Full wwPDB X-ray Structure Validation Report (i)

Jul 31, 2023 – 10:14 PM EDT

PDB ID	:	2FRV
Title	:	CRYSTAL STRUCTURE OF THE OXIDIZED FORM OF NI-FE HYDROGENASE
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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

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

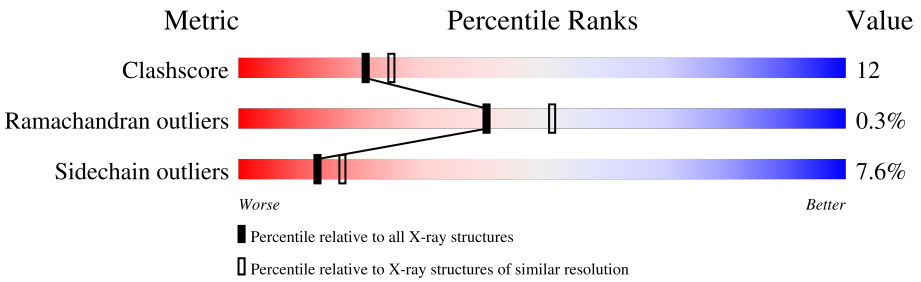
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

1 Overall quality at a glance (i)

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	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	264	69% 26% • •
1	C	264	70% 24% • •
1	E	264	70% 24% 5% •
1	G	264	70% 24% • •
1	I	264	70% 23% 5% •
1	S	264	70% 23% 5% •
2	B	536	63% 31% • ••
2	D	536	63% 30% • ••

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Mol	Chain	Length	Quality of chain
2	F	536	62% 31% 5%
2	H	536	63% 30%
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 (i)

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
			Total	C	N	O	S			
1	S	261	1964	1249	329	367	19	0	0	0
1	A	261	1964	1249	329	367	19	0	0	0
1	C	261	1964	1249	329	367	19	0	0	0
1	E	261	1964	1249	329	367	19	0	0	0
1	G	261	1964	1249	329	367	19	0	0	0
1	I	261	1964	1249	329	367	19	0	0	0

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

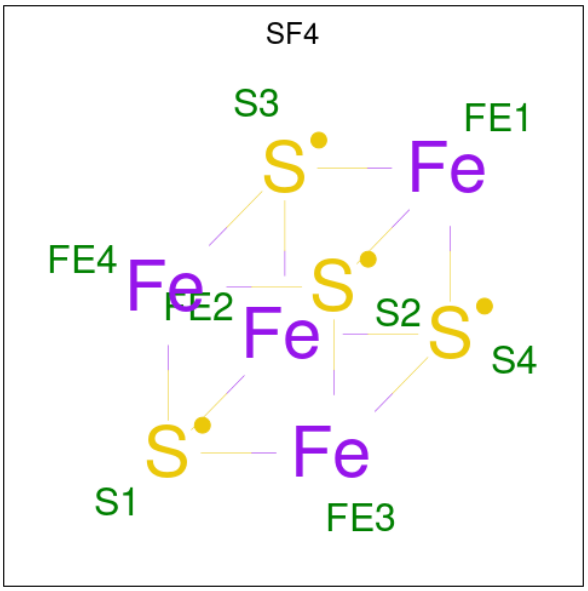
- Molecule 2 is a protein called PERIPLASMIC HYDROGENASE.

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

There are 24 discrepancies between the modelled and reference sequences:

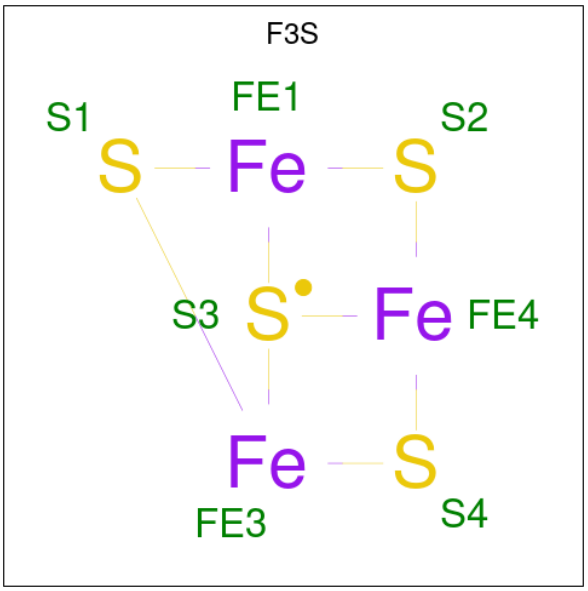
Chain	Residue	Modelled	Actual	Comment	Reference
L	144	LYS	ARG	conflict	UNP P12944
L	332	GLY	ASP	conflict	UNP P12944
L	482	LEU	HIS	conflict	UNP P12944
L	497	GLY	ARG	conflict	UNP P12944
B	144	LYS	ARG	conflict	UNP P12944
B	332	GLY	ASP	conflict	UNP P12944
B	482	LEU	HIS	conflict	UNP P12944
B	497	GLY	ARG	conflict	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 IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



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

- Molecule 4 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4).



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

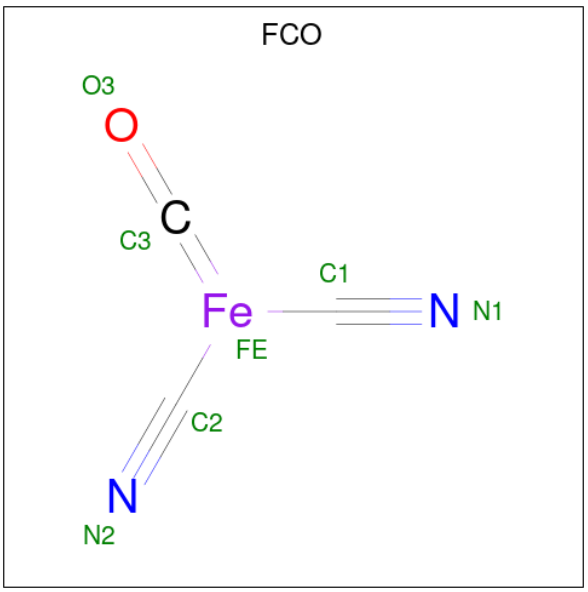
- Molecule 5 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

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

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- 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 7 3 1 2 1	0	0
7	B	1	Total C Fe N O 7 3 1 2 1	0	0
7	D	1	Total C Fe N O 7 3 1 2 1	0	0
7	F	1	Total C Fe N O 7 3 1 2 1	0	0

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

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

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

- Molecule 9 is water.

