	THR	O-C-N	5.26	131.12	122.70
1	A	224	THR	O-C-N	5.26	131.12	122.70
1	E	224	THR	O-C-N	5.26	131.12	122.70
2	H	84	VAL	C-N-CA	5.26	133.34	122.30
2	B	430	ASP	CB-CG-OD1	-5.25	113.57	118.30
2	H	430	ASP	CB-CG-OD1	-5.25	113.57	118.30
2	B	452	GLU	CB-CA-C	-5.25	99.90	110.40
2	D	84	VAL	C-N-CA	5.25	133.32	122.30
2	J	276	LYS	C-N-CA	5.25	134.82	121.70
2	L	84	VAL	C-N-CA	5.25	133.31	122.30
2	D	430	ASP	CB-CG-OD1	-5.24	113.58	118.30
2	L	452	GLU	CB-CA-C	-5.24	99.92	110.40
1	G	224	THR	O-C-N	5.24	131.08	122.70
2	J	430	ASP	CB-CG-OD1	-5.24	113.58	118.30
2	F	84	VAL	C-N-CA	5.24	133.30	122.30
2	J	452	GLU	CB-CA-C	-5.24	99.92	110.40
1	I	224	THR	O-C-N	5.24	131.08	122.70
2	D	452	GLU	CB-CA-C	-5.23	99.94	110.40
1	A	26	ARG	NH1-CZ-NH2	-5.23	113.65	119.40
2	H	452	GLU	CB-CA-C	-5.23	99.94	110.40
2	J	84	VAL	C-N-CA	5.23	133.28	122.30
2	B	84	VAL	C-N-CA	5.23	133.28	122.30
1	E	26	ARG	NH1-CZ-NH2	-5.22	113.65	119.40
2	L	430	ASP	CB-CG-OD1	-5.22	113.60	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	68	PHE	CB-CG-CD2	-5.22	117.14	120.80
2	L	276	LYS	C-N-CA	5.22	134.75	121.70
2	F	276	LYS	C-N-CA	5.21	134.74	121.70
2	B	276	LYS	C-N-CA	5.21	134.73	121.70
2	F	452	GLU	CB-CA-C	-5.21	99.98	110.40
2	H	276	LYS	C-N-CA	5.21	134.73	121.70
1	S	26	ARG	NH1-CZ-NH2	-5.21	113.67	119.40
2	D	276	LYS	C-N-CA	5.21	134.71	121.70
2	F	430	ASP	CB-CG-OD1	-5.20	113.62	118.30
2	F	307	ASP	CB-CG-OD1	5.20	122.98	118.30
1	G	26	ARG	NH1-CZ-NH2	-5.20	113.69	119.40
1	C	26	ARG	NH1-CZ-NH2	-5.19	113.69	119.40
1	G	68	PHE	CB-CG-CD2	-5.19	117.17	120.80
2	B	208	ARG	NE-CZ-NH2	5.18	122.89	120.30
2	B	307	ASP	CB-CG-OD1	5.18	122.96	118.30
1	S	68	PHE	CB-CG-CD2	-5.18	117.18	120.80
1	I	26	ARG	NH1-CZ-NH2	-5.18	113.71	119.40
1	A	68	PHE	CB-CG-CD2	-5.16	117.19	120.80
2	D	530	CYS	O-C-N	5.16	130.95	122.70
2	D	208	ARG	NE-CZ-NH2	5.15	122.88	120.30
2	J	307	ASP	CB-CG-OD1	5.15	122.94	118.30
2	H	208	ARG	NE-CZ-NH2	5.14	122.87	120.30
2	D	307	ASP	CB-CG-OD1	5.14	122.92	118.30
2	H	307	ASP	CB-CG-OD1	5.14	122.93	118.30
2	F	530	CYS	O-C-N	5.14	130.92	122.70
2	L	208	ARG	NE-CZ-NH2	5.13	122.87	120.30
2	L	307	ASP	CB-CG-OD1	5.13	122.92	118.30
1	C	68	PHE	CB-CG-CD2	-5.13	117.21	120.80
2	B	530	CYS	O-C-N	5.13	130.91	122.70
2	L	530	CYS	O-C-N	5.13	130.90	122.70
1	I	68	PHE	CB-CG-CD2	-5.12	117.21	120.80
1	C	207	GLU	CG-CD-OE1	5.12	128.54	118.30
2	J	530	CYS	O-C-N	5.12	130.89	122.70
1	A	207	GLU	CG-CD-OE1	5.12	128.53	118.30
2	J	237	GLU	CG-CD-OE2	-5.12	108.07	118.30
1	G	207	GLU	CG-CD-OE1	5.12	128.53	118.30
1	A	225	TYR	O-C-N	5.11	130.88	122.70
1	G	225	TYR	O-C-N	5.11	130.88	122.70
1	S	207	GLU	CG-CD-OE1	5.11	128.52	118.30
2	H	237	GLU	CG-CD-OE2	-5.11	108.09	118.30
2	H	530	CYS	O-C-N	5.11	130.87	122.70
1	E	207	GLU	CG-CD-OE1	5.10	128.50	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	225	TYR	O-C-N	5.10	130.87	122.70
1	I	225	TYR	O-C-N	5.10	130.86	122.70
2	F	237	GLU	CG-CD-OE2	-5.10	108.10	118.30
2	L	237	GLU	CG-CD-OE2	-5.10	108.10	118.30
2	F	140	ASP	CB-CA-C	5.10	120.59	110.40
2	D	237	GLU	CG-CD-OE2	-5.09	108.11	118.30
1	E	241	GLN	CB-CG-CD	5.09	124.84	111.60
1	I	207	GLU	CG-CD-OE1	5.09	128.49	118.30
1	S	225	TYR	O-C-N	5.09	130.85	122.70
2	J	140	ASP	CB-CA-C	5.09	120.58	110.40
1	I	241	GLN	CB-CG-CD	5.09	124.83	111.60
2	B	237	GLU	CG-CD-OE2	-5.09	108.12	118.30
2	L	140	ASP	CB-CA-C	5.08	120.57	110.40
1	S	241	GLN	CB-CG-CD	5.08	124.81	111.60
1	G	241	GLN	CB-CG-CD	5.08	124.81	111.60
2	F	187	GLU	CG-CD-OE2	5.08	128.45	118.30
1	A	241	GLN	CB-CG-CD	5.08	124.80	111.60
2	B	140	ASP	CB-CA-C	5.08	120.55	110.40
2	H	140	ASP	CB-CA-C	5.08	120.55	110.40
1	C	225	TYR	O-C-N	5.07	130.82	122.70
2	D	140	ASP	CB-CA-C	5.07	120.55	110.40
2	B	187	GLU	CG-CD-OE2	5.07	128.44	118.30
1	C	241	GLN	CB-CG-CD	5.07	124.77	111.60
2	F	208	ARG	NE-CZ-NH2	5.05	122.83	120.30
2	L	187	GLU	CG-CD-OE2	5.05	128.40	118.30
1	C	165	LYS	CA-C-N	5.04	126.28	116.20
2	D	187	GLU	CG-CD-OE2	5.04	128.38	118.30
1	G	165	LYS	CA-C-N	5.04	126.28	116.20
2	H	187	GLU	CG-CD-OE2	5.03	128.36	118.30
2	J	187	GLU	CG-CD-OE2	5.03	128.36	118.30
1	A	165	LYS	CA-C-N	5.02	126.24	116.20
1	I	165	LYS	CA-C-N	5.02	126.23	116.20
1	S	165	LYS	CA-C-N	5.02	126.23	116.20
1	I	251	GLU	CG-CD-OE2	5.01	128.32	118.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	353	ARG	Sidechain
2	D	353	ARG	Sidechain
2	F	353	ARG	Sidechain

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Mol	Chain	Res	Type	Group
2	H	353	ARG	Sidechain
2	J	353	ARG	Sidechain
2	L	353	ARG	Sidechain

## 5.2 Too-close contacts

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	A	1964	0	1895	44	0
1	C	1964	0	1895	38	0
1	E	1964	0	1895	42	0
1	G	1964	0	1895	41	0
1	I	1964	0	1895	40	0
1	S	1964	0	1895	42	0
2	B	4152	0	4114	118	0
2	D	4152	0	4114	114	0
2	F	4152	0	4114	117	0
2	H	4152	0	4114	113	0
2	J	4152	0	4114	117	0
2	L	4152	0	4114	113	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
3	F	1	0	0	0	0
3	H	1	0	0	0	0
3	J	1	0	0	0	0
3	L	1	0	0	0	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
4	F	1	0	0	0	0
4	H	1	0	0	0	0
4	J	1	0	0	0	0
4	L	1	0	0	0	0
5	A	16	0	0	0	0
5	C	16	0	0	0	0
5	E	16	0	0	0	0
5	G	16	0	0	0	0
5	I	16	0	0	0	0
5	S	16	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	7	0	0	0	0
6	C	7	0	0	0	0
6	E	7	0	0	0	0
6	G	7	0	0	0	0
6	I	7	0	0	1	0
6	S	7	0	0	1	0
7	B	7	0	0	2	0
7	D	7	0	0	2	0
7	F	7	0	0	2	0
7	H	7	0	0	2	0
7	J	7	0	0	2	0
7	L	7	0	0	2	0
8	B	1	0	0	0	0
8	D	1	0	0	0	0
8	F	1	0	0	0	0
8	H	1	0	0	0	0
8	J	1	0	0	0	0
8	L	1	0	0	0	0
9	A	78	0	0	0	2
9	B	114	0	0	0	0
9	C	76	0	0	0	1
9	D	114	0	0	0	0
9	E	81	0	0	0	1
9	F	115	0	0	0	0
9	G	76	0	0	0	0
9	H	112	0	0	0	0
9	I	80	0	0	0	1
9	J	113	0	0	0	0
9	L	110	0	0	0	0
9	S	77	0	0	0	1
All	All	38040	0	36054	878	3

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 12.

