Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:26 AM GMT

PDB ID	:	2CV4
Title	:	Crystal Structure of an Archaeal Peroxiredoxin from the Aerobic Hyperthermophilic Crenarchaeon Aeropyrum pernix K1
Authors	:	Mizohata, E.; Sakai, H.; Fusatomi, E.; Terada, T.; Murayama, K.; Shirouzu, M.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on	:	2005-05-31
Resolution	:	2.30 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

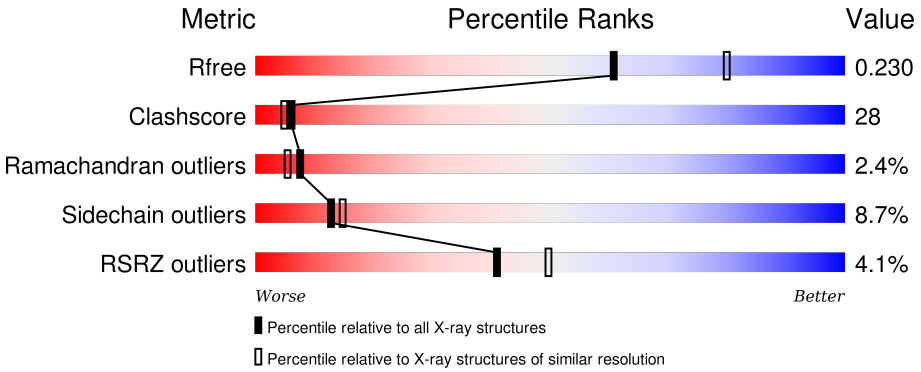
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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

Mol	Chain	Length	Quality of chain
1	A	250	4% 59% 30% 5%
1	B	250	3% 60% 31% 5%
1	C	250	3% 56% 32% 6%
1	D	250	5% 53% 37% 5%
1	E	250	4% 60% 29% 6%

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Mol	Chain	Length	Quality of chain
1	F	250	4% 58% 31% 6%
1	G	250	4% 59% 31% 6%
1	H	250	4% 56% 34% 6%
1	I	250	3% 55% 36%
1	J	250	4% 54% 37%

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
1	OCS	H	50	-	-	X	-
2	MES	F	1002	-	-	-	X
3	IPA	B	2005	-	-	X	-
3	IPA	D	2003	-	-	X	-
3	IPA	E	2006	-	-	-	X
3	IPA	F	2007	-	-	-	X
3	IPA	H	2009	-	-	X	-
3	IPA	J	2001	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 20374 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 peroxiredoxin.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	241	Total	C	N	O	S	Se	0	0	0
			1953	1255	344	347	3	4			
1	B	241	Total	C	N	O	S	Se	0	0	0
			1953	1255	344	347	3	4			
1	C	241	Total	C	N	O	S	Se	0	0	0
			1953	1255	344	347	3	4			
1	D	242	Total	C	N	O	S	Se	0	0	0
			1962	1260	345	350	3	4			
1	E	240	Total	C	N	O	S	Se	0	0	0
			1941	1246	343	345	3	4			
1	F	240	Total	C	N	O	S	Se	0	0	0
			1941	1246	343	345	3	4			
1	G	242	Total	C	N	O	S	Se	0	0	0
			1962	1260	345	350	3	4			
1	H	240	Total	C	N	O	S	Se	0	0	0
			1941	1246	343	345	3	4			
1	I	241	Total	C	N	O	S	Se	0	0	0
			1953	1255	344	347	3	4			
1	J	240	Total	C	N	O	S	Se	0	0	0
			1941	1246	343	345	3	4			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP Q9Y9L0
A	15	MSE	MET	MODIFIED RESIDUE	UNP Q9Y9L0
A	50	OCS	CYS	MODIFIED RESIDUE	UNP Q9Y9L0
A	140	MSE	MET	MODIFIED RESIDUE	UNP Q9Y9L0
A	145	MSE	MET	MODIFIED RESIDUE	UNP Q9Y9L0
A	200	MSE	MET	MODIFIED RESIDUE	UNP Q9Y9L0
B	1	MSE	MET	MODIFIED RESIDUE	UNP Q9Y9L0
B	15	MSE	MET	MODIFIED RESIDUE	UNP Q9Y9L0
B	50	OCS	CYS	MODIFIED RESIDUE	UNP Q9Y9L0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	140	MSE	MET	MODIFIED RESIDUE	UNP Q9Y9L0
B	145	MSE	MET	MODIFIED RESIDUE	UNP Q9Y9L0
B	200	MSE	MET	MODIFIED RESIDUE	UNP Q9Y9L0
C	1	MSE	MET	MODIFIED RESIDUE	UNP Q9Y9L0
C	15	MSE	MET	MODIFIED RESIDUE	UNP Q9Y9L0
C	50	OCS	CYS	MODIFIED RESIDUE	UNP Q9Y9L0
C	140	MSE	MET	MODIFIED RESIDUE	UNP Q9Y9L0
C	145	MSE	MET	MODIFIED RESIDUE	UNP Q9Y9L0
C	200	MSE	MET	MODIFIED RESIDUE	UNP Q9Y9L0
D	1	MSE	MET	MODIFIED RESIDUE	UNP Q9Y9L0
D	15	MSE	MET	MODIFIED RESIDUE	UNP Q9Y9L0
D	50	OCS	CYS	MODIFIED RESIDUE	UNP Q9Y9L0
D	140	MSE	MET	MODIFIED RESIDUE	UNP Q9Y9L0
D	145	MSE	MET	MODIFIED RESIDUE	UNP Q9Y9L0
D	200	MSE	MET	MODIFIED RESIDUE	UNP Q9Y9L0
E	1	MSE	MET	MODIFIED RESIDUE	UNP Q9Y9L0
E	15	MSE	MET	MODIFIED RESIDUE	UNP Q9Y9L0
E	50	OCS	CYS	MODIFIED RESIDUE	UNP Q9Y9L0
E	140	MSE	MET	MODIFIED RESIDUE	UNP Q9Y9L0
E	145	MSE	MET	MODIFIED RESIDUE	UNP Q9Y9L0
E	200	MSE	MET	MODIFIED RESIDUE	UNP Q9Y9L0
F	1	MSE	MET	MODIFIED RESIDUE	UNP Q9Y9L0
F	15	MSE	MET	MODIFIED RESIDUE	UNP Q9Y9L0
F	50	OCS	CYS	MODIFIED RESIDUE	UNP Q9Y9L0
F	140	MSE	MET	MODIFIED RESIDUE	UNP Q9Y9L0
F	145	MSE	MET	MODIFIED RESIDUE	UNP Q9Y9L0
F	200	MSE	MET	MODIFIED RESIDUE	UNP Q9Y9L0
G	1	MSE	MET	MODIFIED RESIDUE	UNP Q9Y9L0
G	15	MSE	MET	MODIFIED RESIDUE	UNP Q9Y9L0
G	50	OCS	CYS	MODIFIED RESIDUE	UNP Q9Y9L0
G	140	MSE	MET	MODIFIED RESIDUE	UNP Q9Y9L0
G	145	MSE	MET	MODIFIED RESIDUE	UNP Q9Y9L0
G	200	MSE	MET	MODIFIED RESIDUE	UNP Q9Y9L0
H	1	MSE	MET	MODIFIED RESIDUE	UNP Q9Y9L0
H	15	MSE	MET	MODIFIED RESIDUE	UNP Q9Y9L0
H	50	OCS	CYS	MODIFIED RESIDUE	UNP Q9Y9L0
H	140	MSE	MET	MODIFIED RESIDUE	UNP Q9Y9L0
H	145	MSE	MET	MODIFIED RESIDUE	UNP Q9Y9L0
H	200	MSE	MET	MODIFIED RESIDUE	UNP Q9Y9L0
I	1	MSE	MET	MODIFIED RESIDUE	UNP Q9Y9L0
I	15	MSE	MET	MODIFIED RESIDUE	UNP Q9Y9L0
I	50	OCS	CYS	MODIFIED RESIDUE	UNP Q9Y9L0