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
9	H	112	112	112	0	0
			Total	O		
9	I	80	80	80	0	0
			Total	O		
9	J	113	113	113	0	0

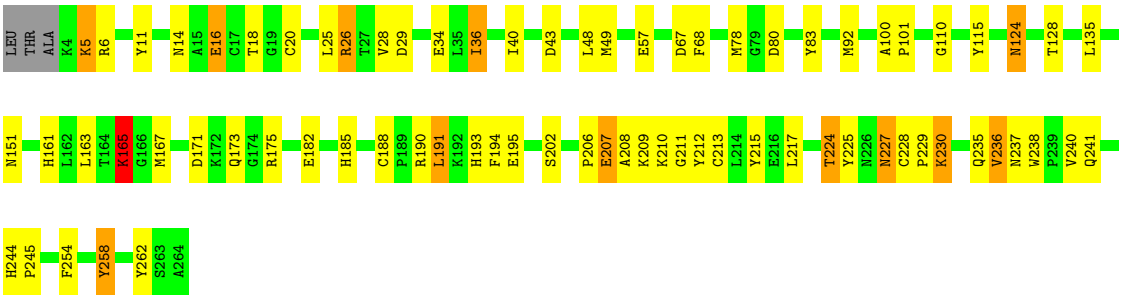
3 Residue-property plots (i)

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

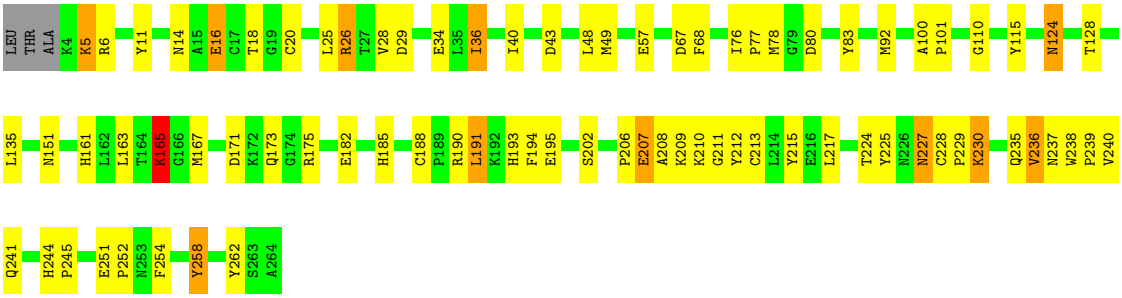
• Molecule 1: PERIPLASMIC HYDROGENASE

Chain S:



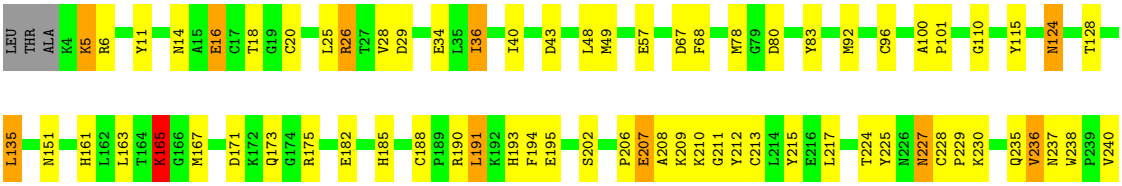
• Molecule 1: PERIPLASMIC HYDROGENASE

Chain A:



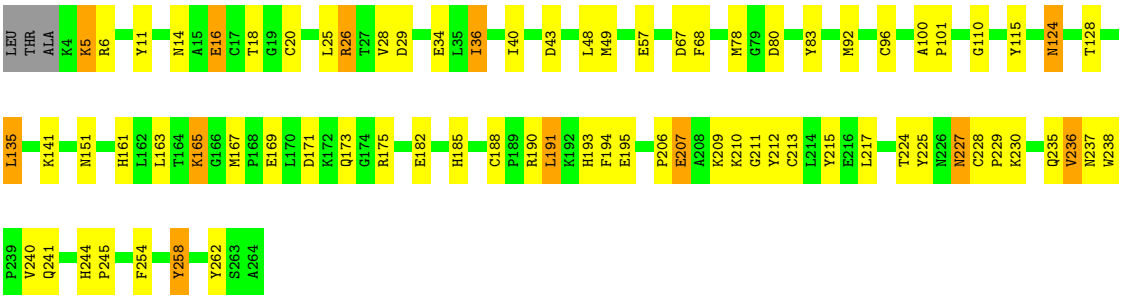
• Molecule 1: PERIPLASMIC HYDROGENASE

Chain C:



• Molecule 1: PERIPLASMIC HYDROGENASE

Chain E:

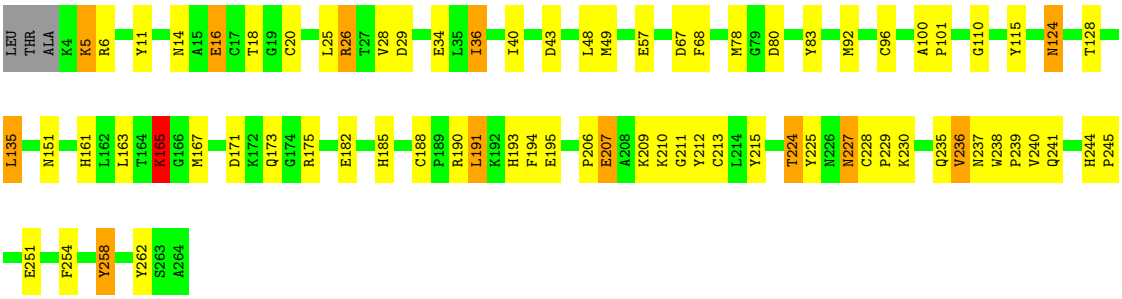


• Molecule 1: PERIPLASMIC HYDROGENASE

Chain G:

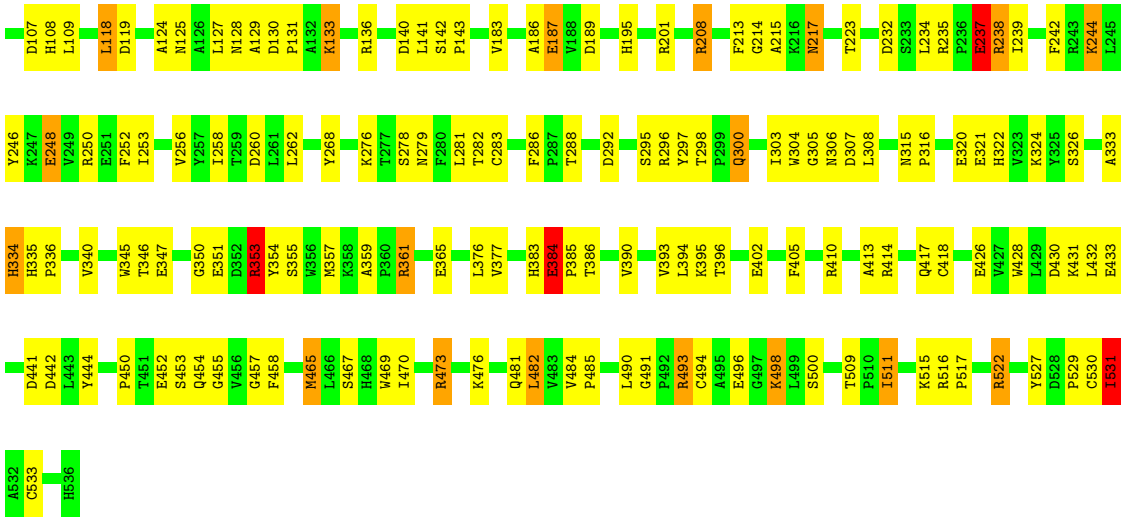
• Molecule 1: PERIPLASMIC HYDROGENASE

Chain I:



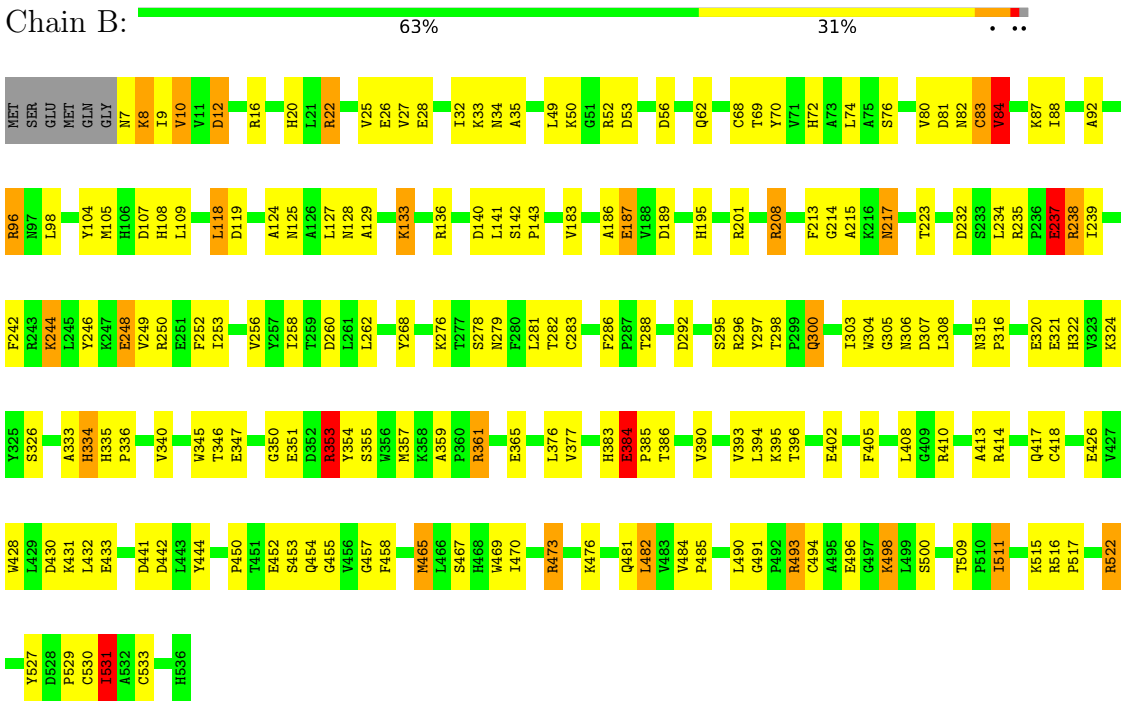
• Molecule 2: PERIPLASMIC HYDROGENASE

Chain L:



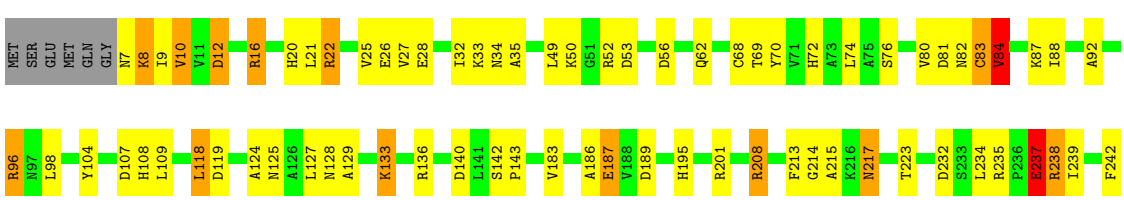
- Molecule 2: PERIPLASMIC HYDROGENASE

Chain B:



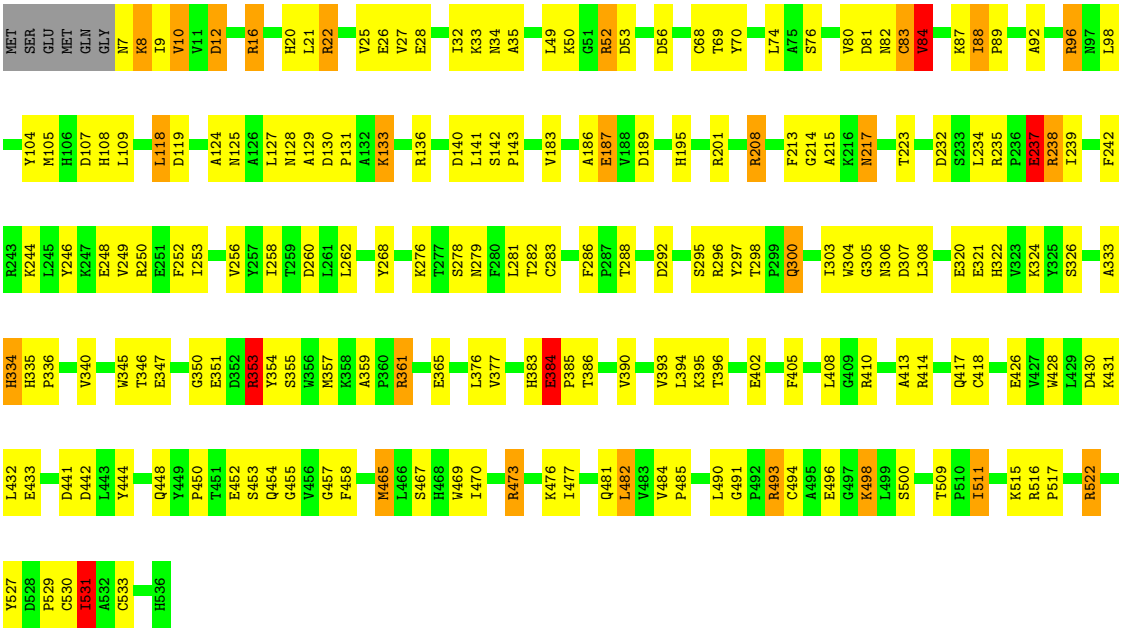
- Molecule 2: PERIPLASMIC HYDROGENASE

Chain D:



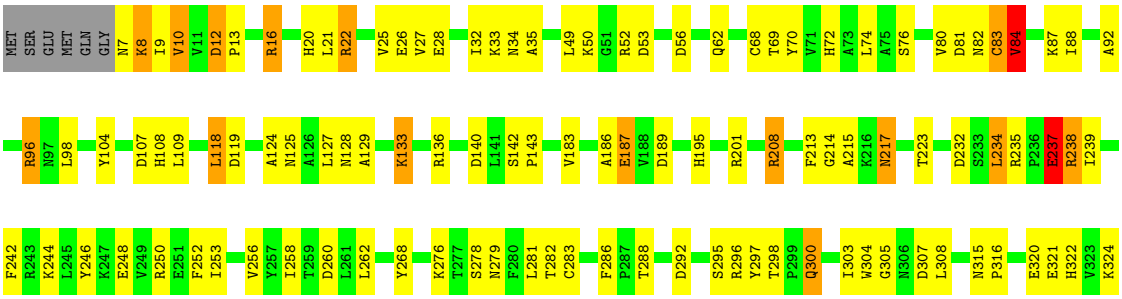
- Molecule 2: PERIPLASMIC HYDROGENASE

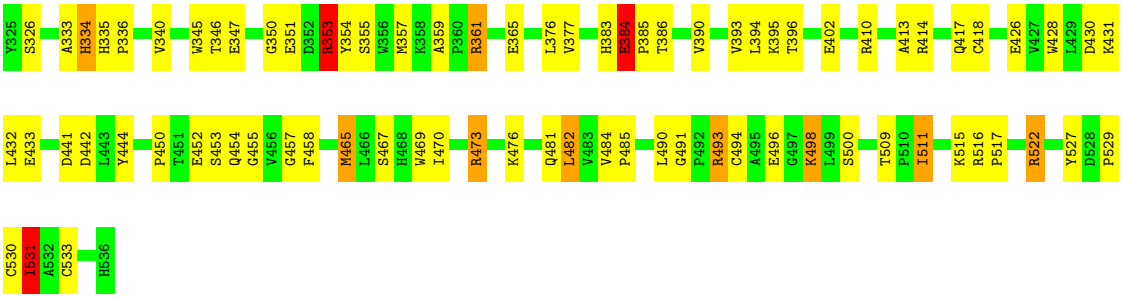
Chain F:



- Molecule 2: PERIPLASMIC HYDROGENASE

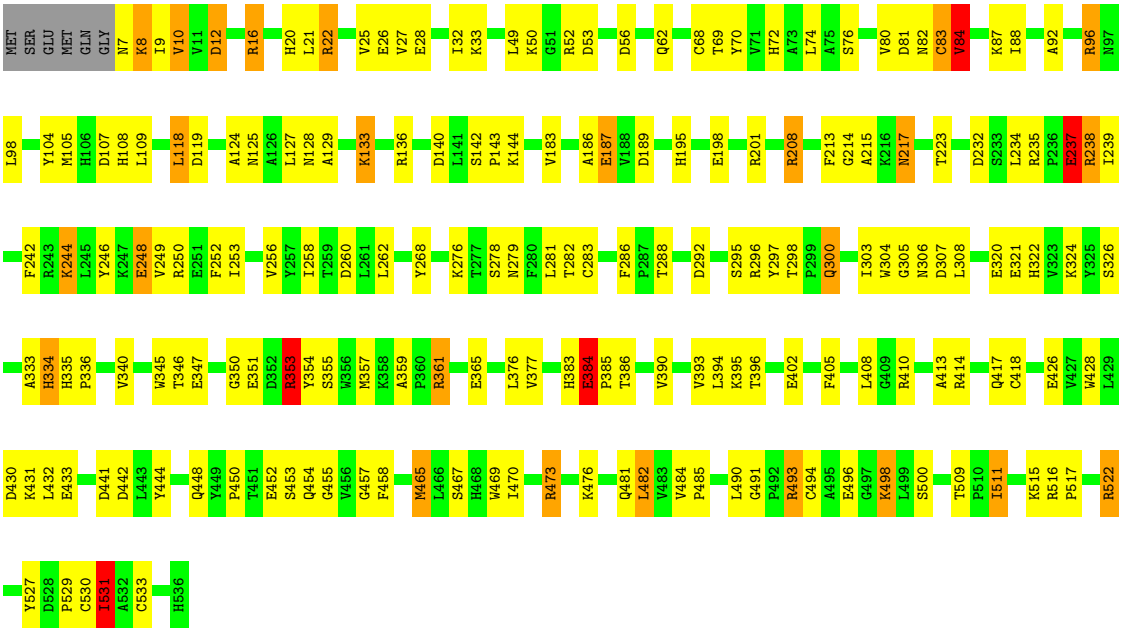
Chain H:





• Molecule 2: PERIPLASMIC HYDROGENASE

Chain J: 63% 30% 5% ••



4 Data and refinement statistics (i)

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, α, β, γ	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^2)	9.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