All (878) 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)
1:I:235:GLN:NE2	2:J:208:ARG:HH21	1.56	1.03
1:E:235:GLN:NE2	2:F:208:ARG:HH21	1.56	1.03
1:C:235:GLN:NE2	2:D:208:ARG:HH21	1.56	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:235:GLN:NE2	2:H:208:ARG:HH21	1.56	1.02
1:A:235:GLN:NE2	2:B:208:ARG:HH21	1.56	1.02
1:S:235:GLN:NE2	2:L:208:ARG:HH21	1.56	1.01
1:C:235:GLN:HE21	2:D:208:ARG:NH2	1.62	0.96
1:S:235:GLN:HE21	2:L:208:ARG:NH2	1.62	0.96
1:G:235:GLN:HE21	2:H:208:ARG:NH2	1.62	0.96
1:A:235:GLN:HE21	2:B:208:ARG:NH2	1.62	0.95
1:I:235:GLN:HE21	2:J:208:ARG:NH2	1.62	0.95
1:E:235:GLN:HE21	2:F:208:ARG:NH2	1.62	0.95
2:B:142:SER:HB2	2:B:143:PRO:CD	2.08	0.84
2:D:142:SER:HB2	2:D:143:PRO:CD	2.08	0.84
2:H:142:SER:HB2	2:H:143:PRO:CD	2.08	0.84
2:L:142:SER:HB2	2:L:143:PRO:CD	2.08	0.84
1:E:26:ARG:HH21	2:F:217:ASN:HD21	1.24	0.84
1:C:26:ARG:HH21	2:D:217:ASN:HD21	1.24	0.83
2:J:142:SER:HB2	2:J:143:PRO:CD	2.08	0.83
1:A:26:ARG:HH21	2:B:217:ASN:HD21	1.24	0.83
2:F:142:SER:HB2	2:F:143:PRO:CD	2.08	0.83
1:G:26:ARG:HH21	2:H:217:ASN:HD21	1.24	0.83
1:I:26:ARG:HH21	2:J:217:ASN:HD21	1.24	0.82
1:S:26:ARG:HH21	2:L:217:ASN:HD21	1.24	0.82
2:F:108:HIS:CE1	2:F:417:GLN:HE21	2.00	0.80
2:J:108:HIS:CE1	2:J:417:GLN:HE21	2.00	0.80
2:L:108:HIS:CE1	2:L:417:GLN:HE21	2.00	0.80
2:D:108:HIS:CE1	2:D:417:GLN:HE21	2.00	0.80
1:G:141:LYS:HD2	2:J:384:GLU:HG3	1.64	0.80
2:D:484:VAL:HG11	2:D:533:CYS:HB3	1.63	0.79
2:H:108:HIS:CE1	2:H:417:GLN:HE21	2.00	0.79
2:H:484:VAL:HG11	2:H:533:CYS:HB3	1.63	0.79
2:B:108:HIS:CE1	2:B:417:GLN:HE21	2.00	0.79
2:B:484:VAL:HG11	2:B:533:CYS:HB3	1.63	0.78
2:L:484:VAL:HG11	2:L:533:CYS:HB3	1.63	0.78
2:J:484:VAL:HG11	2:J:533:CYS:HB3	1.63	0.77
2:F:484:VAL:HG11	2:F:533:CYS:HB3	1.63	0.77
2:H:484:VAL:CG1	2:H:485:PRO:HD2	2.15	0.77
1:I:227:ASN:HD22	1:I:227:ASN:H	1.33	0.77
2:J:484:VAL:CG1	2:J:485:PRO:HD2	2.15	0.77
2:B:484:VAL:CG1	2:B:485:PRO:HD2	2.15	0.76
1:E:227:ASN:H	1:E:227:ASN:HD22	1.33	0.76
2:D:484:VAL:CG1	2:D:485:PRO:HD2	2.15	0.76
1:G:227:ASN:H	1:G:227:ASN:HD22	1.33	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:484:VAL:CG1	2:L:485:PRO:HD2	2.15	0.76
2:F:484:VAL:CG1	2:F:485:PRO:HD2	2.15	0.76
1:C:227:ASN:HD22	1:C:227:ASN:H	1.33	0.75
1:A:227:ASN:HD22	1:A:227:ASN:H	1.33	0.74
2:D:217:ASN:C	2:D:217:ASN:HD22	1.91	0.74
2:B:217:ASN:HD22	2:B:217:ASN:C	1.91	0.74
2:J:217:ASN:HD22	2:J:217:ASN:C	1.91	0.74
1:S:227:ASN:HD22	1:S:227:ASN:H	1.33	0.74
2:H:217:ASN:C	2:H:217:ASN:HD22	1.91	0.74
2:L:217:ASN:C	2:L:217:ASN:HD22	1.91	0.73
2:J:32:ILE:HD12	2:J:509:THR:HB	1.71	0.73
2:B:32:ILE:HD12	2:B:509:THR:HB	1.71	0.73
2:F:217:ASN:HD22	2:F:217:ASN:C	1.91	0.73
2:L:32:ILE:HD12	2:L:509:THR:HB	1.71	0.73
2:D:32:ILE:HD12	2:D:509:THR:HB	1.71	0.72
2:H:346:THR:O	2:H:350:GLY:HA3	1.89	0.72
2:H:32:ILE:HD12	2:H:509:THR:HB	1.71	0.72
2:J:346:THR:O	2:J:350:GLY:HA3	1.89	0.72
2:L:346:THR:O	2:L:350:GLY:HA3	1.89	0.72
2:F:32:ILE:HD12	2:F:509:THR:HB	1.71	0.72
2:B:346:THR:O	2:B:350:GLY:HA3	1.89	0.72
2:F:346:THR:O	2:F:350:GLY:HA3	1.89	0.71
2:D:346:THR:O	2:D:350:GLY:HA3	1.89	0.71
2:F:108:HIS:HE1	2:F:417:GLN:HG2	1.55	0.71
1:E:124:ASN:HD21	1:E:128:THR:H	1.39	0.71
1:A:124:ASN:HD21	1:A:128:THR:H	1.39	0.70
2:J:108:HIS:HE1	2:J:417:GLN:HG2	1.55	0.70
1:I:124:ASN:HD21	1:I:128:THR:H	1.39	0.70
2:L:108:HIS:HE1	2:L:417:GLN:HE21	1.40	0.70
2:L:108:HIS:HE1	2:L:417:GLN:HG2	1.55	0.70
2:D:108:HIS:HE1	2:D:417:GLN:HG2	1.55	0.70
2:D:108:HIS:HE1	2:D:417:GLN:HE21	1.40	0.69
1:S:124:ASN:HD21	1:S:128:THR:H	1.39	0.69
2:B:108:HIS:HE1	2:B:417:GLN:HE21	1.40	0.69
2:H:108:HIS:HE1	2:H:417:GLN:HE21	1.40	0.69
1:G:124:ASN:HD21	1:G:128:THR:H	1.39	0.69
2:B:108:HIS:HE1	2:B:417:GLN:HG2	1.55	0.69
1:C:124:ASN:HD21	1:C:128:THR:H	1.39	0.69
2:J:108:HIS:HE1	2:J:417:GLN:HE21	1.40	0.69
2:F:108:HIS:HE1	2:F:417:GLN:HE21	1.40	0.69
2:H:108:HIS:HE1	2:H:417:GLN:HG2	1.55	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:384:GLU:HG3	1:E:141:LYS:HD2	1.76	0.68
1:C:235:GLN:HE21	2:D:208:ARG:HH21	0.77	0.67
1:S:235:GLN:HE21	2:L:208:ARG:HH21	0.77	0.67
2:D:278:SER:O	2:D:279:ASN:HB2	1.96	0.66
2:H:253:ILE:O	2:H:258:ILE:HG12	1.95	0.66
2:D:253:ILE:O	2:D:258:ILE:HG12	1.96	0.66
2:H:278:SER:O	2:H:279:ASN:HB2	1.96	0.66
2:J:278:SER:O	2:J:279:ASN:HB2	1.96	0.66
1:A:235:GLN:HE21	2:B:208:ARG:HH21	0.77	0.65
2:D:195:HIS:ND1	2:D:260:ASP:OD2	2.24	0.65
2:J:253:ILE:O	2:J:258:ILE:HG12	1.96	0.65
2:B:253:ILE:O	2:B:258:ILE:HG12	1.96	0.65
2:L:253:ILE:O	2:L:258:ILE:HG12	1.96	0.65
2:F:278:SER:O	2:F:279:ASN:HB2	1.96	0.65
1:C:206:PRO:O	1:C:210:LYS:HD3	1.97	0.65
1:G:206:PRO:O	1:G:210:LYS:HD3	1.97	0.65
2:B:278:SER:O	2:B:279:ASN:HB2	1.96	0.64
2:H:133:LYS:HG2	2:H:187:GLU:HG2	1.80	0.64
1:G:235:GLN:HE21	2:H:208:ARG:HH21	0.77	0.64
2:L:278:SER:O	2:L:279:ASN:HB2	1.96	0.64
2:F:253:ILE:O	2:F:258:ILE:HG12	1.96	0.64
2:L:133:LYS:HG2	2:L:187:GLU:HG2	1.80	0.64
2:B:133:LYS:HG2	2:B:187:GLU:HG2	1.80	0.64
2:H:195:HIS:ND1	2:H:260:ASP:OD2	2.24	0.64
2:J:133:LYS:HG2	2:J:187:GLU:HG2	1.80	0.64
2:D:133:LYS:HG2	2:D:187:GLU:HG2	1.80	0.64
1:S:206:PRO:O	1:S:210:LYS:HD3	1.97	0.64
1:I:206:PRO:O	1:I:210:LYS:HD3	1.97	0.64
2:F:133:LYS:HG2	2:F:187:GLU:HG2	1.80	0.64
2:L:195:HIS:ND1	2:L:260:ASP:OD2	2.24	0.63
1:G:141:LYS:CD	2:J:384:GLU:HG3	2.29	0.63
1:A:206:PRO:O	1:A:210:LYS:HD3	1.97	0.63
1:I:235:GLN:HE21	2:J:208:ARG:HH21	0.76	0.63
2:L:383:HIS:HD2	2:L:386:THR:OG1	1.82	0.63
1:A:171:ASP:OD1	1:A:173:GLN:N	2.31	0.63
2:D:383:HIS:HD2	2:D:386:THR:OG1	1.82	0.63
2:D:129:ALA:HB2	2:D:186:ALA:O	1.99	0.63
1:G:228:CYS:HB2	1:G:229:PRO:HD3	1.81	0.63
2:H:383:HIS:HD2	2:H:386:THR:OG1	1.82	0.63
2:F:484:VAL:HG12	2:F:485:PRO:HD2	1.81	0.62
2:H:129:ALA:HB2	2:H:186:ALA:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:484:VAL:HG12	2:J:485:PRO:HD2	1.81	0.62
2:B:129:ALA:HB2	2:B:186:ALA:O	1.99	0.62
2:B:383:HIS:HD2	2:B:386:THR:OG1	1.82	0.62
1:E:235:GLN:HE21	2:F:208:ARG:HH21	0.77	0.62
2:J:383:HIS:HD2	2:J:386:THR:OG1	1.82	0.62
1:E:206:PRO:O	1:E:210:LYS:HD3	1.97	0.62
2:J:195:HIS:ND1	2:J:260:ASP:OD2	2.24	0.62
2:F:129:ALA:HB2	2:F:186:ALA:O	1.99	0.62
2:F:383:HIS:HD2	2:F:386:THR:OG1	1.82	0.62
2:L:129:ALA:HB2	2:L:186:ALA:O	1.99	0.62
1:A:228:CYS:HB2	1:A:229:PRO:HD3	1.81	0.62
1:C:14:ASN:OD1	1:C:92:MET:HB3	2.00	0.62
2:D:351:GLU:HB2	2:D:353:ARG:HD2	1.82	0.62
2:B:484:VAL:HG12	2:B:485:PRO:HD2	1.81	0.62
2:D:484:VAL:HG12	2:D:485:PRO:HD2	1.81	0.62
1:G:171:ASP:OD1	1:G:173:GLN:N	2.31	0.62
1:C:171:ASP:OD1	1:C:173:GLN:N	2.31	0.62
1:E:161:HIS:HD2	1:E:165:LYS:NZ	1.98	0.62
1:I:228:CYS:HB2	1:I:229:PRO:HD3	1.81	0.62
1:E:171:ASP:OD1	1:E:173:GLN:N	2.31	0.61
1:E:228:CYS:HB2	1:E:229:PRO:HD3	1.81	0.61
2:J:129:ALA:HB2	2:J:186:ALA:O	1.99	0.61
1:S:171:ASP:OD1	1:S:173:GLN:N	2.31	0.61
1:E:14:ASN:OD1	1:E:92:MET:HB3	2.00	0.61
1:G:14:ASN:OD1	1:G:92:MET:HB3	2.00	0.61
2:H:351:GLU:HB2	2:H:353:ARG:HD2	1.82	0.61
1:S:228:CYS:HB2	1:S:229:PRO:HD3	1.81	0.61
1:S:14:ASN:OD1	1:S:92:MET:HB3	2.00	0.61
2:F:195:HIS:ND1	2:F:260:ASP:OD2	2.24	0.61
1:C:161:HIS:HD2	1:C:165:LYS:NZ	1.98	0.61
2:L:484:VAL:HG12	2:L:485:PRO:HD2	1.81	0.61
1:E:188:CYS:O	1:E:191:LEU:HB2	2.01	0.61
2:F:351:GLU:HB2	2:F:353:ARG:HD2	1.82	0.61
1:S:161:HIS:HD2	1:S:165:LYS:NZ	1.98	0.61
2:B:351:GLU:HB2	2:B:353:ARG:HD2	1.82	0.61
1:A:161:HIS:HD2	1:A:165:LYS:NZ	1.98	0.61
1:I:161:HIS:HD2	1:I:165:LYS:NZ	1.98	0.61
1:I:188:CYS:O	1:I:191:LEU:HB2	2.01	0.61
2:L:351:GLU:HB2	2:L:353:ARG:HD2	1.82	0.61
1:A:14:ASN:OD1	1:A:92:MET:HB3	2.00	0.60
1:G:161:HIS:HD2	1:G:165:LYS:NZ	1.98	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:188:CYS:O	1:C:191:LEU:HB2	2.01	0.60
2:J:351:GLU:HB2	2:J:353:ARG:HD2	1.82	0.60
1:C:228:CYS:HB2	1:C:229:PRO:HD3	1.81	0.60
2:H:484:VAL:HG12	2:H:485:PRO:HD2	1.81	0.60
1:I:14:ASN:OD1	1:I:92:MET:HB3	2.00	0.60
1:S:188:CYS:O	1:S:191:LEU:HB2	2.01	0.60
1:A:188:CYS:O	1:A:191:LEU:HB2	2.01	0.60
2:B:195:HIS:ND1	2:B:260:ASP:OD2	2.24	0.60
1:S:26:ARG:NH2	2:L:217:ASN:HD21	1.98	0.60
2:F:108:HIS:CE1	2:F:417:GLN:HG2	2.37	0.59
2:D:108:HIS:CE1	2:D:417:GLN:HG2	2.36	0.59
2:H:108:HIS:CE1	2:H:417:GLN:HG2	2.37	0.59
2:L:322:HIS:HB2	2:L:359:ALA:HB3	1.84	0.59
2:D:322:HIS:HB2	2:D:359:ALA:HB3	1.84	0.59
2:J:108:HIS:CE1	2:J:417:GLN:HG2	2.36	0.59
2:B:108:HIS:CE1	2:B:417:GLN:HG2	2.36	0.59
1:G:188:CYS:O	1:G:191:LEU:HB2	2.01	0.59
2:J:458:PHE:CD1	2:J:465:MET:HE3	2.37	0.59
2:J:232:ASP:O	2:J:235:ARG:HG3	2.03	0.59
2:J:322:HIS:HB2	2:J:359:ALA:HB3	1.84	0.59
2:B:142:SER:HB2	2:B:143:PRO:HD3	1.85	0.59
2:B:217:ASN:ND2	2:B:217:ASN:C	2.56	0.58
2:D:232:ASP:O	2:D:235:ARG:HG3	2.03	0.58
2:F:232:ASP:O	2:F:235:ARG:HG3	2.03	0.58
2:B:458:PHE:CD1	2:B:465:MET:HE3	2.38	0.58
1:C:26:ARG:NH2	2:D:217:ASN:HD21	1.98	0.58
2:F:484:VAL:CG1	2:F:533:CYS:HB3	2.33	0.58
2:J:217:ASN:C	2:J:217:ASN:ND2	2.57	0.58
2:L:217:ASN:C	2:L:217:ASN:ND2	2.57	0.58
2:L:458:PHE:CD1	2:L:465:MET:HE3	2.38	0.58
2:B:232:ASP:O	2:B:235:ARG:HG3	2.03	0.58
2:D:142:SER:HB2	2:D:143:PRO:HD2	1.85	0.58
2:F:322:HIS:HB2	2:F:359:ALA:HB3	1.84	0.58
2:L:232:ASP:O	2:L:235:ARG:HG3	2.03	0.58
2:F:142:SER:HB2	2:F:143:PRO:HD3	1.85	0.58
1:I:171:ASP:OD1	1:I:173:GLN:N	2.31	0.58
2:L:32:ILE:HD11	2:L:511:ILE:HD11	1.86	0.58
2:H:322:HIS:HB2	2:H:359:ALA:HB3	1.84	0.58
2:D:32:ILE:HD11	2:D:511:ILE:HD11	1.86	0.58
2:D:8:LYS:HG3	2:D:25:VAL:O	2.04	0.58
2:H:217:ASN:ND2	2:H:217:ASN:C	2.57	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:142:SER:HB2	2:B:143:PRO:HD2	1.85	0.58
2:B:32:ILE:HD11	2:B:511:ILE:HD11	1.86	0.58
1:G:26:ARG:NH2	2:H:217:ASN:HD21	1.98	0.58
2:H:484:VAL:CG1	2:H:533:CYS:HB3	2.33	0.58
2:L:108:HIS:CE1	2:L:417:GLN:HG2	2.37	0.58
2:L:8:LYS:HG3	2:L:25:VAL:O	2.04	0.58
2:D:484:VAL:CG1	2:D:533:CYS:HB3	2.33	0.57
2:J:484:VAL:CG1	2:J:533:CYS:HB3	2.33	0.57
2:H:8:LYS:HG3	2:H:25:VAL:O	2.04	0.57
2:F:217:ASN:C	2:F:217:ASN:ND2	2.57	0.57
2:H:232:ASP:O	2:H:235:ARG:HG3	2.03	0.57
2:B:322:HIS:HB2	2:B:359:ALA:HB3	1.84	0.57
2:H:32:ILE:HD11	2:H:511:ILE:HD11	1.86	0.57
1:E:26:ARG:NH2	2:F:217:ASN:HD21	1.98	0.57
2:B:8:LYS:HG3	2:B:25:VAL:O	2.04	0.57
2:F:32:ILE:HD11	2:F:511:ILE:HD11	1.86	0.57
2:J:142:SER:HB2	2:J:143:PRO:HD3	1.85	0.57
2:J:8:LYS:HG3	2:J:25:VAL:O	2.04	0.57
2:D:308:LEU:HD21	2:D:376:LEU:HD22	1.87	0.57
2:F:142:SER:HB2	2:F:143:PRO:HD2	1.85	0.57
2:J:32:ILE:HD11	2:J:511:ILE:HD11	1.86	0.57
2:J:308:LEU:HD21	2:J:376:LEU:HD22	1.87	0.57
2:F:458:PHE:CD1	2:F:465:MET:HE3	2.39	0.56
2:H:308:LEU:HD21	2:H:376:LEU:HD22	1.87	0.56
2:J:142:SER:HB2	2:J:143:PRO:HD2	1.85	0.56
2:L:308:LEU:HD21	2:L:376:LEU:HD22	1.87	0.56
1:S:18:THR:O	1:S:18:THR:HG22	2.05	0.56
1:A:26:ARG:NH2	2:B:217:ASN:HD21	1.98	0.56
2:D:217:ASN:C	2:D:217:ASN:ND2	2.57	0.56
1:E:18:THR:O	1:E:18:THR:HG22	2.05	0.56
2:F:8:LYS:HG3	2:F:25:VAL:O	2.04	0.56
1:G:18:THR:O	1:G:18:THR:HG22	2.05	0.56
2:F:308:LEU:HD21	2:F:376:LEU:HD22	1.87	0.56
1:G:141:LYS:HD2	2:J:384:GLU:CG	2.35	0.56
1:I:18:THR:HG22	1:I:18:THR:O	2.06	0.56
2:L:484:VAL:CG1	2:L:533:CYS:HB3	2.33	0.56
2:L:69:THR:O	2:L:70:TYR:HB3	2.06	0.56
2:B:308:LEU:HD21	2:B:376:LEU:HD22	1.87	0.56
1:A:18:THR:HG22	1:A:18:THR:O	2.05	0.56
1:C:18:THR:HG22	1:C:18:THR:O	2.05	0.56
2:H:458:PHE:CD1	2:H:465:MET:HE3	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:283:CYS:SG	2:F:465:MET:HG3	2.46	0.56
1:I:26:ARG:NH2	2:J:217:ASN:HD21	1.98	0.56
2:J:283:CYS:SG	2:J:465:MET:HG3	2.46	0.56
2:H:142:SER:HB2	2:H:143:PRO:HD3	1.85	0.55
2:B:69:THR:O	2:B:70:TYR:HB3	2.06	0.55
2:J:119:ASP:O	2:J:522:ARG:NE	2.36	0.55
2:D:458:PHE:CD1	2:D:465:MET:HE3	2.41	0.55
2:B:283:CYS:SG	2:B:465:MET:HG3	2.46	0.55
2:J:69:THR:O	2:J:70:TYR:HB3	2.06	0.55
2:D:283:CYS:SG	2:D:465:MET:HG3	2.46	0.55
2:L:283:CYS:SG	2:L:465:MET:HG3	2.46	0.55
2:L:278:SER:HB3	2:L:305:GLY:HA2	1.88	0.55
2:B:278:SER:HB3	2:B:305:GLY:HA2	1.89	0.55
2:L:142:SER:HB2	2:L:143:PRO:HD2	1.85	0.55
2:B:297:TYR:CD2	2:B:298:THR:HG23	2.42	0.55
2:F:8:LYS:HA	2:F:25:VAL:O	2.07	0.55
2:H:69:THR:O	2:H:70:TYR:HB3	2.06	0.55
2:F:297:TYR:CD2	2:F:298:THR:HG23	2.42	0.54
2:H:278:SER:HB3	2:H:305:GLY:HA2	1.88	0.54
2:J:278:SER:HB3	2:J:305:GLY:HA2	1.88	0.54
2:J:8:LYS:HA	2:J:25:VAL:O	2.08	0.54
2:L:8:LYS:HA	2:L:25:VAL:O	2.08	0.54
2:F:69:THR:O	2:F:70:TYR:HB3	2.06	0.54
2:B:484:VAL:CG1	2:B:533:CYS:HB3	2.33	0.54
2:D:142:SER:HB2	2:D:143:PRO:HD3	1.85	0.54
1:E:26:ARG:HE	2:F:217:ASN:ND2	2.06	0.54
2:B:8:LYS:HA	2:B:25:VAL:O	2.07	0.54
2:D:8:LYS:HA	2:D:25:VAL:O	2.08	0.54
2:H:8:LYS:HA	2:H:25:VAL:O	2.07	0.54
2:L:297:TYR:CD2	2:L:298:THR:HG23	2.42	0.54
1:A:238:TRP:CH2	1:A:240:VAL:HB	2.43	0.54
2:H:283:CYS:SG	2:H:465:MET:HG3	2.46	0.54
2:J:297:TYR:CD2	2:J:298:THR:HG23	2.42	0.54
1:C:238:TRP:CH2	1:C:240:VAL:HB	2.43	0.54
1:G:238:TRP:CH2	1:G:240:VAL:HB	2.43	0.54
2:H:142:SER:HB2	2:H:143:PRO:HD2	1.85	0.54
2:L:484:VAL:HG13	2:L:485:PRO:HD2	1.89	0.54
2:D:278:SER:HB3	2:D:305:GLY:HA2	1.89	0.54
2:J:237:GLU:H	2:J:237:GLU:CD	2.11	0.54
1:A:26:ARG:HE	2:B:217:ASN:ND2	2.06	0.54