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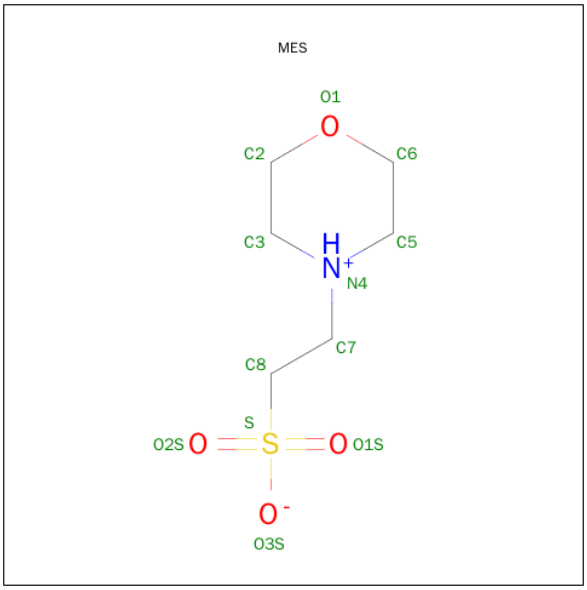
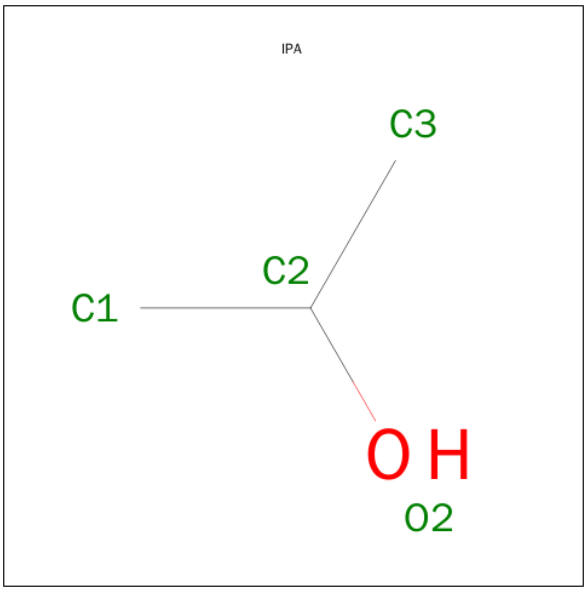
Chain	Residue	Modelled	Actual	Comment	Reference
I	140	MSE	MET	MODIFIED RESIDUE	UNP Q9Y9L0
I	145	MSE	MET	MODIFIED RESIDUE	UNP Q9Y9L0
I	200	MSE	MET	MODIFIED RESIDUE	UNP Q9Y9L0
J	1	MSE	MET	MODIFIED RESIDUE	UNP Q9Y9L0
J	15	MSE	MET	MODIFIED RESIDUE	UNP Q9Y9L0
J	50	OCS	CYS	MODIFIED RESIDUE	UNP Q9Y9L0
J	140	MSE	MET	MODIFIED RESIDUE	UNP Q9Y9L0
J	145	MSE	MET	MODIFIED RESIDUE	UNP Q9Y9L0
J	200	MSE	MET	MODIFIED RESIDUE	UNP Q9Y9L0