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

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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	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	A	16	0	0	0	0
3	C	16	0	0	0	0
3	E	16	0	0	0	0
3	G	16	0	0	0	0
3	I	16	0	0	0	0
3	S	16	0	0	0	0
4	A	7	0	0	0	0
4	C	7	0	0	0	0
4	E	7	0	0	0	0
4	G	7	0	0	0	0
4	I	7	0	0	1	0
4	S	7	0	0	1	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
5	F	1	0	0	0	0
5	H	1	0	0	0	0
5	J	1	0	0	0	0
5	L	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
6	H	1	0	0	0	0
6	J	1	0	0	0	0
6	L	1	0	0	0	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:A:235:GLN:NE2	2:B:208:ARG:HH21	1.56	1.02
1:G:235:GLN:NE2	2:H: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:L:142:SER:HB2	2:L:143:PRO:CD	2.08	0.84
2:H:142:SER:HB2	2:H: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:L:108:HIS:CE1	2:L:417:GLN:HE21	2.00	0.80
2:J:108:HIS:CE1	2:J: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:C	2:B:217:ASN:HD22	1.91	0.74
1:S:227:ASN:H	1:S:227:ASN:HD22	1.33	0.74
2:J:217:ASN:C	2:J:217:ASN:HD22	1.91	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:L:32:ILE:HD12	2:L: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:C	2:F:217:ASN:HD22	1.91	0.73
2:D:32:ILE:HD12	2:D:509:THR:HB	1.71	0.72
2:H:32:ILE:HD12	2:H:509:THR:HB	1.71	0.72
2:H:346:THR:O	2:H:350:GLY:HA3	1.89	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
1:S:124:ASN:HD21	1:S:128:THR:H	1.39	0.69
2:D:108:HIS:HE1	2:D:417:GLN:HE21	1.40	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: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
2:J:108:HIS:HE1	2:J:417:GLN:HE21	1.40	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
2:L:278:SER:O	2:L:279:ASN:HB2	1.96	0.64
1:G:235:GLN:HE21	2:H:208:ARG:HH21	0.77	0.64
2:L:133:LYS:HG2	2:L:187:GLU:HG2	1.80	0.64
2:F:253:ILE:O	2:F:258:ILE:HG12	1.96	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
1:S:206:PRO:O	1:S:210:LYS:HD3	1.97	0.64
2:D:133:LYS:HG2	2:D:187:GLU:HG2	1.80	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
2:L:383:HIS:HD2	2:L:386:THR:OG1	1.82	0.63
1:I:235:GLN:HE21	2:J:208:ARG:HH21	0.76	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:L:129:ALA:HB2	2:L:186:ALA:O	1.99	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
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:S:171:ASP:OD1	1:S:173:GLN:N	2.31	0.61
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: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
2:L:484:VAL:HG12	2:L:485:PRO:HD2	1.81	0.61
1:C:161:HIS:HD2	1:C:165:LYS:NZ	1.98	0.61
1:S:161:HIS:HD2	1:S:165:LYS:NZ	1.98	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
2:B:351:GLU:HB2	2:B:353:ARG:HD2	1.82	0.61
2:L:351:GLU:HB2	2:L: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
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:S:188:CYS:O	1:S:191:LEU:HB2	2.01	0.60
1:I:14:ASN:OD1	1:I:92:MET:HB3	2.00	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:C	2:B:217:ASN:ND2	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: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: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: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:8:LYS:HG3	2:D:25:VAL:O	2.04	0.58
2:D:32:ILE:HD11	2:D:511:ILE:HD11	1.86	0.58
2:H:217:ASN:C	2:H:217:ASN:ND2	2.57	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:8:LYS:HG3	2:L:25:VAL:O	2.04	0.58
2:L:108:HIS:CE1	2:L:417:GLN:HG2	2.37	0.58
2:B:32:ILE:HD11	2:B:511:ILE:HD11	1.86	0.58
2:B:142:SER:HB2	2:B:143:PRO:HD2	1.85	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: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:8:LYS:HG3	2:J:25:VAL:O	2.04	0.57
2:J:142:SER:HB2	2:J:143:PRO:HD3	1.85	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
1:S:18:THR:O	1:S:18:THR:HG22	2.05	0.56
2:L:308:LEU:HD21	2:L:376:LEU:HD22	1.87	0.56
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
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:HG22	1:E:18:THR:O	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:L:69:THR:O	2:L:70:TYR:HB3	2.06	0.56
2:L:484:VAL:CG1	2:L:533:CYS:HB3	2.33	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:O	1:I:18:THR:HG22	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:L:283:CYS:SG	2:L:465:MET:HG3	2.46	0.55
2:D:283:CYS:SG	2:D:465:MET:HG3	2.46	0.55
2:L:278:SER:HB3	2:L:305:GLY:HA2	1.88	0.55
2:L:142:SER:HB2	2:L:143:PRO:HD2	1.85	0.55
2:B:278:SER:HB3	2:B:305:GLY:HA2	1.89	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:L:8:LYS:HA	2:L:25:VAL:O	2.08	0.54
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:8:LYS:HA	2:J:25:VAL:O	2.08	0.54
2:J:278:SER:HB3	2:J:305:GLY:HA2	1.88	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:L:297:TYR:CD2	2:L:298:THR:HG23	2.42	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
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:CD	2:J:237:GLU:H	2.11	0.54
1:S:238:TRP:CH2	1:S:240:VAL:HB	2.43	0.54
1:A:26:ARG:HE	2:B:217:ASN:ND2	2.06	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:D:297:TYR:CD2	2:D:298:THR:HG23	2.42	0.54
2:F:278:SER:HB3	2:F:305:GLY:HA2	1.89	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:L:494:CYS:SG	2:L:498:LYS:HG3	2.48	0.53
2:H:282:THR:HG22	2:H:377:VAL:HG21	1.90	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:C:26:ARG:HE	2:D:217:ASN:ND2	2.06	0.53
2:D:237:GLU:H	2:D:237:GLU:CD	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
1:S:26:ARG:HE	2:L:217:ASN:ND2	2.06	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:CD	2:H:237:GLU:H	2.11	0.53
1:S:227:ASN:H	1:S:227:ASN:ND2	2.04	0.53
1:S:227:ASN:HD22	1:S:227:ASN:N	2.04	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: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:S:20:CYS:SG	1:S:110:GLY:HA3	2.49	0.52
1:A:237:ASN:HB3	2:B:215:ALA:O	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)
2:B:354:TYR:OH	2:B:493:ARG:HD2	2.09	0.52
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: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:108:HIS:ND1	2:D:418:CYS:HB2	2.24	0.52
2:D:383:HIS:NE2	2:D:385:PRO:HG2	2.25	0.52
2:J:494:CYS:SG	2:J:498:LYS:HG3	2.49	0.52
2:L:108:HIS:ND1	2:L:418:CYS:HB2	2.24	0.52
2:L:383:HIS:NE2	2:L:385:PRO:HG2	2.25	0.52
1:A:227:ASN:H	1:A:227:ASN:ND2	2.04	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
2:L:354:TYR:OH	2:L:493:ARG:HD2	2.09	0.52
1:G:185:HIS:CE1	1:G:191:LEU:HD23	2.45	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:S:185:HIS:CE1	1:S:191:LEU:HD23	2.45	0.51
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: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
2:L:282:THR:HG22	2:L:377:VAL:HG21	1.90	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
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:S:185:HIS:CE1	1:S:191:LEU:CD2	2.94	0.51
1:E:244:HIS:CG	1:E:245:PRO:HD2	2.46	0.51
2:L:346:THR:O	2:L:347:GLU:HB2	2.10	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:H	1:I:227:ASN:ND2	2.04	0.51
1:A:209:LYS:NZ	2:B:442:ASP:OD1	2.43	0.51
2:B:119:ASP:O	2:B:522:ARG:NE	2.36	0.51
1:G:185:HIS:CE1	1:G:191:LEU:CD2	2.94	0.51
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:L:485:PRO:HG2	7:L:537:FCO:N1	2.26	0.50
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: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:L:20:HIS:O	2:L:531:ILE:HG21	2.12	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:262:LEU:HD21	2:L:393:VAL:HG22	1.93	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: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:CD1	1:I:36:ILE:N	2.76	0.49
2:L:195:HIS:HD1	2:L:260:ASP:CG	2.14	0.49
1:A:36:ILE:N	1:A:36:ILE:CD1	2.76	0.49
1:A:100:ALA:HB3	1:A:101:PRO:HD3	1.95	0.49
1:E:36:ILE:N	1:E:36:ILE:CD1	2.76	0.49
1:E:235:GLN:NE2	2:F:208:ARG:NH2	2.39	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
1:S:36:ILE:CD1	1:S:36:ILE:N	2.76	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:100:ALA:HB3	1:S:101:PRO:HD3	1.95	0.49
2:L:491:GLY:O	2:L:500:SER:HB3	2.12	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:92:ALA:O	2:L:96:ARG:HD3	2.12	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: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:L:321:GLU:O	2:L:333:ALA:HA	2.13	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: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:L:82:ASN:HD22	2:L: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:334:HIS:CD2	2:L:340:VAL:HG22	2.49	0.48