2:D:297:TYR:CD2	2:D:298:THR:HG23	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:69:THR:O	2:D:70:TYR:HB3	2.06	0.54
2:F:278:SER:HB3	2:F:305:GLY:HA2	1.89	0.54
1:S:238:TRP:CH2	1:S:240:VAL:HB	2.43	0.54
1:E:227:ASN:H	1:E:227:ASN:ND2	2.04	0.53
2:F:237:GLU:H	2:F:237:GLU:CD	2.11	0.53
1:I:238:TRP:CH2	1:I:240:VAL:HB	2.43	0.53
2:D:494:CYS:SG	2:D:498:LYS:HG3	2.48	0.53
2:H:297:TYR:CD2	2:H:298:THR:HG23	2.42	0.53
2:H:484:VAL:HG13	2:H:485:PRO:HD2	1.89	0.53
2:H:282:THR:HG22	2:H:377:VAL:HG21	1.90	0.53
2:L:494:CYS:SG	2:L:498:LYS:HG3	2.48	0.53
1:C:26:ARG:HE	2:D:217:ASN:ND2	2.06	0.53
2:D:237:GLU:CD	2:D:237:GLU:H	2.11	0.53
2:L:142:SER:HB2	2:L:143:PRO:HD3	1.85	0.53
2:L:237:GLU:CD	2:L:237:GLU:H	2.11	0.53
1:E:238:TRP:CH2	1:E:240:VAL:HB	2.43	0.53
2:H:108:HIS:ND1	2:H:418:CYS:HB2	2.24	0.53
2:J:282:THR:HG22	2:J:377:VAL:HG21	1.90	0.53
2:B:237:GLU:CD	2:B:237:GLU:H	2.11	0.53
1:C:20:CYS:SG	1:C:110:GLY:HA3	2.49	0.53
1:E:237:ASN:HB3	2:F:215:ALA:O	2.09	0.53
2:B:108:HIS:ND1	2:B:418:CYS:HB2	2.24	0.53
1:C:237:ASN:HB3	2:D:215:ALA:O	2.09	0.53
2:F:494:CYS:SG	2:F:498:LYS:HG3	2.48	0.53
2:H:237:GLU:H	2:H:237:GLU:CD	2.11	0.53
1:S:26:ARG:HE	2:L:217:ASN:ND2	2.06	0.53
2:H:119:ASP:O	2:H:522:ARG:NE	2.36	0.53
1:I:237:ASN:HB3	2:J:215:ALA:O	2.09	0.53
2:J:108:HIS:ND1	2:J:418:CYS:HB2	2.24	0.53
1:S:227:ASN:HD22	1:S:227:ASN:N	2.04	0.53
1:S:227:ASN:ND2	1:S:227:ASN:H	2.04	0.53
1:A:20:CYS:SG	1:A:110:GLY:HA3	2.49	0.53
2:H:494:CYS:SG	2:H:498:LYS:HG3	2.48	0.53
2:B:484:VAL:HG13	2:B:485:PRO:HD2	1.89	0.53
2:B:494:CYS:SG	2:B:498:LYS:HG3	2.48	0.53
2:D:484:VAL:HG13	2:D:485:PRO:HD2	1.89	0.53
2:F:354:TYR:OH	2:F:493:ARG:HD2	2.09	0.53
1:G:20:CYS:SG	1:G:110:GLY:HA3	2.49	0.53
1:A:237:ASN:HB3	2:B:215:ALA:O	2.09	0.52
2:B:354:TYR:OH	2:B:493:ARG:HD2	2.09	0.52
2:B:282:THR:HG22	2:B:377:VAL:HG21	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:20:CYS:SG	1:E:110:GLY:HA3	2.49	0.52
1:G:26:ARG:HE	2:H:217:ASN:ND2	2.06	0.52
1:S:20:CYS:SG	1:S:110:GLY:HA3	2.49	0.52
1:S:237:ASN:HB3	2:L:215:ALA:O	2.09	0.52
2:D:282:THR:HG22	2:D:377:VAL:HG21	1.90	0.52
2:F:282:THR:HG22	2:F:377:VAL:HG21	1.90	0.52
1:I:26:ARG:HE	2:J:217:ASN:ND2	2.06	0.52
2:J:484:VAL:HG13	2:J:485:PRO:HD2	1.89	0.52
2:D:383:HIS:NE2	2:D:385:PRO:HG2	2.25	0.52
2:D:108:HIS:ND1	2:D:418:CYS:HB2	2.24	0.52
2:J:494:CYS:SG	2:J:498:LYS:HG3	2.49	0.52
1:A:227:ASN:ND2	1:A:227:ASN:H	2.04	0.52
2:L:383:HIS:NE2	2:L:385:PRO:HG2	2.25	0.52
2:L:108:HIS:ND1	2:L:418:CYS:HB2	2.24	0.52
1:I:20:CYS:SG	1:I:110:GLY:HA3	2.49	0.52
1:G:237:ASN:HB3	2:H:215:ALA:O	2.09	0.52
1:G:185:HIS:CE1	1:G:191:LEU:HD23	2.45	0.52
2:L:354:TYR:OH	2:L:493:ARG:HD2	2.09	0.52
1:C:227:ASN:H	1:C:227:ASN:ND2	2.05	0.52
2:F:108:HIS:ND1	2:F:418:CYS:HB2	2.24	0.52
2:H:383:HIS:NE2	2:H:385:PRO:HG2	2.25	0.52
2:J:354:TYR:OH	2:J:493:ARG:HD2	2.09	0.52
1:A:185:HIS:CE1	1:A:191:LEU:HD23	2.45	0.52
2:D:354:TYR:OH	2:D:493:ARG:HD2	2.09	0.52
1:C:185:HIS:CE1	1:C:191:LEU:HD23	2.45	0.51
1:I:185:HIS:CE1	1:I:191:LEU:HD23	2.45	0.51
1:S:185:HIS:CE1	1:S:191:LEU:HD23	2.45	0.51
1:A:185:HIS:CE1	1:A:191:LEU:CD2	2.94	0.51
1:E:185:HIS:CE1	1:E:191:LEU:CD2	2.94	0.51
2:F:484:VAL:HG13	2:F:485:PRO:HD2	1.89	0.51
1:G:244:HIS:CG	1:G:245:PRO:HD2	2.46	0.51
1:I:185:HIS:CE1	1:I:191:LEU:CD2	2.94	0.51
2:J:383:HIS:NE2	2:J:385:PRO:HG2	2.25	0.51
2:B:383:HIS:NE2	2:B:385:PRO:HG2	2.25	0.51
1:C:244:HIS:CG	1:C:245:PRO:HD2	2.46	0.51
1:A:244:HIS:CG	1:A:245:PRO:HD2	2.46	0.51
1:E:185:HIS:CE1	1:E:191:LEU:HD23	2.45	0.51
2:F:383:HIS:NE2	2:F:385:PRO:HG2	2.25	0.51
2:H:354:TYR:OH	2:H:493:ARG:HD2	2.09	0.51
2:L:282:THR:HG22	2:L:377:VAL:HG21	1.90	0.51
1:A:207:GLU:HB3	1:A:212:TYR:CD2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:244:HIS:CG	1:E:245:PRO:HD2	2.46	0.51
1:S:185:HIS:CE1	1:S:191:LEU:CD2	2.94	0.51
2:F:346:THR:O	2:F:347:GLU:HB2	2.10	0.51
1:G:207:GLU:HB3	1:G:212:TYR:CD2	2.46	0.51
1:I:207:GLU:HB3	1:I:212:TYR:CD2	2.46	0.51
1:I:227:ASN:ND2	1:I:227:ASN:H	2.04	0.51
2:L:346:THR:O	2:L:347:GLU:HB2	2.10	0.51
2:B:119:ASP:O	2:B:522:ARG:NE	2.36	0.51
1:A:209:LYS:NZ	2:B:442:ASP:OD1	2.43	0.51
1:G:185:HIS:CE1	1:G:191:LEU:CD2	2.94	0.51
2:F:119:ASP:O	2:F:522:ARG:NE	2.36	0.50
1:G:227:ASN:H	1:G:227:ASN:ND2	2.04	0.50
2:H:346:THR:O	2:H:347:GLU:HB2	2.11	0.50
2:J:346:THR:O	2:J:347:GLU:HB2	2.10	0.50
2:L:485:PRO:HG2	7:L:537:FCO:N1	2.26	0.50
1:S:207:GLU:HB3	1:S:212:TYR:CD2	2.46	0.50
1:S:244:HIS:CG	1:S:245:PRO:HD2	2.46	0.50
2:B:195:HIS:HD1	2:B:260:ASP:CG	2.14	0.50
2:H:20:HIS:O	2:H:531:ILE:HG21	2.12	0.50
1:I:244:HIS:CG	1:I:245:PRO:HD2	2.46	0.50
2:B:346:THR:O	2:B:347:GLU:HB2	2.10	0.50
2:B:485:PRO:HG2	7:B:537:FCO:N1	2.26	0.50
1:E:207:GLU:HB3	1:E:212:TYR:CD2	2.46	0.50
2:J:20:HIS:O	2:J:531:ILE:HG21	2.12	0.50
2:D:20:HIS:O	2:D:531:ILE:HG21	2.12	0.50
2:D:491:GLY:O	2:D:500:SER:HB3	2.12	0.50
2:F:20:HIS:O	2:F:531:ILE:HG21	2.12	0.50
2:J:491:GLY:O	2:J:500:SER:HB3	2.12	0.50
1:C:185:HIS:CE1	1:C:191:LEU:CD2	2.94	0.50
2:D:119:ASP:O	2:D:522:ARG:NE	2.36	0.50
2:H:262:LEU:HD21	2:H:393:VAL:HG22	1.93	0.50
2:J:262:LEU:HD21	2:J:393:VAL:HG22	1.93	0.50
2:B:262:LEU:HD21	2:B:393:VAL:HG22	1.93	0.50
1:C:207:GLU:HB3	1:C:212:TYR:CD2	2.46	0.50
2:L:20:HIS:O	2:L:531:ILE:HG21	2.12	0.50
2:B:20:HIS:O	2:B:531:ILE:HG21	2.12	0.50
2:D:346:THR:O	2:D:347:GLU:HB2	2.10	0.50
2:L:262:LEU:HD21	2:L:393:VAL:HG22	1.93	0.50
2:B:491:GLY:O	2:B:500:SER:HB3	2.12	0.49
2:H:491:GLY:O	2:H:500:SER:HB3	2.12	0.49
2:J:214:GLY:O	2:J:215:ALA:HB3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:92:ALA:O	2:D:96:ARG:HD3	2.12	0.49
2:F:214:GLY:O	2:F:215:ALA:HB3	2.12	0.49
2:J:485:PRO:HG2	7:J:537:FCO:N1	2.26	0.49
2:D:262:LEU:HD21	2:D:393:VAL:HG22	1.93	0.49
1:I:36:ILE:N	1:I:36:ILE:CD1	2.76	0.49
1:A:100:ALA:HB3	1:A:101:PRO:HD3	1.95	0.49
1:A:36:ILE:N	1:A:36:ILE:CD1	2.76	0.49
1:E:235:GLN:NE2	2:F:208:ARG:NH2	2.39	0.49
1:E:36:ILE:CD1	1:E:36:ILE:N	2.76	0.49
2:F:491:GLY:O	2:F:500:SER:HB3	2.12	0.49
2:H:485:PRO:HG2	7:H:537:FCO:N1	2.26	0.49
2:L:195:HIS:HD1	2:L:260:ASP:CG	2.14	0.49
1:C:100:ALA:HB3	1:C:101:PRO:HD3	1.95	0.49
2:D:321:GLU:O	2:D:333:ALA:HA	2.13	0.49
1:G:100:ALA:HB3	1:G:101:PRO:HD3	1.95	0.49
1:I:100:ALA:HB3	1:I:101:PRO:HD3	1.95	0.49
1:I:235:GLN:NE2	2:J:208:ARG:NH2	2.39	0.49
1:S:36:ILE:CD1	1:S:36:ILE:N	2.76	0.49
1:A:235:GLN:NE2	2:B:208:ARG:NH2	2.39	0.49
2:D:214:GLY:O	2:D:215:ALA:HB3	2.13	0.49
2:D:485:PRO:HG2	7:D:537:FCO:N1	2.26	0.49
2:F:321:GLU:O	2:F:333:ALA:HA	2.13	0.49
2:F:485:PRO:HG2	7:F:537:FCO:N1	2.26	0.49
2:H:214:GLY:O	2:H:215:ALA:HB3	2.13	0.49
2:L:491:GLY:O	2:L:500:SER:HB3	2.12	0.49
1:S:100:ALA:HB3	1:S:101:PRO:HD3	1.95	0.49
2:H:82:ASN:HD22	2:H:455:GLY:HA2	1.77	0.49
2:H:92:ALA:O	2:H:96:ARG:HD3	2.12	0.49
2:J:92:ALA:O	2:J:96:ARG:HD3	2.12	0.49
2:L:92:ALA:O	2:L:96:ARG:HD3	2.12	0.49
2:B:92:ALA:O	2:B:96:ARG:HD3	2.12	0.49
1:E:100:ALA:HB3	1:E:101:PRO:HD3	1.95	0.49
2:F:262:LEU:HD21	2:F:393:VAL:HG22	1.93	0.49
2:B:82:ASN:HD22	2:B:455:GLY:HA2	1.77	0.49
2:F:92:ALA:O	2:F:96:ARG:HD3	2.12	0.49
2:L:321:GLU:O	2:L:333:ALA:HA	2.13	0.49
2:B:321:GLU:O	2:B:333:ALA:HA	2.13	0.48
2:J:82:ASN:HD22	2:J:455:GLY:HA2	1.77	0.48
2:D:82:ASN:HD22	2:D:455:GLY:HA2	1.77	0.48
1:G:36:ILE:CD1	1:G:36:ILE:N	2.76	0.48
2:H:321:GLU:O	2:H:333:ALA:HA	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:303:ILE:HD13	2:J:308:LEU:HD23	1.95	0.48
1:A:36:ILE:N	1:A:36:ILE:HD12	2.29	0.48
2:B:384:GLU:HG3	1:E:141:LYS:CD	2.43	0.48
2:F:82:ASN:HD22	2:F:455:GLY:HA2	1.77	0.48
2:B:214:GLY:O	2:B:215:ALA:HB3	2.12	0.48
2:B:334:HIS:CD2	2:B:340:VAL:HG22	2.49	0.48
2:H:303:ILE:HD13	2:H:308:LEU:HD23	1.95	0.48
2:J:321:GLU:O	2:J:333:ALA:HA	2.13	0.48
2:L:82:ASN:HD22	2:L:455:GLY:HA2	1.77	0.48
2:F:303:ILE:HD13	2:F:308:LEU:HD23	1.95	0.48
1:G:36:ILE:HD12	1:G:36:ILE:N	2.29	0.48
1:I:36:ILE:N	1:I:36:ILE:HD12	2.29	0.48
2:L:334:HIS:CD2	2:L:340:VAL:HG22	2.49	0.48
1:C:36:ILE:N	1:C:36:ILE:CD1	2.76	0.48
2:F:457:GLY:O	2:F:467:SER:HA	2.14	0.48
2:J:334:HIS:CD2	2:J:340:VAL:HG22	2.49	0.48
2:B:283:CYS:SG	2:B:465:MET:CG	3.02	0.48
2:J:457:GLY:O	2:J:467:SER:HA	2.14	0.48
2:J:283:CYS:SG	2:J:465:MET:CG	3.02	0.48
2:L:214:GLY:O	2:L:215:ALA:HB3	2.12	0.48
2:B:303:ILE:HD13	2:B:308:LEU:HD23	1.95	0.48
2:D:283:CYS:SG	2:D:465:MET:CG	3.02	0.48
2:D:303:ILE:HD13	2:D:308:LEU:HD23	1.95	0.48
2:H:334:HIS:CD2	2:H:340:VAL:HG22	2.49	0.48
2:F:283:CYS:SG	2:F:465:MET:CG	3.02	0.48
1:C:209:LYS:NZ	2:D:442:ASP:OD1	2.43	0.47
2:F:334:HIS:CD2	2:F:340:VAL:HG22	2.49	0.47
1:S:36:ILE:HD12	1:S:36:ILE:N	2.29	0.47
2:D:195:HIS:HD1	2:D:260:ASP:CG	2.14	0.47
2:B:457:GLY:O	2:B:467:SER:HA	2.14	0.47
2:H:457:GLY:O	2:H:467:SER:HA	2.14	0.47
2:J:390:VAL:O	2:J:394:LEU:HG	2.15	0.47
2:L:283:CYS:SG	2:L:465:MET:CG	3.02	0.47
2:D:334:HIS:CD2	2:D:340:VAL:HG22	2.49	0.47
1:E:161:HIS:HD2	1:E:165:LYS:HZ3	1.60	0.47
2:L:119:ASP:O	2:L:522:ARG:NE	2.36	0.47
2:H:390:VAL:O	2:H:394:LEU:HG	2.15	0.47
2:H:493:ARG:HA	2:H:498:LYS:O	2.15	0.47
2:L:303:ILE:HD13	2:L:308:LEU:HD23	1.95	0.47
2:B:68:CYS:CB	7:B:537:FCO:C2	2.93	0.47
1:C:161:HIS:HD2	1:C:165:LYS:HZ3	1.61	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:390:VAL:O	2:D:394:LEU:HG	2.15	0.47
1:E:209:LYS:NZ	2:F:442:ASP:OD1	2.43	0.47
2:F:493:ARG:HA	2:F:498:LYS:O	2.15	0.47
2:H:283:CYS:SG	2:H:465:MET:CG	3.02	0.47
1:E:36:ILE:N	1:E:36:ILE:HD12	2.29	0.47
2:F:390:VAL:O	2:F:394:LEU:HG	2.15	0.47
2:L:457:GLY:O	2:L:467:SER:HA	2.14	0.47
2:L:304:TRP:HZ3	2:L:365:GLU:HG3	1.80	0.47
2:D:304:TRP:HZ3	2:D:365:GLU:HG3	1.80	0.47
2:J:335:HIS:HE1	2:J:469:TRP:CZ3	2.33	0.47
2:J:68:CYS:CB	7:J:537:FCO:C2	2.93	0.47
1:S:124:ASN:HD21	1:S:128:THR:N	2.10	0.47
2:B:304:TRP:HZ3	2:B:365:GLU:HG3	1.80	0.47
1:C:36:ILE:N	1:C:36:ILE:HD12	2.29	0.47
2:D:457:GLY:O	2:D:467:SER:HA	2.14	0.47
2:D:493:ARG:HA	2:D:498:LYS:O	2.15	0.47
1:G:235:GLN:NE2	2:H:208:ARG:NH2	2.39	0.47
2:H:335:HIS:HE1	2:H:469:TRP:CZ3	2.33	0.47
2:J:320:GLU:OE1	2:J:333:ALA:C	2.54	0.47
1:I:209:LYS:NZ	2:J:442:ASP:OD1	2.43	0.47
2:L:390:VAL:O	2:L:394:LEU:HG	2.15	0.47
2:D:239:ILE:HG21	2:D:433:GLU:HG3	1.97	0.46
2:F:68:CYS:CB	7:F:537:FCO:C2	2.93	0.46
2:H:68:CYS:CB	7:H:537:FCO:C2	2.93	0.46
2:J:304:TRP:HZ3	2:J:365:GLU:HG3	1.80	0.46
2:L:239:ILE:HG21	2:L:433:GLU:HG3	1.97	0.46
2:D:458:PHE:HD1	2:D:465:MET:CE	2.29	0.46
1:G:161:HIS:HD2	1:G:165:LYS:HZ3	1.62	0.46
2:B:408:LEU:HA	2:B:408:LEU:HD12	1.65	0.46
2:F:304:TRP:HZ3	2:F:365:GLU:HG3	1.80	0.46
2:F:335:HIS:HE1	2:F:469:TRP:CZ3	2.33	0.46
2:B:493:ARG:HA	2:B:498:LYS:O	2.15	0.46
2:L:320:GLU:OE1	2:L:333:ALA:C	2.54	0.46
2:L:493:ARG:HA	2:L:498:LYS:O	2.15	0.46
2:L:68:CYS:CB	7:L:537:FCO:C2	2.93	0.46
1:A:124:ASN:HD21	1:A:128:THR:N	2.10	0.46
1:A:217:LEU:HD23	1:A:217:LEU:HA	1.72	0.46
1:C:124:ASN:HD21	1:C:128:THR:N	2.10	0.46
2:H:304:TRP:HZ3	2:H:365:GLU:HG3	1.80	0.46
2:J:493:ARG:HA	2:J:498:LYS:O	2.15	0.46
2:L:458:PHE:CD1	2:L:465:MET:CE	2.99	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:217:LEU:HA	1:S:217:LEU:HD23	1.73	0.46
2:B:278:SER:O	2:B:279:ASN:CB	2.63	0.46
2:B:390:VAL:O	2:B:394:LEU:HG	2.15	0.46
2:D:335:HIS:HE1	2:D:469:TRP:CZ3	2.33	0.46
2:F:34:ASN:OD1	2:F:35:ALA:N	2.49	0.46
2:F:458:PHE:HD1	2:F:465:MET:CE	2.28	0.46
2:H:76:SER:O	2:H:80:VAL:HG23	2.16	0.46
2:J:458:PHE:HD1	2:J:465:MET:CE	2.29	0.46
2:B:239:ILE:HG21	2:B:433:GLU:HG3	1.97	0.46
2:B:335:HIS:HE1	2:B:469:TRP:CZ3	2.33	0.46
1:C:217:LEU:HD23	1:C:217:LEU:HA	1.72	0.46
1:C:235:GLN:NE2	2:D:208:ARG:NH2	2.39	0.46
2:F:239:ILE:HG21	2:F:433:GLU:HG3	1.97	0.46
2:H:195:HIS:HD1	2:H:260:ASP:CG	2.14	0.46
2:B:320:GLU:OE1	2:B:333:ALA:C	2.54	0.45
2:B:34:ASN:OD1	2:B:35:ALA:N	2.49	0.45
2:D:68:CYS:CB	7:D:537:FCO:C2	2.93	0.45
2:D:76:SER:O	2:D:80:VAL:HG23	2.16	0.45
2:F:458:PHE:CD1	2:F:465:MET:CE	2.99	0.45
2:H:235:ARG:HD2	2:H:235:ARG:HH11	1.64	0.45
2:H:239:ILE:HG21	2:H:433:GLU:HG3	1.97	0.45
2:J:16:ARG:HD2	2:J:16:ARG:HH11	1.47	0.45
2:J:408:LEU:HA	2:J:408:LEU:HD12	1.65	0.45
2:J:239:ILE:HG21	2:J:433:GLU:HG3	1.97	0.45
2:F:76:SER:O	2:F:80:VAL:HG23	2.16	0.45
2:H:320:GLU:OE1	2:H:333:ALA:C	2.54	0.45
2:L:335:HIS:HE1	2:L:469:TRP:CZ3	2.33	0.45
2:B:306:ASN:ND2	2:B:405:PHE:CD1	2.80	0.45
2:B:458:PHE:CD1	2:B:465:MET:CE	2.99	0.45
2:B:288:THR:OG1	2:B:295:SER:HB2	2.17	0.45
2:B:458:PHE:HD1	2:B:465:MET:CE	2.29	0.45
1:E:217:LEU:HA	1:E:217:LEU:HD23	1.72	0.45
2:F:320:GLU:OE1	2:F:333:ALA:C	2.54	0.45
2:J:458:PHE:CD1	2:J:465:MET:CE	2.99	0.45
2:L:458:PHE:HD1	2:L:465:MET:CE	2.29	0.45
2:B:76:SER:O	2:B:80:VAL:HG23	2.16	0.45
2:D:458:PHE:CD1	2:D:465:MET:CE	2.99	0.45
2:D:491:GLY:O	2:D:500:SER:CB	2.65	0.45
2:L:491:GLY:O	2:L:500:SER:CB	2.65	0.45
1:S:254:PHE:HA	1:S:258:TYR:HD2	1.82	0.45
2:F:288:THR:OG1	2:F:295:SER:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:491:GLY:O	2:F:500:SER:CB	2.65	0.45
1:A:254:PHE:HA	1:A:258:TYR:HD2	1.82	0.45
2:B:491:GLY:O	2:B:500:SER:CB	2.65	0.45
2:D:16:ARG:HH11	2:D:16:ARG:HD2	1.47	0.45
2:D:408:LEU:HD12	2:D:408:LEU:HA	1.65	0.45