- Molecule 2 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	F	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 3 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C_3H_8O).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	J	1	Total C O 4 3 1	0	0
3	J	1	Total C O 4 3 1	0	0
3	D	1	Total C O 4 3 1	0	0
3	H	1	Total C O 4 3 1	0	0
3	B	1	Total C O 4 3 1	0	0
3	E	1	Total C O 4 3 1	0	0
3	F	1	Total C O 4 3 1	0	0
3	G	1	Total C O 4 3 1	0	0
3	H	1	Total C O 4 3 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	123	Total O 123 123	0	0
4	B	69	Total O 69 69	0	0
4	C	70	Total O 70 70	0	0

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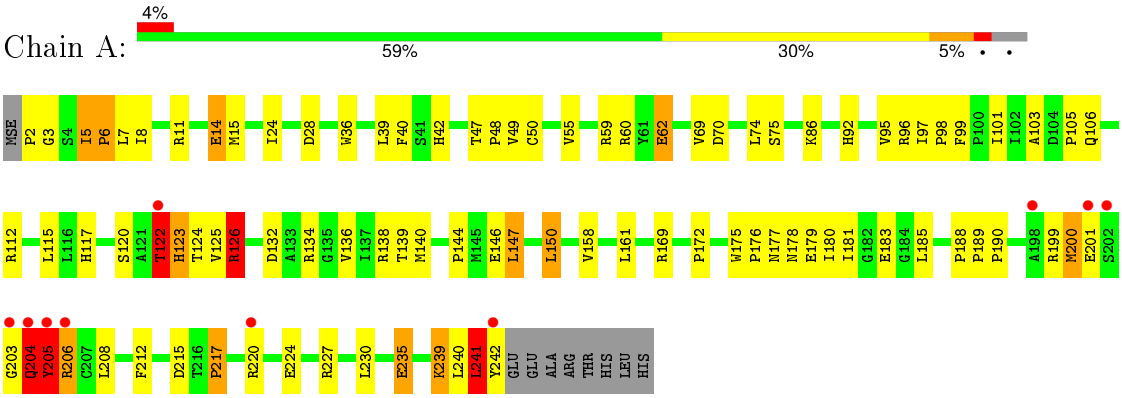
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	66	Total O 66 66	0	0
4	E	70	Total O 70 70	0	0
4	F	75	Total O 75 75	0	0
4	G	85	Total O 85 85	0	0
4	H	82	Total O 82 82	0	0
4	I	82	Total O 82 82	0	0
4	J	92	Total O 92 92	0	0

3 Residue-property plots (i)

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

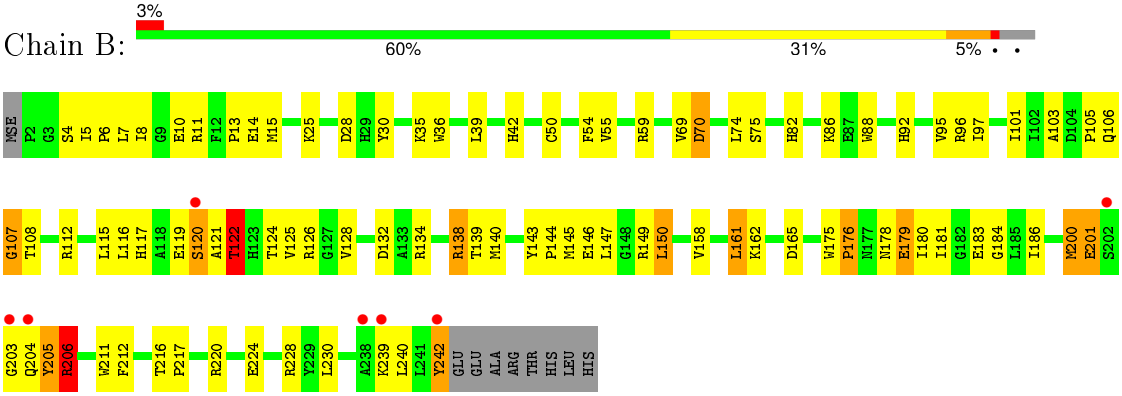
- Molecule 1: peroxiredoxin

Chain A:



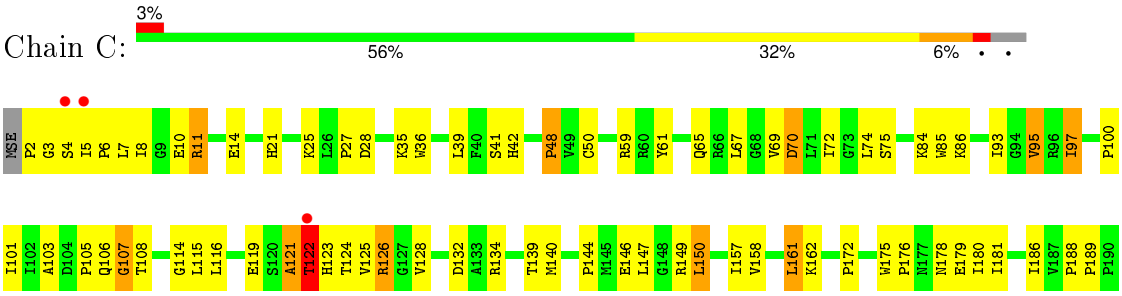
- Molecule 1: peroxiredoxin

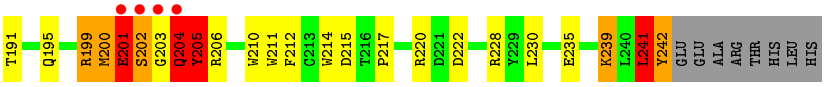
Chain B:



- Molecule 1: peroxiredoxin

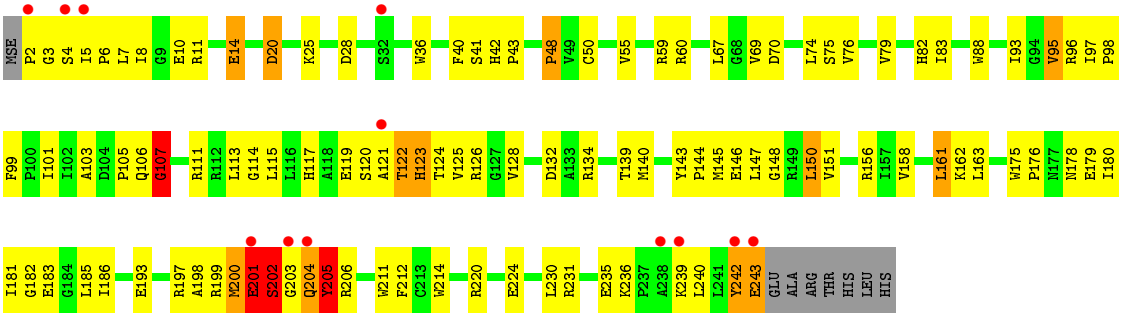
Chain C:





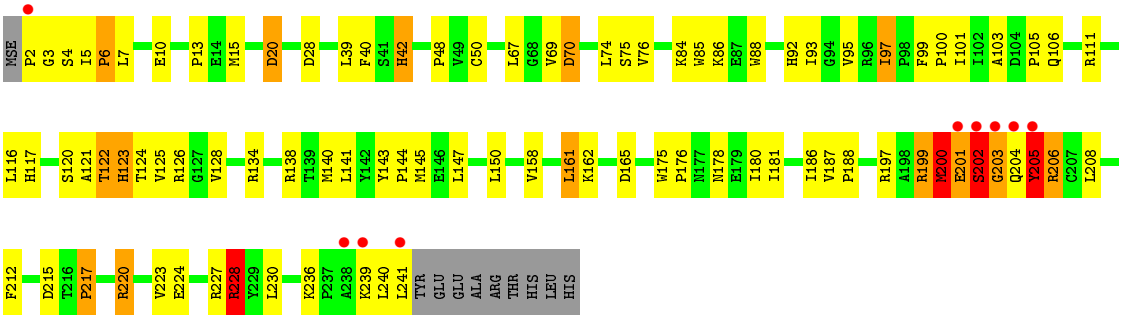
• Molecule 1: peroxiredoxin

Chain D:



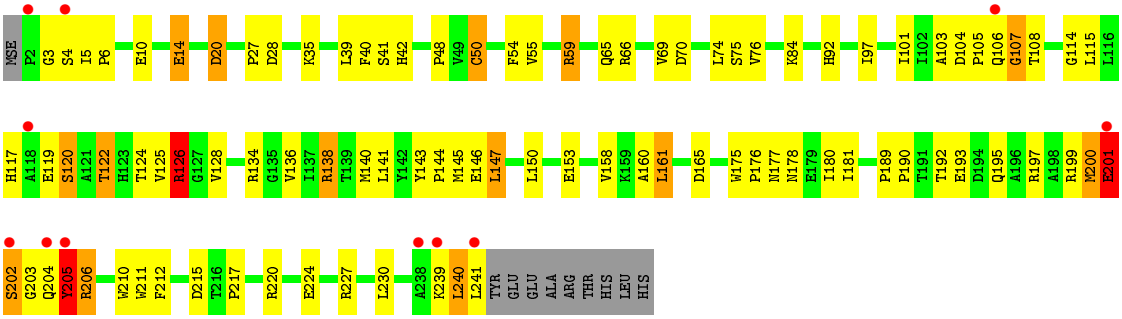
• Molecule 1: peroxiredoxin

Chain E:



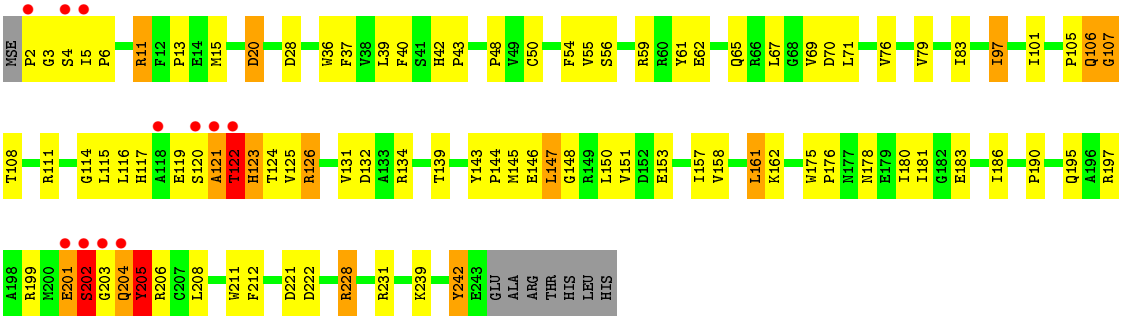
• Molecule 1: peroxiredoxin

Chain F:



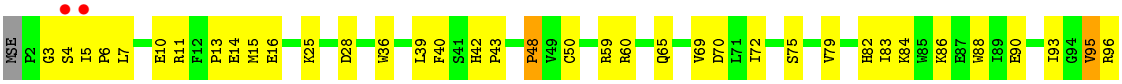
• Molecule 1: peroxiredoxin

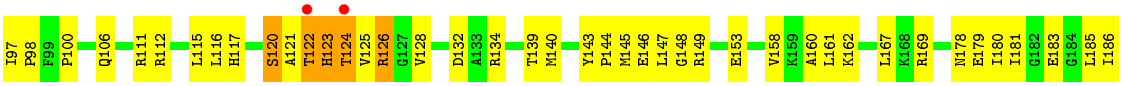
Chain G:



• Molecule 1: peroxiredoxin

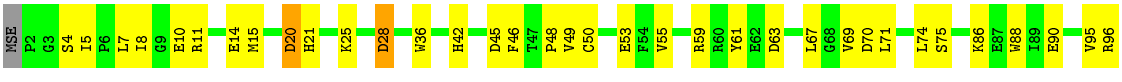
Chain H:

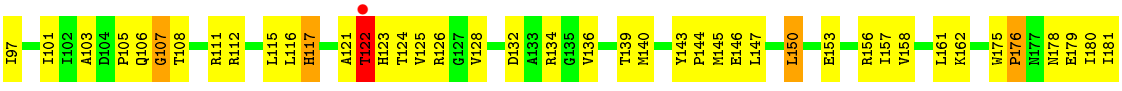


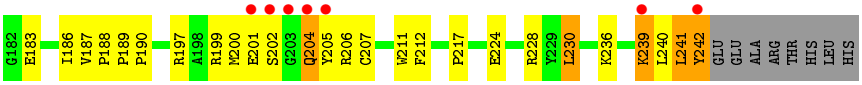


• Molecule 1: peroxiredoxin

Chain I:

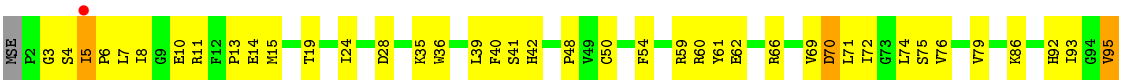


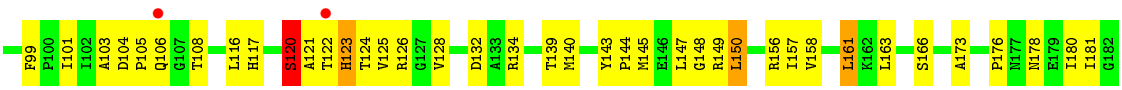


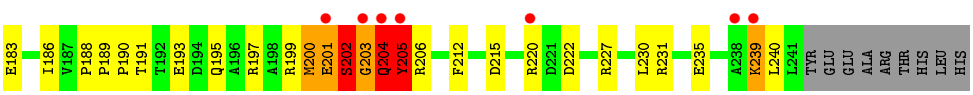


• Molecule 1: peroxiredoxin

Chain J:







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	76.74Å 103.43Å 102.81Å 105.18° 92.91° 105.39°	Depositor
Resolution (Å)	49.20 – 2.30 49.20 – 2.31	Depositor EDS
% Data completeness (in resolution range)	93.4 (49.20-2.30) 85.1 (49.20-2.31)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.45 (at 2.32Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.178 , 0.230 0.179 , 0.230	Depositor DCC
R_{free} test set	6058 reflections (5.05%)	DCC
Wilson B-factor (Å^2)	28.4	Xtriage
Anisotropy	0.306	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 60.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 120086 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	20374	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.18% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OCS, IPA, MES