2:F:303:ILE:HD13	2:F:308:LEU:HD23	1.95	0.48
1:G:36:ILE:N	1:G:36:ILE:HD12	2.29	0.48
1:I:36:ILE:N	1:I:36:ILE:HD12	2.29	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:L:214:GLY:O	2:L:215:ALA:HB3	2.12	0.48
2:B:283:CYS:SG	2:B:465:MET:CG	3.02	0.48
2:J:283:CYS:SG	2:J:465:MET:CG	3.02	0.48
2:J:457:GLY:O	2:J:467:SER:HA	2.14	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:S:36:ILE:N	1:S:36:ILE:HD12	2.29	0.47
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
2:D:195:HIS:HD1	2:D:260:ASP:CG	2.14	0.47
2:L:283:CYS:SG	2:L:465:MET:CG	3.02	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: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:L:303:ILE:HD13	2:L:308:LEU:HD23	1.95	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:457:GLY:O	2:L:467:SER:HA	2.14	0.47
2:B:68:CYS:CB	7:B:537:FCO:C2	2.93	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:161:HIS:HD2	1:C:165:LYS:HZ3	1.61	0.47
2:D:390:VAL:O	2:D:394:LEU:HG	2.15	0.47
1:E:36:ILE:N	1:E:36:ILE:HD12	2.29	0.47
1:E:209:LYS:NZ	2:F:442:ASP:OD1	2.43	0.47
2:F:390:VAL:O	2:F:394:LEU:HG	2.15	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
2:L:304:TRP:HZ3	2:L:365:GLU:HG3	1.80	0.47
1:S:124:ASN:HD21	1:S:128:THR:N	2.10	0.47
2:D:304:TRP:HZ3	2:D:365:GLU:HG3	1.80	0.47
2:J:68:CYS:CB	7:J:537:FCO:C2	2.93	0.47
2:J:335:HIS:HE1	2:J:469:TRP:CZ3	2.33	0.47
2:L:390:VAL:O	2:L:394:LEU:HG	2.15	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
1:I:209:LYS:NZ	2:J:442:ASP:OD1	2.43	0.47
2:J:320:GLU:OE1	2:J:333:ALA:C	2.54	0.47
2:L:239:ILE:HG21	2:L:433:GLU:HG3	1.97	0.46
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: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:HD12	2:B:408:LEU:HA	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:L:68:CYS:CB	7:L:537:FCO:C2	2.93	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:B:493:ARG:HA	2:B:498:LYS:O	2.15	0.46
1:A:124:ASN:HD21	1:A:128:THR:N	2.10	0.46
1:A:217:LEU:HA	1:A:217:LEU:HD23	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
1:S:217:LEU:HD23	1:S:217:LEU:HA	1.73	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:458:PHE:CD1	2:L:465:MET:CE	2.99	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:HA	1:C:217:LEU:HD23	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:34:ASN:OD1	2:B:35:ALA:N	2.49	0.45
2:B:320:GLU:OE1	2:B:333:ALA:C	2.54	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:HH11	2:H:235:ARG:HD2	1.64	0.45
2:H:239:ILE:HG21	2:H:433:GLU:HG3	1.97	0.45
2:J:16:ARG:HH11	2:J:16:ARG:HD2	1.47	0.45
2:J:239:ILE:HG21	2:J:433:GLU:HG3	1.97	0.45
2:J:408:LEU:HD12	2:J:408:LEU:HA	1.65	0.45
2:L:335:HIS:HE1	2:L:469:TRP:CZ3	2.33	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: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:L:458:PHE:HD1	2:L:465:MET:CE	2.29	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
1:S:254:PHE:HA	1:S:258:TYR:HD2	1.82	0.45
2:L:491:GLY:O	2:L:500:SER:CB	2.65	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: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:80:VAL:O	2:D:84:VAL:HB	2.17	0.45
2:D:408:LEU:HA	2:D:408:LEU:HD12	1.65	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:L:235:ARG:HH11	2:L:235:ARG:HD2	1.64	0.45
2:D:320:GLU:OE1	2:D:333:ALA:C	2.54	0.45
2:L:278:SER:O	2:L:279:ASN:CB	2.63	0.45
2:F:335:HIS:CE1	2:F:469:TRP:CZ3	3.05	0.45
2:H:80:VAL:O	2:H:84:VAL:HB	2.17	0.45
2:H:458:PHE:HD1	2:H:465:MET:CE	2.29	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:76:SER:O	2:J:80:VAL:HG23	2.16	0.45
2:J:491:GLY:O	2:J:500:SER:CB	2.65	0.45
2:L:76:SER:O	2:L:80:VAL:HG23	2.16	0.44
2:L:336:PRO:O	2:L:481:GLN:HG3	2.17	0.44
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:HD12	2:F:408:LEU:HA	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:431:LYS:O	2:L:432:LEU:C	2.55	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:80:VAL:O	2:L:84:VAL:HB	2.17	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: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:384:GLU:CG	1:E:141:LYS:HD2	2.45	0.44
2:B:431:LYS:O	2:B:432:LEU:C	2.55	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:315:ASN:HA	2:D:316:PRO:HD2	1.95	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
2:L:326:SER:HA	2:L:355:SER:O	2.18	0.44
1:A:161:HIS:HD2	1:A:165:LYS:HZ2	1.63	0.44
2:B:235:ARG:HH11	2:B:235:ARG:HD2	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:84:VAL:HG13	2:H:84:VAL:O	2.18	0.44
2:H:454:GLN:HA	2:H:470:ILE: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:335:HIS:CE1	2:L:469:TRP:CZ3	3.05	0.44
1:A:80:ASP:HB3	1:A:83:TYR:CE2	2.53	0.44
2:B:119:ASP:HB3	2:B:522:ARG:HG3	2.00	0.44
2:B:336:PRO:O	2:B:481:GLN:HG3	2.17	0.44
2:B:454:GLN:HA	2:B:470:ILE:O	2.18	0.44
2:F:324:LYS:O	2:F:324:LYS:HG2	2.18	0.44
2:L:454:GLN:HA	2:L:470:ILE:O	2.18	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:HG13	2:J:84:VAL:O	2.18	0.44
2:L:324:LYS:O	2:L:324:LYS:HG2	2.18	0.43
2:B:431:LYS:NZ	1:E:169:GLU:OE1	2.43	0.43
1:C:194:PHE:HD1	1:C:213:CYS:SG	2.41	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:O	2:H:324:LYS:HG2	2.18	0.43
2:D:454:GLN:HA	2:D:470:ILE:O	2.18	0.43
2:F:80:VAL:O	2:F:84:VAL:HB	2.17	0.43
2:F:431:LYS:O	2:F:432:LEU:C	2.55	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:L:12:ASP:OD2	2:L:22:ARG:HB2	2.18	0.43
2:B:80:VAL:O	2:B:84:VAL:HB	2.17	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:D:246:TYR:HE2	2:D:426:GLU:OE1	2.02	0.43
2:D:252:PHE:CE1	2:D:256:VAL:HG11	2.54	0.43
2:F:119:ASP:HB3	2:F:522:ARG:HG3	2.00	0.43
2:F:448:GLN:HE21	2:F:448:GLN:HB3	1.67	0.43
2:H:239:ILE:HD11	2:H:432:LEU:HD23	2.00	0.43
2:H:252:PHE:CE1	2:H:256:VAL:HG11	2.54	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:124:ALA:O	2:L:127:LEU: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:80:ASP:HB3	1:I:83:TYR:CE2	2.53	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
2:J:278:SER:O	2:J:279:ASN:CB	2.63	0.43
2:L:84:VAL:O	2:L:84:VAL:HG13	2.18	0.43
2:L:246:TYR:HE2	2:L:426:GLU:OE1	2.02	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:235:ARG:NH2	2:L:238:ARG:HD3	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:84:VAL:O	2:F:84:VAL:HG13	2.18	0.43
2:J:239:ILE:HD11	2:J:432:LEU:HD23	2.00	0.43
1:S:80:ASP:HB3	1:S:83:TYR:CE2	2.53	0.43
2:L:119:ASP:HB3	2:L:522:ARG:HG3	2.00	0.43
2:L:288:THR:OG1	2:L:295:SER:HB2	2.17	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:HG2	2:D:324:LYS:O	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:262:LEU:HD13	2:L:396:THR:HG21	2.01	0.43
2:B:450:PRO:HG2	2:B:453:SER:CB	2.49	0.43
2:D:84:VAL:O	2:D:84:VAL:HG13	2.18	0.43
2:D:119:ASP:HB3	2:D:522:ARG:HG3	2.00	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
1:S:194:PHE:HD1	1:S:213:CYS:SG	2.41	0.42
2:L:252:PHE:CE1	2:L:256:VAL:HG11	2.54	0.42
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
1:S:161:HIS:HD2	1:S:165:LYS:HZ2	1.66	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:9:ILE:HB	2:J:25:VAL:CG2	2.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:450:PRO:HG2	2:L:453:SER:HB3	2.00	0.42
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:9:ILE:HB	2:H:25:VAL:CG2	2.50	0.42
2:H:242:PHE:CD1	2:H:242:PHE:C	2.92	0.42
1:A:230:LYS:H	1:A:230:LYS:HG3	1.68	0.42
2:H:9:ILE:HB	2:H:25:VAL:HG22	2.01	0.42
1:S:193:HIS:CD2	1:S:211:GLY:O	2.72	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
2:D:9:ILE:HB	2:D:25:VAL:HG22	2.01	0.42
2:D:286:PHE:CD1	2:D:428:TRP:CH2	3.07	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: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:CD1	2:D:242:PHE:C	2.92	0.42
2:F:242:PHE:CD1	2:F:242:PHE:C	2.92	0.42
2:L:286:PHE:CD1	2:L:428:TRP:CH2	3.07	0.42
2:B:242:PHE:CD1	2:B:242:PHE:C	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:9:ILE:HB	2:L:25:VAL:CG2	2.50	0.42
2:L:384:GLU:N	2:L:385:PRO:CD	2.83	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:12:ASP:HA	2:L:13:PRO:HA	1.91	0.42
1:A:193:HIS:CD2	1:A:211:GLY:O	2.72	0.42
2:B:84:VAL:O	2:B:84:VAL:HG13	2.18	0.42
2:J:324:LYS:O	2:J:324:LYS:HG2	2.18	0.42
1:S:235:GLN:NE2	2:L:208:ARG:NH2	2.39	0.42
2:L:242:PHE:CD1	2:L:242:PHE:C	2.92	0.42
2:L:306:ASN:ND2	2:L:405:PHE:CD1	2.80	0.42
2:B:141:LEU:HD23	2:B:141:LEU:HA	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