2:D:80:VAL:O	2:D:84:VAL:HB	2.17	0.45
2:F:278:SER:O	2:F:279:ASN:CB	2.63	0.45
1:I:161:HIS:HD2	1:I:165:LYS:HZ3	1.64	0.45
2:D:320:GLU:OE1	2:D:333:ALA:C	2.54	0.45
2:L:235:ARG:HH11	2:L:235:ARG:HD2	1.64	0.45
2:F:335:HIS:CE1	2:F:469:TRP:CZ3	3.05	0.45
2:H:458:PHE:HD1	2:H:465:MET:CE	2.29	0.45
2:H:80:VAL:O	2:H:84:VAL:HB	2.17	0.45
2:L:278:SER:O	2:L:279:ASN:CB	2.63	0.45
2:B:335:HIS:CE1	2:B:469:TRP:CZ3	3.05	0.45
1:E:124:ASN:HD21	1:E:128:THR:N	2.10	0.45
2:J:491:GLY:O	2:J:500:SER:CB	2.65	0.45
2:J:76:SER:O	2:J:80:VAL:HG23	2.16	0.45
1:C:254:PHE:HA	1:C:258:TYR:HD2	1.82	0.44
2:D:288:THR:OG1	2:D:295:SER:HB2	2.16	0.44
2:D:335:HIS:CE1	2:D:469:TRP:CZ3	3.05	0.44
2:F:408:LEU:HA	2:F:408:LEU:HD12	1.65	0.44
1:G:124:ASN:HD21	1:G:128:THR:N	2.10	0.44
2:H:288:THR:OG1	2:H:295:SER:HB2	2.16	0.44
2:J:288:THR:OG1	2:J:295:SER:HB2	2.17	0.44
2:J:336:PRO:O	2:J:481:GLN:HG3	2.18	0.44
2:L:336:PRO:O	2:L:481:GLN:HG3	2.17	0.44
2:L:76:SER:O	2:L:80:VAL:HG23	2.16	0.44
2:D:142:SER:CB	2:D:143:PRO:CD	2.81	0.44
2:D:431:LYS:O	2:D:432:LEU:C	2.55	0.44
2:F:336:PRO:O	2:F:481:GLN:HG3	2.17	0.44
2:J:244:LYS:NZ	2:J:248:GLU:OE1	2.44	0.44
2:L:431:LYS:O	2:L:432:LEU:C	2.55	0.44
2:H:336:PRO:O	2:H:481:GLN:HG3	2.17	0.44
2:H:458:PHE:CD1	2:H:465:MET:CE	2.99	0.44
2:J:80:VAL:O	2:J:84:VAL:HB	2.17	0.44
2:L:80:VAL:O	2:L:84:VAL:HB	2.17	0.44
2:B:326:SER:HA	2:B:355:SER:O	2.18	0.44
2:H:335:HIS:CE1	2:H:469:TRP:CZ3	3.05	0.44
2:B:431:LYS:O	2:B:432:LEU:C	2.55	0.44
2:D:315:ASN:HA	2:D:316:PRO:HD2	1.95	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:384:GLU:CG	1:E:141:LYS:HD2	2.45	0.44
1:G:254:PHE:HA	1:G:258:TYR:HD2	1.82	0.44
2:H:431:LYS:O	2:H:432:LEU:C	2.55	0.44
2:H:491:GLY:O	2:H:500:SER:CB	2.65	0.44
2:H:124:ALA:O	2:H:127:LEU:HB2	2.18	0.44
2:J:335:HIS:CE1	2:J:469:TRP:CZ3	3.05	0.44
1:A:161:HIS:HD2	1:A:165:LYS:HZ2	1.63	0.44
2:B:235:ARG:HD2	2:B:235:ARG:HH11	1.64	0.44
2:B:244:LYS:NZ	2:B:248:GLU:OE1	2.44	0.44
2:F:454:GLN:HA	2:F:470:ILE:O	2.18	0.44
2:H:454:GLN:HA	2:H:470:ILE:O	2.18	0.44
2:H:84:VAL:HG13	2:H:84:VAL:O	2.18	0.44
1:I:254:PHE:HA	1:I:258:TYR:HD2	1.82	0.44
2:J:454:GLN:HA	2:J:470:ILE:O	2.18	0.44
2:L:326:SER:HA	2:L:355:SER:O	2.18	0.44
1:A:80:ASP:HB3	1:A:83:TYR:CE2	2.53	0.44
2:B:454:GLN:HA	2:B:470:ILE:O	2.18	0.44
2:B:336:PRO:O	2:B:481:GLN:HG3	2.17	0.44
2:B:119:ASP:HB3	2:B:522:ARG:HG3	2.00	0.44
2:F:324:LYS:HG2	2:F:324:LYS:O	2.18	0.44
2:L:335:HIS:CE1	2:L:469:TRP:CZ3	3.05	0.44
2:D:124:ALA:O	2:D:127:LEU:HB2	2.18	0.44
2:D:450:PRO:HG2	2:D:453:SER:HB3	2.00	0.44
2:J:84:VAL:O	2:J:84:VAL:HG13	2.18	0.44
2:L:454:GLN:HA	2:L:470:ILE:O	2.18	0.44
1:C:194:PHE:HD1	1:C:213:CYS:SG	2.41	0.43
2:B:431:LYS:NZ	1:E:169:GLU:OE1	2.43	0.43
2:F:16:ARG:HH11	2:F:16:ARG:HD2	1.47	0.43
2:F:326:SER:HA	2:F:355:SER:O	2.18	0.43
2:F:450:PRO:HG2	2:F:453:SER:HB3	2.00	0.43
2:H:324:LYS:HG2	2:H:324:LYS:O	2.18	0.43
2:L:324:LYS:HG2	2:L:324:LYS:O	2.18	0.43
2:D:454:GLN:HA	2:D:470:ILE:O	2.18	0.43
2:F:431:LYS:O	2:F:432:LEU:C	2.55	0.43
2:F:80:VAL:O	2:F:84:VAL:HB	2.17	0.43
2:J:124:ALA:O	2:J:127:LEU:HB2	2.18	0.43
2:J:431:LYS:O	2:J:432:LEU:C	2.56	0.43
2:B:124:ALA:O	2:B:127:LEU:HB2	2.18	0.43
2:B:324:LYS:O	2:B:324:LYS:HG2	2.18	0.43
1:C:80:ASP:HB3	1:C:83:TYR:CE2	2.53	0.43
2:F:246:TYR:HE2	2:F:426:GLU:OE1	2.02	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:246:TYR:HE2	2:H:426:GLU:OE1	2.02	0.43
2:H:326:SER:HA	2:H:355:SER:O	2.18	0.43
2:B:105:MET:HE2	2:B:249:VAL:HG12	2.00	0.43
2:B:246:TYR:HE2	2:B:426:GLU:OE1	2.02	0.43
2:B:80:VAL:O	2:B:84:VAL:HB	2.17	0.43
2:D:252:PHE:CE1	2:D:256:VAL:HG11	2.54	0.43
2:D:246:TYR:HE2	2:D:426:GLU:OE1	2.02	0.43
2:F:448:GLN:HB3	2:F:448:GLN:HE21	1.67	0.43
2:F:119:ASP:HB3	2:F:522:ARG:HG3	2.00	0.43
2:H:252:PHE:CE1	2:H:256:VAL:HG11	2.54	0.43
2:H:239:ILE:HD11	2:H:432:LEU:HD23	2.00	0.43
2:H:450:PRO:HG2	2:H:453:SER:HB3	2.00	0.43
2:J:12:ASP:OD2	2:J:22:ARG:HB2	2.18	0.43
2:J:246:TYR:HE2	2:J:426:GLU:OE1	2.02	0.43
2:L:12:ASP:OD2	2:L:22:ARG:HB2	2.18	0.43
2:B:12:ASP:OD2	2:B:22:ARG:HB2	2.18	0.43
2:B:235:ARG:NH2	2:B:238:ARG:HD3	2.34	0.43
2:B:262:LEU:HD13	2:B:396:THR:HG21	2.01	0.43
1:E:254:PHE:HA	1:E:258:TYR:HD2	1.82	0.43
2:H:16:ARG:HH11	2:H:16:ARG:HD2	1.47	0.43
1:I:124:ASN:HD21	1:I:128:THR:N	2.10	0.43
1:I:194:PHE:HD1	1:I:213:CYS:SG	2.41	0.43
1:I:80:ASP:HB3	1:I:83:TYR:CE2	2.53	0.43
2:J:278:SER:O	2:J:279:ASN:CB	2.63	0.43
2:L:124:ALA:O	2:L:127:LEU:HB2	2.18	0.43
1:A:194:PHE:HD1	1:A:213:CYS:SG	2.41	0.43
2:B:239:ILE:HD11	2:B:432:LEU:HD23	2.00	0.43
2:D:278:SER:O	2:D:279:ASN:CB	2.63	0.43
2:D:336:PRO:O	2:D:481:GLN:HG3	2.17	0.43
2:F:12:ASP:OD2	2:F:22:ARG:HB2	2.18	0.43
2:F:252:PHE:CE1	2:F:256:VAL:HG11	2.54	0.43
2:J:195:HIS:HD1	2:J:260:ASP:CG	2.14	0.43
2:L:246:TYR:HE2	2:L:426:GLU:OE1	2.02	0.43
2:L:84:VAL:O	2:L:84:VAL:HG13	2.18	0.43
2:B:450:PRO:HG2	2:B:453:SER:HB3	2.00	0.43
2:D:262:LEU:HD13	2:D:396:THR:HG21	2.01	0.43
1:E:80:ASP:HB3	1:E:83:TYR:CE2	2.53	0.43
2:F:124:ALA:O	2:F:127:LEU:HB2	2.18	0.43
2:H:12:ASP:OD2	2:H:22:ARG:HB2	2.19	0.43
2:J:450:PRO:HG2	2:J:453:SER:HB3	2.00	0.43
2:L:235:ARG:NH2	2:L:238:ARG:HD3	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:84:VAL:HG13	2:F:84:VAL:O	2.18	0.43
2:J:239:ILE:HD11	2:J:432:LEU:HD23	2.00	0.43
2:B:119:ASP:O	2:B:522:ARG:NH2	2.51	0.43
2:D:12:ASP:OD2	2:D:22:ARG:HB2	2.18	0.43
2:D:239:ILE:HD11	2:D:432:LEU:HD23	2.00	0.43
2:D:324:LYS:O	2:D:324:LYS:HG2	2.18	0.43
1:G:80:ASP:HB3	1:G:83:TYR:CE2	2.53	0.43
2:H:262:LEU:HD13	2:H:396:THR:HG21	2.01	0.43
2:J:119:ASP:O	2:J:522:ARG:NH2	2.51	0.43
2:J:252:PHE:CE1	2:J:256:VAL:HG11	2.54	0.43
2:J:262:LEU:HD13	2:J:396:THR:HG21	2.01	0.43
2:L:288:THR:OG1	2:L:295:SER:HB2	2.17	0.43
2:L:119:ASP:HB3	2:L:522:ARG:HG3	2.00	0.43
1:S:80:ASP:HB3	1:S:83:TYR:CE2	2.53	0.43
2:B:450:PRO:HG2	2:B:453:SER:CB	2.49	0.43
2:D:119:ASP:HB3	2:D:522:ARG:HG3	2.00	0.43
2:D:84:VAL:O	2:D:84:VAL:HG13	2.18	0.43
2:F:262:LEU:HD13	2:F:396:THR:HG21	2.01	0.43
2:F:306:ASN:ND2	2:F:405:PHE:CD1	2.80	0.43
1:G:193:HIS:CD2	1:G:211:GLY:O	2.72	0.43
2:H:278:SER:O	2:H:279:ASN:CB	2.63	0.43
2:H:450:PRO:HG2	2:H:453:SER:CB	2.49	0.43
2:J:326:SER:HA	2:J:355:SER:O	2.18	0.43
2:L:262:LEU:HD13	2:L:396:THR:HG21	2.01	0.43
2:D:326:SER:HA	2:D:355:SER:O	2.18	0.42
2:D:450:PRO:HG2	2:D:453:SER:CB	2.49	0.42
1:E:194:PHE:HD1	1:E:213:CYS:SG	2.41	0.42
2:F:235:ARG:NH2	2:F:238:ARG:HD3	2.34	0.42
2:H:12:ASP:HA	2:H:13:PRO:HA	1.91	0.42
1:I:193:HIS:CD2	1:I:211:GLY:O	2.72	0.42
2:J:235:ARG:HH11	2:J:235:ARG:HD2	1.64	0.42
2:L:252:PHE:CE1	2:L:256:VAL:HG11	2.54	0.42
1:S:194:PHE:HD1	1:S:213:CYS:SG	2.41	0.42
2:D:235:ARG:NH2	2:D:238:ARG:HD3	2.34	0.42
2:F:239:ILE:HD11	2:F:432:LEU:HD23	2.00	0.42
1:G:194:PHE:HD1	1:G:213:CYS:SG	2.41	0.42
2:H:119:ASP:O	2:H:522:ARG:NH2	2.51	0.42
2:J:286:PHE:CD1	2:J:428:TRP:CH2	3.07	0.42
2:J:306:ASN:ND2	2:J:405:PHE:CD1	2.80	0.42
2:J:9:ILE:HB	2:J:25:VAL:CG2	2.50	0.42
1:S:161:HIS:HD2	1:S:165:LYS:HZ2	1.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:193:HIS:CD2	1:C:211:GLY:O	2.72	0.42
2:F:286:PHE:CD1	2:F:428:TRP:CH2	3.07	0.42
2:F:450:PRO:HG2	2:F:453:SER:CB	2.49	0.42
2:H:242:PHE:CD1	2:H:242:PHE:C	2.92	0.42
2:H:9:ILE:HB	2:H:25:VAL:CG2	2.50	0.42
2:L:450:PRO:HG2	2:L:453:SER:HB3	2.00	0.42
1:A:230:LYS:HG3	1:A:230:LYS:H	1.68	0.42
2:H:9:ILE:HB	2:H:25:VAL:HG22	2.01	0.42
2:D:286:PHE:CD1	2:D:428:TRP:CH2	3.07	0.42
2:D:9:ILE:HB	2:D:25:VAL:HG22	2.01	0.42
2:F:105:MET:HE2	2:F:249:VAL:HG12	2.02	0.42
2:H:119:ASP:HB3	2:H:522:ARG:HG3	2.00	0.42
2:J:450:PRO:HG2	2:J:453:SER:CB	2.49	0.42
2:L:239:ILE:HD11	2:L:432:LEU:HD23	2.00	0.42
2:L:450:PRO:HG2	2:L:453:SER:CB	2.49	0.42
1:S:193:HIS:CD2	1:S:211:GLY:O	2.72	0.42
2:B:252:PHE:CE1	2:B:256:VAL:HG11	2.54	0.42
2:B:383:HIS:CD2	2:B:386:THR:OG1	2.70	0.42
2:D:242:PHE:C	2:D:242:PHE:CD1	2.92	0.42
2:F:242:PHE:CD1	2:F:242:PHE:C	2.92	0.42
2:B:242:PHE:C	2:B:242:PHE:CD1	2.92	0.42
2:B:286:PHE:CD1	2:B:428:TRP:CH2	3.07	0.42
2:D:490:LEU:HD13	2:D:529:PRO:HB3	2.02	0.42
2:H:235:ARG:NH2	2:H:238:ARG:HD3	2.34	0.42
2:J:119:ASP:HB3	2:J:522:ARG:HG3	2.00	0.42
2:L:286:PHE:CD1	2:L:428:TRP:CH2	3.07	0.42
2:B:9:ILE:HB	2:B:25:VAL:CG2	2.50	0.42
2:D:9:ILE:HB	2:D:25:VAL:CG2	2.50	0.42
2:H:490:LEU:HD13	2:H:529:PRO:HB3	2.02	0.42
2:L:384:GLU:N	2:L:385:PRO:CD	2.83	0.42
2:L:9:ILE:HB	2:L:25:VAL:CG2	2.50	0.42
1:A:193:HIS:CD2	1:A:211:GLY:O	2.72	0.42
2:B:84:VAL:HG13	2:B:84:VAL:O	2.18	0.42
2:J:324:LYS:HG2	2:J:324:LYS:O	2.18	0.42
2:L:12:ASP:HA	2:L:13:PRO:HA	1.91	0.42
2:B:141:LEU:HA	2:B:141:LEU:HD23	1.78	0.42
2:F:9:ILE:HB	2:F:25:VAL:CG2	2.50	0.42
2:J:490:LEU:HD13	2:J:529:PRO:HB3	2.02	0.42
2:L:242:PHE:C	2:L:242:PHE:CD1	2.92	0.42
2:L:306:ASN:ND2	2:L:405:PHE:CD1	2.80	0.42
1:S:235:GLN:NE2	2:L:208:ARG:NH2	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:315:ASN:HA	2:B:316:PRO:HD2	1.95	0.41
2:F:125:ASN:HA	2:F:128:ASN:ND2	2.35	0.41
2:H:286:PHE:CD1	2:H:428:TRP:CH2	3.07	0.41
1:G:209:LYS:NZ	2:H:442:ASP:OD1	2.43	0.41
2:J:125:ASN:HA	2:J:128:ASN:ND2	2.35	0.41
2:B:384:GLU:N	2:B:385:PRO:CD	2.83	0.41
2:D:125:ASN:HA	2:D:128:ASN:ND2	2.35	0.41
2:D:21:LEU:HB2	2:D:531:ILE:HG12	2.02	0.41
2:D:384:GLU:N	2:D:385:PRO:CD	2.83	0.41
1:E:193:HIS:CD2	1:E:211:GLY:O	2.72	0.41
2:F:119:ASP:O	2:F:522:ARG:NH2	2.51	0.41
1:G:244:HIS:ND1	1:G:245:PRO:HD2	2.36	0.41
2:H:125:ASN:HA	2:H:128:ASN:ND2	2.35	0.41
2:J:21:LEU:HB2	2:J:531:ILE:HG12	2.02	0.41
2:L:490:LEU:HD13	2:L:529:PRO:HB3	2.02	0.41
2:J:9:ILE:HB	2:J:25:VAL:HG22	2.01	0.41
2:B:125:ASN:HA	2:B:128:ASN:ND2	2.35	0.41
1:E:244:HIS:ND1	1:E:245:PRO:HD2	2.36	0.41
2:J:242:PHE:CD1	2:J:242:PHE:C	2.92	0.41
2:L:125:ASN:HA	2:L:128:ASN:ND2	2.35	0.41
1:C:244:HIS:ND1	1:C:245:PRO:HD2	2.36	0.41
2:D:119:ASP:O	2:D:522:ARG:NH2	2.51	0.41
2:F:384:GLU:N	2:F:385:PRO:CD	2.83	0.41
2:H:21:LEU:HB2	2:H:531:ILE:HG12	2.02	0.41
2:H:315:ASN:HA	2:H:316:PRO:HD2	1.95	0.41
1:I:18:THR:CG2	1:I:18:THR:O	2.69	0.41
2:J:235:ARG:NH2	2:J:238:ARG:HD3	2.34	0.41
2:L:16:ARG:HH11	2:L:16:ARG:HD2	1.47	0.41
2:B:490:LEU:HD13	2:B:529:PRO:HB3	2.02	0.41
1:E:228:CYS:HB2	1:E:229:PRO:CD	2.50	0.41
2:F:195:HIS:HD1	2:F:260:ASP:CG	2.14	0.41
2:L:9:ILE:HB	2:L:25:VAL:HG22	2.01	0.41
1:S:230:LYS:HG3	1:S:230:LYS:H	1.68	0.41
2:D:244:LYS:NZ	2:D:248:GLU:OE1	2.44	0.41
2:F:141:LEU:HA	2:F:141:LEU:HD23	1.78	0.41
2:J:448:GLN:HB3	2:J:448:GLN:HE21	1.67	0.41
2:L:130:ASP:HA	2:L:131:PRO:HD2	1.93	0.41
2:L:244:LYS:NZ	2:L:248:GLU:OE1	2.44	0.41
1:A:227:ASN:HD22	1:A:227:ASN:N	2.04	0.41
2:B:9:ILE:HB	2:B:25:VAL:HG22	2.01	0.41
2:F:490:LEU:HD13	2:F:529:PRO:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:384:GLU:N	2:H:385:PRO:CD	2.83	0.41
1:I:96:CYS:HB3	1:I:135:LEU:HD11	2.03	0.41
1:I:244:HIS:ND1	1:I:245:PRO:HD2	2.36	0.41
2:L:141:LEU:HD23	2:L:141:LEU:HA	1.78	0.41
1:S:209:LYS:NZ	2:L:442:ASP:OD1	2.43	0.41
1:A:18:THR:CG2	1:A:18:THR:O	2.69	0.41
2:F:477:ILE:HG21	2:F:477:ILE:HD13	1.90	0.41
2:F:52:ARG:HH11	2:F:52:ARG:HD3	1.69	0.41
2:H:62:GLN:HA	2:H:72:HIS:HB2	2.03	0.41
2:J:105:MET:HE2	2:J:249:VAL:HG12	2.03	0.41
2:J:83:CYS:HB2	2:J:454:GLN:C	2.41	0.41
2:J:62:GLN:HA	2:J:72:HIS:HB2	2.03	0.41
1:S:18:THR:O	1:S:18:THR:CG2	2.69	0.41
1:A:251:GLU:HA	1:A:252:PRO:HD3	1.95	0.41
1:A:76:ILE:HA	1:A:77:PRO:HD3	1.95	0.41
2:D:294:ASN:OD1	2:D:300:GLN:NE2	2.47	0.41
2:D:34:ASN:OD1	2:D:35:ALA:N	2.49	0.41
2:D:83:CYS:HB2	2:D:454:GLN:C	2.42	0.41
1:G:96:CYS:HB3	1:G:135:LEU:HD11	2.03	0.41
2:H:383:HIS:CD2	2:H:386:THR:OG1	2.70	0.41
2:L:83:CYS:HB2	2:L:454:GLN:C	2.41	0.41
1:A:244:HIS:ND1	1:A:245:PRO:HD2	2.36	0.41
2:F:21:LEU:HB2	2:F:531:ILE:HG12	2.02	0.41
2:F:83:CYS:HB2	2:F:454:GLN:C	2.41	0.41
2:F:9:ILE:HB	2:F:25:VAL:HG22	2.01	0.41
2:H:34:ASN:OD1	2:H:35:ALA:N	2.48	0.41
2:L:21:LEU:HB2	2:L:531:ILE:HG12	2.02	0.41
1:S:202:SER:O	1:S:208:ALA:HB2	2.22	0.41
1:A:238:TRP:HB2	1:A:239:PRO:HD2	2.04	0.40
1:E:96:CYS:HB3	1:E:135:LEU:HD11	2.03	0.40
2:H:83:CYS:HB2	2:H:454:GLN:C	2.42	0.40
1:I:224:THR:HG21	6:I:266:F3S:S3	2.62	0.40
1:I:227:ASN:ND2	1:I:227:ASN:N	2.68	0.40
2:F:130:ASP:HA	2:F:131:PRO:HD2	1.93	0.40
1:G:238:TRP:HB2	1:G:239:PRO:HD2	2.03	0.40
1:I:238:TRP:HB2	1:I:239:PRO:HD2	2.04	0.40
2:J:144:LYS:NZ	2:J:198:GLU:OE2	2.53	0.40
2:J:384:GLU:N	2:J:385:PRO:CD	2.83	0.40
2:L:315:ASN:HA	2:L:316:PRO:HD2	1.95	0.40
1:S:228:CYS:HB2	1:S:229:PRO:CD	2.50	0.40
1:A:202:SER:O	1:A:208:ALA:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:CYS:HB2	1:A:229:PRO:CD	2.51	0.40
2:B:62:GLN:HA	2:B:72:HIS:HB2	2.03	0.40
2:D:62:GLN:HA	2:D:72:HIS:HB2	2.03	0.40
2:F:88:ILE:HA	2:F:89:PRO:HD3	1.90	0.40
2:L:119:ASP:O	2:L:522:ARG:NH2	2.51	0.40
1:S:244:HIS:ND1	1:S:245:PRO:HD2	2.36	0.40
1:S:224:THR:HG21	6:S:266:F3S:S3	2.62	0.40
2:B:83:CYS:HB2	2:B:454:GLN:C	2.42	0.40
1:C:202:SER:O	1:C:208:ALA:HB2	2.22	0.40
1:C:96:CYS:HB3	1:C:135:LEU:HD11	2.03	0.40
2:D:320:GLU:OE1	2:D:334:HIS:CA	2.70	0.40
2:F:235:ARG:HD2	2:F:235:ARG:HH11	1.64	0.40
1:G:18:THR:CG2	1:G:18:THR:O	2.69	0.40
2:H:234:LEU:HD12	2:H:234:LEU:HA	1.95	0.40