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	0.79	1/1994 (0.1%)	1.00	8/2703 (0.3%)
1	B	0.76	0/1994	0.91	3/2703 (0.1%)
1	C	0.77	0/1994	0.98	4/2703 (0.1%)
1	D	0.76	0/2003	1.02	8/2715 (0.3%)
1	E	0.73	0/1981	0.95	9/2685 (0.3%)
1	F	0.75	0/1981	1.01	11/2685 (0.4%)
1	G	0.75	0/2003	0.97	9/2715 (0.3%)
1	H	0.74	0/1981	0.92	3/2685 (0.1%)
1	I	0.72	0/1994	0.89	1/2703 (0.0%)
1	J	0.71	0/1981	0.96	4/2685 (0.1%)
All	All	0.75	1/19906 (0.0%)	0.96	60/26982 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	E	0	1
1	F	0	1
All	All	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	126	ARG	CB-CG	-5.33	1.38	1.52

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	203	GLY	N-CA-C	-9.93	88.28	113.10
1	E	202	SER	N-CA-C	8.54	134.05	111.00
1	J	204	GLN	N-CA-C	7.68	131.74	111.00
1	A	241	LEU	CA-CB-CG	7.68	132.97	115.30
1	F	202	SER	CB-CA-C	7.67	124.68	110.10
1	A	60	ARG	NE-CZ-NH2	-7.54	116.53	120.30
1	F	241	LEU	CA-CB-CG	7.50	132.54	115.30
1	H	205	TYR	N-CA-C	7.41	130.99	111.00
1	H	203	GLY	N-CA-C	7.32	131.40	113.10
1	G	204	GLN	N-CA-C	-7.31	91.28	111.00
1	D	200	MSE	N-CA-C	-7.12	91.78	111.00
1	D	201	GLU	CA-C-N	-7.07	101.65	117.20
1	G	202	SER	N-CA-C	7.04	130.00	111.00
1	J	202	SER	N-CA-C	-6.97	92.17	111.00
1	D	121	ALA	N-CA-C	-6.75	92.78	111.00
1	G	205	TYR	N-CA-C	6.71	129.10	111.00
1	H	201	GLU	N-CA-CB	-6.61	98.71	110.60
1	E	205	TYR	N-CA-C	6.60	128.82	111.00
1	E	205	TYR	CB-CG-CD2	-6.58	117.05	121.00
1	D	202	SER	CA-C-N	-6.35	103.50	116.20
1	C	241	LEU	CA-CB-CG	6.34	129.87	115.30
1	C	204	GLN	N-CA-C	-6.32	93.94	111.00
1	F	205	TYR	CB-CG-CD2	-6.29	117.23	121.00
1	F	147	LEU	CA-CB-CG	5.95	128.98	115.30
1	F	203	GLY	N-CA-C	-5.91	98.32	113.10
1	G	122	THR	N-CA-CB	5.91	121.53	110.30
1	E	202	SER	CA-C-N	-5.80	104.60	116.20
1	A	6	PRO	N-CA-C	-5.76	97.11	112.10
1	G	147	LEU	CA-CB-CG	5.73	128.48	115.30
1	F	201	GLU	N-CA-C	5.71	126.41	111.00
1	D	205	TYR	CB-CG-CD1	5.70	124.42	121.00
1	F	122	THR	N-CA-C	5.68	126.34	111.00
1	E	205	TYR	CB-CA-C	-5.67	99.05	110.40
1	A	138	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	G	97	ILE	CG1-CB-CG2	-5.58	99.13	111.40
1	B	206	ARG	NE-CZ-NH2	-5.57	117.51	120.30
1	F	205	TYR	CB-CA-C	-5.55	99.30	110.40
1	B	138	ARG	NE-CZ-NH1	-5.52	117.54	120.30
1	A	138	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	F	126	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	I	121	ALA	N-CA-C	-5.50	96.16	111.00
1	G	106	GLN	N-CA-C	-5.48	96.21	111.00
1	B	206	ARG	NE-CZ-NH1	5.46	123.03	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	203	GLY	CA-C-N	-5.42	105.28	117.20
1	E	6	PRO	N-CA-C	-5.41	98.03	112.10
1	D	107	GLY	N-CA-C	-5.36	99.70	113.10
1	E	228	ARG	CA-CB-CG	5.33	125.13	113.40
1	G	121	ALA	N-CA-C	-5.30	96.70	111.00
1	C	121	ALA	N-CA-C	-5.22	96.90	111.00
1	A	60	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	F	205	TYR	CB-CG-CD1	5.20	124.12	121.00
1	F	203	GLY	CA-C-N	-5.17	105.82	117.20
1	C	126	ARG	NE-CZ-NH1	-5.15	117.73	120.30
1	A	70	ASP	CB-CG-OD2	-5.13	113.68	118.30
1	D	205	TYR	CB-CG-CD2	-5.12	117.92	121.00
1	A	126	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	D	202	SER	O-C-N	5.10	131.87	123.20
1	G	201	GLU	CA-C-N	-5.10	105.99	117.20
1	E	228	ARG	N-CA-CB	5.05	119.70	110.60
1	E	205	TYR	CA-CB-CG	5.02	122.94	113.40

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	205	TYR	Sidechain
1	B	30	TYR	Sidechain
1	C	205	TYR	Sidechain
1	E	205	TYR	Sidechain
1	F	50	OCS	Mainchain