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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
1:G:209:LYS:NZ	2:H:442:ASP:OD1	2.43	0.41
2:H:286:PHE:CD1	2:H:428:TRP:CH2	3.07	0.41
2:J:125:ASN:HA	2:J:128:ASN:ND2	2.35	0.41
2:L:490:LEU:HD13	2:L:529:PRO:HB3	2.02	0.41
2:B:384:GLU:N	2:B:385:PRO:CD	2.83	0.41
2:D:21:LEU:HB2	2:D:531:ILE:HG12	2.02	0.41
2:D:125:ASN:HA	2:D:128:ASN:ND2	2.35	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:J:9:ILE:HB	2:J:25:VAL:HG22	2.01	0.41
2:L:125:ASN:HA	2:L:128:ASN:ND2	2.35	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:16:ARG:HH11	2:L:16:ARG:HD2	1.47	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:O	1:I:18:THR:CG2	2.69	0.41
2:J:235:ARG:NH2	2:J:238:ARG:HD3	2.34	0.41
1:S:230:LYS:H	1:S:230:LYS:HG3	1.68	0.41
2:L:9:ILE:HB	2:L:25:VAL:HG22	2.01	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: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
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:HE21	2:J:448:GLN:HB3	1.67	0.41
1:S:209:LYS:NZ	2:L:442:ASP:OD1	2.43	0.41
2:L:141:LEU:HD23	2:L:141:LEU:HA	1.78	0.41
1:A:227:ASN:HD22	1:A:227:ASN:N	2.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:S:18:THR:O	1:S:18:THR:CG2	2.69	0.41
2:L:83:CYS:HB2	2:L:454:GLN:C	2.41	0.41
1:A:18:THR:O	1:A:18:THR:CG2	2.69	0.41
1:A:76:ILE:HA	1:A:77:PRO:HD3	1.95	0.41
1:A:251:GLU:HA	1:A:252:PRO:HD3	1.95	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
2:D:294:ASN:OD1	2:D:300:GLN:NE2	2.47	0.41
2:F:52:ARG:HH11	2:F:52:ARG:HD3	1.69	0.41
2:F:477:ILE:HD13	2:F:477:ILE:HG21	1.90	0.41
1:G:96:CYS:HB3	1:G:135:LEU:HD11	2.03	0.41
2:H:62:GLN:HA	2:H:72:HIS:HB2	2.03	0.41
2:H:383:HIS:CD2	2:H:386:THR:OG1	2.70	0.41
2:J:62:GLN:HA	2:J:72:HIS:HB2	2.03	0.41
2:J:83:CYS:HB2	2:J:454:GLN:C	2.41	0.41
2:J:105:MET:HE2	2:J:249:VAL:HG12	2.03	0.41
1:S:202:SER:O	1:S:208:ALA:HB2	2.22	0.41
2:L:21:LEU:HB2	2:L:531:ILE:HG12	2.02	0.41
1:A:244:HIS:ND1	1:A:245:PRO:HD2	2.36	0.41
2:F:9:ILE:HB	2:F:25:VAL:HG22	2.01	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:H:34:ASN:OD1	2:H:35:ALA:N	2.48	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	4:I:266:F3S:S3	2.62	0.40
1:I:227:ASN:ND2	1:I:227:ASN:N	2.68	0.40
1:S:228:CYS:HB2	1:S:229:PRO:CD	2.50	0.40
2:L:315:ASN:HA	2:L:316:PRO:HD2	1.95	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
1:S:224:THR:HG21	4:S:266:F3S:S3	2.62	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:244:HIS:ND1	1:S:245:PRO:HD2	2.36	0.40
2:L:119:ASP:O	2:L:522:ARG:NH2	2.51	0.40
1:A:202:SER:O	1:A:208:ALA:HB2	2.21	0.40
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:B:83:CYS:HB2	2:B:454:GLN:C	2.42	0.40
1:C:96:CYS:HB3	1:C:135:LEU:HD11	2.03	0.40
1:C:202:SER:O	1:C:208:ALA:HB2	2.22	0.40
2:D:320:GLU:OE1	2:D:334:HIS:CA	2.70	0.40
2:F:235:ARG:HH11	2:F:235:ARG:HD2	1.64	0.40
1:G:18:THR:O	1:G:18:THR:CG2	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 (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	259/264 (98%)	244 (94%)	14 (5%)	1 (0%)	34	46
1	C	259/264 (98%)	244 (94%)	14 (5%)	1 (0%)	34	46
1	E	259/264 (98%)	244 (94%)	14 (5%)	1 (0%)	34	46
1	G	259/264 (98%)	244 (94%)	14 (5%)	1 (0%)	34	46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	259/264 (98%)	244 (94%)	14 (5%)	1 (0%)	34	46
1	S	259/264 (98%)	244 (94%)	14 (5%)	1 (0%)	34	46
2	B	528/536 (98%)	506 (96%)	21 (4%)	1 (0%)	47	60
2	D	528/536 (98%)	506 (96%)	21 (4%)	1 (0%)	47	60
2	F	528/536 (98%)	506 (96%)	21 (4%)	1 (0%)	47	60
2	H	528/536 (98%)	506 (96%)	21 (4%)	1 (0%)	47	60
2	J	528/536 (98%)	506 (96%)	21 (4%)	1 (0%)	47	60
2	L	528/536 (98%)	506 (96%)	21 (4%)	1 (0%)	47	60
All	All	4722/4800 (98%)	4500 (95%)	210 (4%)	12 (0%)	41	51