All (3) 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)
9:A:340:HOH:O	9:I:1015:HOH:O[1_445]	1.32	0.88
9:A:341:HOH:O	9:C:450:HOH:O[1_444]	1.34	0.86
9:S:338:HOH:O	9:E:639:HOH:O[1_556]	1.41	0.79

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	Percentiles
1	A	259/264 (98%)	244 (94%)	14 (5%)	1 (0%)	38 57
1	C	259/264 (98%)	244 (94%)	14 (5%)	1 (0%)	38 57
1	E	259/264 (98%)	244 (94%)	14 (5%)	1 (0%)	38 57
1	G	259/264 (98%)	244 (94%)	14 (5%)	1 (0%)	38 57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	259/264 (98%)	244 (94%)	14 (5%)	1 (0%)	38	57
1	S	259/264 (98%)	244 (94%)	14 (5%)	1 (0%)	38	57
2	B	528/536 (98%)	506 (96%)	21 (4%)	1 (0%)	51	71
2	D	528/536 (98%)	506 (96%)	21 (4%)	1 (0%)	51	71
2	F	528/536 (98%)	506 (96%)	21 (4%)	1 (0%)	51	71
2	H	528/536 (98%)	506 (96%)	21 (4%)	1 (0%)	51	71
2	J	528/536 (98%)	506 (96%)	21 (4%)	1 (0%)	51	71
2	L	528/536 (98%)	506 (96%)	21 (4%)	1 (0%)	51	71
All	All	4722/4800 (98%)	4500 (95%)	210 (4%)	12 (0%)	44	64