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	1953	0	1939	115	0
1	B	1953	0	1940	108	0
1	C	1953	0	1940	131	0
1	D	1962	0	1946	151	0
1	E	1941	0	1931	115	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1941	0	1931	112	0
1	G	1962	0	1946	118	1
1	H	1941	0	1931	131	0
1	I	1953	0	1940	121	0
1	J	1941	0	1931	145	0
2	A	12	0	13	1	0
2	F	12	0	13	0	0
3	B	4	0	8	6	0
3	D	4	0	8	8	0
3	E	4	0	8	3	0
3	F	4	0	8	1	0
3	G	4	0	8	0	0
3	H	8	0	16	7	0
3	J	8	0	16	7	0
4	A	123	0	0	7	0
4	B	69	0	0	4	1
4	C	70	0	0	7	0
4	D	66	0	0	5	0
4	E	70	0	0	6	0
4	F	75	0	0	8	0
4	G	85	0	0	8	0
4	H	82	0	0	9	0
4	I	82	0	0	6	0
4	J	92	0	0	11	0
All	All	20374	0	19473	1101	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 28.

All (1101) 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:H:199:ARG:O	1:H:200:MSE:HE3	1.41	1.20
1:D:202:SER:C	1:D:204:GLN:H	1.49	1.11
1:G:121:ALA:O	1:G:122:THR:HG23	1.48	1.11
1:I:117:HIS:HB2	1:I:125:VAL:CG2	1.84	1.08
1:J:200:MSE:HE3	1:J:203:GLY:HA3	1.30	1.07
1:D:202:SER:O	1:D:204:GLN:HB2	1.53	1.07
1:I:117:HIS:HB2	1:I:125:VAL:HG21	1.35	1.07
1:I:5:ILE:HG12	1:J:5:ILE:HD13	1.38	1.06
1:A:126:ARG:HG3	1:A:126:ARG:HH11	0.95	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:ILE:HG13	1:A:6:PRO:O	1.58	1.03
1:F:178:ASN:HD22	1:F:181:ILE:H	1.06	1.02
1:D:202:SER:O	1:D:204:GLN:N	1.92	1.02
1:A:240:LEU:HB2	1:A:242:TYR:HE2	1.22	1.01
1:G:4:SER:C	1:G:5:ILE:HD12	1.81	1.01
1:B:69:VAL:HG21	1:B:158:VAL:HG11	1.42	1.01
1:A:240:LEU:HB2	1:A:242:TYR:CE2	1.97	1.00
1:J:178:ASN:HD22	1:J:181:ILE:H	1.08	0.98
1:A:106:GLN:OE1	1:J:121:ALA:O	1.83	0.97
1:D:243:GLU:HA	1:D:243:GLU:OE1	1.63	0.97
1:G:69:VAL:HG21	1:G:158:VAL:HG11	1.46	0.97
1:C:106:GLN:O	1:C:108:THR:N	1.96	0.97
1:A:201:GLU:OE1	1:A:206:ARG:HA	1.64	0.96
1:F:200:MSE:HG2	1:F:210:TRP:HB3	1.47	0.95
1:C:10:GLU:OE1	1:D:2:PRO:HG2	1.66	0.95
1:H:4:SER:C	1:H:5:ILE:HD12	1.88	0.94
1:E:178:ASN:HD22	1:E:181:ILE:H	1.13	0.94
1:A:126:ARG:CG	1:A:126:ARG:HH11	1.81	0.94
1:D:178:ASN:HD22	1:D:181:ILE:H	1.14	0.93
1:G:178:ASN:HD22	1:G:181:ILE:H	1.16	0.92
1:H:200:MSE:HE2	1:H:200:MSE:HA	1.51	0.92
1:H:200:MSE:CE	1:H:200:MSE:HA	2.00	0.92
1:J:204:GLN:HA	1:J:204:GLN:HE21	1.33	0.91
1:A:126:ARG:HG3	1:A:126:ARG:NH1	1.74	0.91
1:C:242:TYR:HE2	1:D:206:ARG:HH11	1.18	0.90
1:F:106:GLN:O	1:F:108:THR:N	2.04	0.90
1:E:5:ILE:HG22	1:E:6:PRO:O	1.71	0.90
1:B:106:GLN:HE22	1:C:107:GLY:H	1.14	0.89
1:A:178:ASN:HD22	1:A:181:ILE:H	1.14	0.89
1:I:69:VAL:HG21	1:I:158:VAL:HG11	1.50	0.89
1:E:202:SER:O	1:E:204:GLN:N	2.04	0.89
1:B:201:GLU:HB2	1:B:205:TYR:O	1.72	0.88
1:F:106:GLN:HE22	1:G:107:GLY:H	1.22	0.88
1:J:204:GLN:O	1:J:205:TYR:CG	2.27	0.87
1:G:40:PHE:HD1	1:G:42:HIS:HE1	1.19	0.87
1:H:43:PRO:HB2	1:H:123:HIS:HB3	1.56	0.87
1:A:92:HIS:HE1	3:J:2001:IPA:H12	1.40	0.87
1:B:178:ASN:HD22	1:B:181:ILE:H	1.15	0.87