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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	208/210 (99%)	194 (93%)	14 (7%)	16	21
1	C	208/210 (99%)	194 (93%)	14 (7%)	16	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	208/210 (99%)	194 (93%)	14 (7%)	16	21
1	G	208/210 (99%)	194 (93%)	14 (7%)	16	21
1	I	208/210 (99%)	194 (93%)	14 (7%)	16	21
1	S	208/210 (99%)	194 (93%)	14 (7%)	16	21
2	B	434/439 (99%)	399 (92%)	35 (8%)	11	14
2	D	434/439 (99%)	399 (92%)	35 (8%)	11	14
2	F	434/439 (99%)	399 (92%)	35 (8%)	11	14
2	H	434/439 (99%)	399 (92%)	35 (8%)	11	14
2	J	434/439 (99%)	399 (92%)	35 (8%)	11	14
2	L	434/439 (99%)	399 (92%)	35 (8%)	11	14
All	All	3852/3894 (99%)	3558 (92%)	294 (8%)	13	17

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

Sometimes 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 (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 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	$\#\|Z\| > 2$
3	SF4	I	267	1	0,12,12	-	-	-		
4	F3S	S	266	1	0,9,9	-	-	-		
3	SF4	S	267	1	0,12,12	-	-	-		
4	F3S	G	266	1	0,9,9	-	-	-		
7	FCO	F	537	8,2	0,6,6	-	-	-		
3	SF4	C	267	1	0,12,12	-	-	-		
4	F3S	I	266	1	0,9,9	-	-	-		
4	F3S	C	266	1	0,9,9	-	-	-		
7	FCO	L	537	8,2	0,6,6	-	-	-		
7	FCO	J	537	8,2	0,6,6	-	-	-		
7	FCO	H	537	8,2	0,6,6	-	-	-		
4	F3S	E	266	1	0,9,9	-	-	-		
7	FCO	B	537	8,2	0,6,6	-	-	-		
3	SF4	A	267	1	0,12,12	-	-	-		
3	SF4	S	265	1	0,12,12	-	-	-		
3	SF4	G	265	1	0,12,12	-	-	-		
7	FCO	D	537	8,2	0,6,6	-	-	-		
3	SF4	G	267	1	0,12,12	-	-	-		
3	SF4	A	265	1	0,12,12	-	-	-		
3	SF4	E	265	1	0,12,12	-	-	-		
3	SF4	C	265	1	0,12,12	-	-	-		
3	SF4	I	265	1	0,12,12	-	-	-		
3	SF4	E	267	1	0,12,12	-	-	-		
4	F3S	A	266	1	0,9,9	-	-	-		

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
3	SF4	E	265	1	-	-	0/6/5/5

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

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.