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	S	5	LYS
2	L	118	LEU
1	A	5	LYS
2	B	118	LEU
1	C	5	LYS
2	D	118	LEU
1	E	5	LYS
2	F	118	LEU
1	G	5	LYS
2	H	118	LEU
1	I	5	LYS
2	J	118	LEU

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	208/210 (99%)	194 (93%)	14 (7%)	19	33
1	C	208/210 (99%)	194 (93%)	14 (7%)	19	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	208/210 (99%)	194 (93%)	14 (7%)	19	33
1	G	208/210 (99%)	194 (93%)	14 (7%)	19	33
1	I	208/210 (99%)	194 (93%)	14 (7%)	19	33
1	S	208/210 (99%)	194 (93%)	14 (7%)	19	33
2	B	434/439 (99%)	399 (92%)	35 (8%)	14	24
2	D	434/439 (99%)	399 (92%)	35 (8%)	14	24
2	F	434/439 (99%)	399 (92%)	35 (8%)	14	24
2	H	434/439 (99%)	399 (92%)	35 (8%)	14	24
2	J	434/439 (99%)	399 (92%)	35 (8%)	14	24
2	L	434/439 (99%)	399 (92%)	35 (8%)	14	24
All	All	3852/3894 (99%)	3558 (92%)	294 (8%)	15	27

All (294) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	S	5	LYS
1	S	16	GLU
1	S	25	LEU
1	S	28	VAL
1	S	48	LEU
1	S	67	ASP
1	S	124	ASN
1	S	163	LEU
1	S	165	LYS
1	S	191	LEU
1	S	195	GLU
1	S	227	ASN
1	S	230	LYS
1	S	236	VAL
2	L	7	ASN
2	L	8	LYS
2	L	10	VAL
2	L	28	GLU
2	L	33	LYS
2	L	49	LEU
2	L	50	LYS
2	L	74	LEU
2	L	83	CYS

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Mol	Chain	Res	Type
2	L	84	VAL
2	L	87	LYS
2	L	88	ILE
2	L	109	LEU
2	L	118	LEU
2	L	217	ASN
2	L	234	LEU
2	L	237	GLU
2	L	244	LYS
2	L	281	LEU
2	L	300	GLN
2	L	353	ARG
2	L	361	ARG
2	L	384	GLU
2	L	395	LYS
2	L	402	GLU
2	L	465	MET
2	L	473	ARG
2	L	476	LYS
2	L	482	LEU
2	L	496	GLU
2	L	498	LYS
2	L	511	ILE
2	L	515	LYS
2	L	517	PRO
2	L	531	ILE
1	A	5	LYS
1	A	16	GLU
1	A	25	LEU
1	A	28	VAL
1	A	48	LEU
1	A	67	ASP
1	A	124	ASN
1	A	163	LEU
1	A	165	LYS
1	A	191	LEU
1	A	195	GLU
1	A	227	ASN
1	A	230	LYS
1	A	236	VAL
2	B	7	ASN
2	B	8	LYS

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Mol	Chain	Res	Type
2	B	10	VAL
2	B	28	GLU
2	B	33	LYS
2	B	49	LEU
2	B	50	LYS
2	B	74	LEU
2	B	83	CYS
2	B	84	VAL
2	B	87	LYS
2	B	88	ILE
2	B	109	LEU
2	B	118	LEU
2	B	217	ASN
2	B	234	LEU
2	B	237	GLU
2	B	244	LYS
2	B	281	LEU
2	B	300	GLN
2	B	353	ARG
2	B	361	ARG
2	B	384	GLU
2	B	395	LYS
2	B	402	GLU
2	B	465	MET
2	B	473	ARG
2	B	476	LYS
2	B	482	LEU
2	B	496	GLU
2	B	498	LYS
2	B	511	ILE
2	B	515	LYS
2	B	517	PRO
2	B	531	ILE
1	C	5	LYS
1	C	16	GLU
1	C	25	LEU
1	C	28	VAL
1	C	48	LEU
1	C	67	ASP
1	C	124	ASN
1	C	163	LEU
1	C	165	LYS

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Mol	Chain	Res	Type
1	C	191	LEU
1	C	195	GLU
1	C	227	ASN
1	C	230	LYS
1	C	236	VAL
2	D	7	ASN
2	D	8	LYS
2	D	10	VAL
2	D	28	GLU
2	D	33	LYS
2	D	49	LEU
2	D	50	LYS
2	D	74	LEU
2	D	83	CYS
2	D	84	VAL
2	D	87	LYS
2	D	88	ILE
2	D	109	LEU
2	D	118	LEU
2	D	217	ASN
2	D	234	LEU
2	D	237	GLU
2	D	244	LYS
2	D	281	LEU
2	D	300	GLN
2	D	353	ARG
2	D	361	ARG
2	D	384	GLU
2	D	395	LYS
2	D	402	GLU
2	D	465	MET
2	D	473	ARG
2	D	476	LYS
2	D	482	LEU
2	D	496	GLU
2	D	498	LYS
2	D	511	ILE
2	D	515	LYS
2	D	517	PRO
2	D	531	ILE
1	E	5	LYS
1	E	16	GLU

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Mol	Chain	Res	Type
1	E	25	LEU
1	E	28	VAL
1	E	48	LEU
1	E	67	ASP
1	E	124	ASN
1	E	163	LEU
1	E	165	LYS
1	E	191	LEU
1	E	195	GLU
1	E	227	ASN
1	E	230	LYS
1	E	236	VAL
2	F	7	ASN
2	F	8	LYS
2	F	10	VAL
2	F	28	GLU
2	F	33	LYS
2	F	49	LEU
2	F	50	LYS
2	F	74	LEU
2	F	83	CYS
2	F	84	VAL
2	F	87	LYS
2	F	88	ILE
2	F	109	LEU
2	F	118	LEU
2	F	217	ASN
2	F	234	LEU
2	F	237	GLU
2	F	244	LYS
2	F	281	LEU
2	F	300	GLN
2	F	353	ARG
2	F	361	ARG
2	F	384	GLU
2	F	395	LYS
2	F	402	GLU
2	F	465	MET
2	F	473	ARG
2	F	476	LYS
2	F	482	LEU
2	F	496	GLU

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Mol	Chain	Res	Type
2	F	498	LYS
2	F	511	ILE
2	F	515	LYS
2	F	517	PRO
2	F	531	ILE
1	G	5	LYS
1	G	16	GLU
1	G	25	LEU
1	G	28	VAL
1	G	48	LEU
1	G	67	ASP
1	G	124	ASN
1	G	163	LEU
1	G	165	LYS
1	G	191	LEU
1	G	195	GLU
1	G	227	ASN
1	G	230	LYS
1	G	236	VAL
2	H	7	ASN
2	H	8	LYS
2	H	10	VAL
2	H	28	GLU
2	H	33	LYS
2	H	49	LEU
2	H	50	LYS
2	H	74	LEU
2	H	83	CYS
2	H	84	VAL
2	H	87	LYS
2	H	88	ILE
2	H	109	LEU
2	H	118	LEU
2	H	217	ASN
2	H	234	LEU
2	H	237	GLU
2	H	244	LYS
2	H	281	LEU
2	H	300	GLN
2	H	353	ARG
2	H	361	ARG
2	H	384	GLU

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Mol	Chain	Res	Type
2	H	395	LYS
2	H	402	GLU
2	H	465	MET
2	H	473	ARG
2	H	476	LYS
2	H	482	LEU
2	H	496	GLU
2	H	498	LYS
2	H	511	ILE
2	H	515	LYS
2	H	517	PRO
2	H	531	ILE
1	I	5	LYS
1	I	16	GLU
1	I	25	LEU
1	I	28	VAL
1	I	48	LEU
1	I	67	ASP
1	I	124	ASN
1	I	163	LEU
1	I	165	LYS
1	I	191	LEU
1	I	195	GLU
1	I	227	ASN
1	I	230	LYS
1	I	236	VAL
2	J	7	ASN
2	J	8	LYS
2	J	10	VAL
2	J	28	GLU
2	J	33	LYS
2	J	49	LEU
2	J	50	LYS
2	J	74	LEU
2	J	83	CYS
2	J	84	VAL
2	J	87	LYS
2	J	88	ILE
2	J	109	LEU
2	J	118	LEU
2	J	217	ASN
2	J	234	LEU

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Mol	Chain	Res	Type
2	J	237	GLU
2	J	244	LYS
2	J	281	LEU
2	J	300	GLN
2	J	353	ARG
2	J	361	ARG
2	J	384	GLU
2	J	395	LYS
2	J	402	GLU
2	J	465	MET
2	J	473	ARG
2	J	476	LYS
2	J	482	LEU
2	J	496	GLU
2	J	498	LYS
2	J	511	ILE
2	J	515	LYS
2	J	517	PRO
2	J	531	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (86) such sidechains are listed below:

Mol	Chain	Res	Type
1	S	124	ASN
1	S	154	ASN
1	S	161	HIS
1	S	227	ASN
1	S	231	GLN
1	S	235	GLN
2	L	82	ASN
2	L	108	HIS
2	L	217	ASN
2	L	334	HIS
2	L	335	HIS
2	L	383	HIS
2	L	448	GLN
2	L	460	ASN
2	L	481	GLN
1	A	124	ASN
1	A	154	ASN
1	A	161	HIS
1	A	227	ASN

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Mol	Chain	Res	Type
1	A	231	GLN
1	A	235	GLN
2	B	82	ASN
2	B	108	HIS
2	B	217	ASN
2	B	334	HIS
2	B	383	HIS
2	B	448	GLN
2	B	460	ASN
2	B	481	GLN
1	C	124	ASN
1	C	154	ASN
1	C	161	HIS
1	C	227	ASN
1	C	231	GLN
1	C	235	GLN
2	D	82	ASN
2	D	108	HIS
2	D	217	ASN
2	D	334	HIS
2	D	383	HIS
2	D	448	GLN
2	D	460	ASN
2	D	481	GLN
1	E	124	ASN
1	E	154	ASN
1	E	161	HIS
1	E	227	ASN
1	E	231	GLN
1	E	235	GLN
2	F	82	ASN
2	F	108	HIS
2	F	217	ASN
2	F	334	HIS
2	F	383	HIS
2	F	448	GLN
2	F	460	ASN
2	F	481	GLN
1	G	124	ASN
1	G	154	ASN
1	G	161	HIS
1	G	227	ASN

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Mol	Chain	Res	Type
1	G	231	GLN
1	G	235	GLN
2	H	82	ASN
2	H	108	HIS
2	H	217	ASN
2	H	334	HIS
2	H	383	HIS
2	H	448	GLN
2	H	460	ASN
2	H	481	GLN
1	I	124	ASN
1	I	154	ASN
1	I	161	HIS
1	I	227	ASN
1	I	231	GLN
1	I	235	GLN
2	J	82	ASN
2	J	108	HIS
2	J	217	ASN
2	J	334	HIS
2	J	335	HIS
2	J	383	HIS
2	J	448	GLN
2	J	460	ASN
2	J	481	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 42 ligands modelled in this entry, 18 are monoatomic - leaving 24 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
5	SF4	A	265	1	0,12,12	0.00	-	0,24,24	0.00	-
6	F3S	A	266	1	0,9,9	0.00	-	0,15,15	0.00	-
5	SF4	A	267	1	0,12,12	0.00	-	0,24,24	0.00	-
7	FCO	B	537	8,2	0,6,6	0.00	-	0,6,6	0.00	-
5	SF4	C	265	1	0,12,12	0.00	-	0,24,24	0.00	-
6	F3S	C	266	1	0,9,9	0.00	-	0,15,15	0.00	-
5	SF4	C	267	1	0,12,12	0.00	-	0,24,24	0.00	-
7	FCO	D	537	8,2	0,6,6	0.00	-	0,6,6	0.00	-
5	SF4	E	265	1	0,12,12	0.00	-	0,24,24	0.00	-
6	F3S	E	266	1	0,9,9	0.00	-	0,15,15	0.00	-
5	SF4	E	267	1	0,12,12	0.00	-	0,24,24	0.00	-
7	FCO	F	537	8,2	0,6,6	0.00	-	0,6,6	0.00	-
5	SF4	G	265	1	0,12,12	0.00	-	0,24,24	0.00	-
6	F3S	G	266	1	0,9,9	0.00	-	0,15,15	0.00	-
5	SF4	G	267	1	0,12,12	0.00	-	0,24,24	0.00	-
7	FCO	H	537	8,2	0,6,6	0.00	-	0,6,6	0.00	-
5	SF4	I	265	1	0,12,12	0.00	-	0,24,24	0.00	-
6	F3S	I	266	1	0,9,9	0.00	-	0,15,15	0.00	-
5	SF4	I	267	1	0,12,12	0.00	-	0,24,24	0.00	-
7	FCO	J	537	8,2	0,6,6	0.00	-	0,6,6	0.00	-
7	FCO	L	537	8,2	0,6,6	0.00	-	0,6,6	0.00	-
5	SF4	S	265	1	0,12,12	0.00	-	0,24,24	0.00	-
6	F3S	S	266	1	0,9,9	0.00	-	0,15,15	0.00	-
5	SF4	S	267	1	0,12,12	0.00	-	0,24,24	0.00	-

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
5	SF4	A	265	1	-	0/0/48/48	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	F3S	A	266	1	-	0/0/24/24	0/0/3/3
5	SF4	A	267	1	-	0/0/48/48	0/6/5/5
7	FCO	B	537	8,2	-	0/0/6/6	0/0/0/0
5	SF4	C	265	1	-	0/0/48/48	0/6/5/5
6	F3S	C	266	1	-	0/0/24/24	0/0/3/3
5	SF4	C	267	1	-	0/0/48/48	0/6/5/5
7	FCO	D	537	8,2	-	0/0/6/6	0/0/0/0
5	SF4	E	265	1	-	0/0/48/48	0/6/5/5
6	F3S	E	266	1	-	0/0/24/24	0/0/3/3
5	SF4	E	267	1	-	0/0/48/48	0/6/5/5
7	FCO	F	537	8,2	-	0/0/6/6	0/0/0/0
5	SF4	G	265	1	-	0/0/48/48	0/6/5/5
6	F3S	G	266	1	-	0/0/24/24	0/0/3/3
5	SF4	G	267	1	-	0/0/48/48	0/6/5/5
7	FCO	H	537	8,2	-	0/0/6/6	0/0/0/0
5	SF4	I	265	1	-	0/0/48/48	0/6/5/5
6	F3S	I	266	1	-	0/0/24/24	0/0/3/3
5	SF4	I	267	1	-	0/0/48/48	0/6/5/5
7	FCO	J	537	8,2	-	0/0/6/6	0/0/0/0
7	FCO	L	537	8,2	-	0/0/6/6	0/0/0/0
5	SF4	S	265	1	-	0/0/48/48	0/6/5/5
6	F3S	S	266	1	-	0/0/24/24	0/0/3/3
5	SF4	S	267	1	-	0/0/48/48	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	537	FCO	2	0
7	D	537	FCO	2	0
7	F	537	FCO	2	0
7	H	537	FCO	2	0
6	I	266	F3S	1	0
7	J	537	FCO	2	0
7	L	537	FCO	2	0
6	S	266	F3S	1	0



## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.