1:H:50:OCS:OD2	1:H:126:ARG:NH2	2.08	0.86
1:G:183:GLU:OE2	4:G:2086:HOH:O	1.94	0.86
1:A:59:ARG:HG3	1:B:179:GLU:OE2	1.76	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:VAL:CG1	1:A:126:ARG:NH2	2.39	0.85
1:A:5:ILE:HG21	1:B:5:ILE:HG12	1.58	0.85
1:J:204:GLN:O	1:J:205:TYR:CD2	2.28	0.85
1:J:4:SER:O	1:J:5:ILE:HD12	1.74	0.85
1:H:178:ASN:HD22	1:H:181:ILE:H	1.20	0.85
1:I:187:VAL:HG21	1:I:205:TYR:HE2	1.39	0.85
3:D:2003:IPA:H32	1:E:84:LYS:HZ1	1.40	0.85
1:I:178:ASN:HD22	1:I:181:ILE:H	1.25	0.85
1:B:200:MSE:HE2	1:B:200:MSE:H	1.43	0.84
1:C:241:LEU:HD23	1:D:179:GLU:O	1.76	0.84
1:A:124:THR:HG22	1:A:125:VAL:O	1.78	0.84
1:F:40:PHE:CD1	1:F:42:HIS:HE1	1.95	0.84
1:G:4:SER:CA	1:G:5:ILE:HD12	2.07	0.84
1:H:121:ALA:O	1:H:122:THR:HG22	1.77	0.84
1:H:169:ARG:NH2	1:H:205:TYR:OH	2.09	0.84
1:H:40:PHE:HD1	1:H:42:HIS:HE1	1.26	0.83
1:J:200:MSE:CE	1:J:203:GLY:HA3	2.08	0.83
1:C:59:ARG:HD3	1:D:179:GLU:OE2	1.79	0.83
1:H:69:VAL:HG21	1:H:158:VAL:HG11	1.59	0.83
1:C:3:GLY:O	1:D:4:SER:HA	1.79	0.83
1:E:42:HIS:CD2	1:E:75:SER:HB2	2.13	0.83
3:D:2003:IPA:H32	1:E:84:LYS:NZ	1.94	0.83
1:D:106:GLN:O	1:E:106:GLN:NE2	2.12	0.82
1:D:69:VAL:HG21	1:D:158:VAL:HG11	1.61	0.82
1:J:204:GLN:HA	1:J:204:GLN:NE2	1.94	0.82
1:F:40:PHE:HD1	1:F:42:HIS:HE1	1.26	0.82
1:E:199:ARG:C	1:E:201:GLU:H	1.83	0.81
1:I:42:HIS:CE1	1:I:75:SER:HB2	2.15	0.81
1:B:106:GLN:O	1:B:108:THR:N	2.12	0.81
1:E:42:HIS:NE2	1:E:75:SER:HB2	1.96	0.81
1:G:43:PRO:CB	1:G:123:HIS:HB3	2.10	0.81
1:I:20:ASP:HB2	1:I:101:ILE:H	1.46	0.81
1:H:122:THR:OG1	1:H:123:HIS:CD2	2.34	0.81
1:G:117:HIS:CG	1:G:125:VAL:HG21	2.17	0.80
1:C:42:HIS:NE2	1:C:75:SER:HB2	1.97	0.80
1:C:2:PRO:N	1:D:10:GLU:OE2	2.15	0.80
1:A:117:HIS:CG	1:A:125:VAL:HG21	2.16	0.80
1:A:49:VAL:CG1	1:A:126:ARG:HH21	1.95	0.80
1:F:106:GLN:NE2	1:G:107:GLY:H	1.78	0.80
1:I:201:GLU:OE1	1:I:206:ARG:HA	1.81	0.80
1:B:106:GLN:NE2	1:C:107:GLY:H	1.80	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:65:GLN:HG3	4:H:2037:HOH:O	1.82	0.79
1:B:178:ASN:ND2	1:B:181:ILE:H	1.81	0.79
1:B:8:ILE:HG13	1:B:140:MSE:HE2	1.65	0.79
1:I:242:TYR:CE2	4:I:321:HOH:O	2.36	0.79
1:G:2:PRO:HB2	1:H:10:GLU:OE2	1.82	0.79
1:H:40:PHE:CD1	1:H:42:HIS:HE1	2.00	0.79
1:A:62:GLU:OE1	2:A:1001:MES:H52	1.82	0.79
1:C:203:GLY:O	1:C:204:GLN:O	1.99	0.79
1:E:42:HIS:HE1	1:E:85:TRP:HZ3	1.30	0.78
1:A:49:VAL:HG11	1:A:126:ARG:NH2	1.98	0.78
1:I:117:HIS:CE1	1:J:8:ILE:H	2.02	0.78
1:E:42:HIS:HE1	1:E:85:TRP:CZ3	2.00	0.78
1:H:187:VAL:CG2	1:H:205:TYR:HE2	1.97	0.78
1:E:69:VAL:HG21	1:E:158:VAL:HG11	1.64	0.78
1:D:42:HIS:CE1	1:D:75:SER:HB2	2.19	0.77
1:B:106:GLN:HE22	1:C:107:GLY:N	1.81	0.77
1:G:40:PHE:CD1	1:G:42:HIS:HE1	2.03	0.77
1:G:4:SER:N	1:G:5:ILE:HD12	1.99	0.77
1:J:178:ASN:ND2	1:J:181:ILE:H	1.80	0.77
1:I:117:HIS:CB	1:I:125:VAL:HG21	2.15	0.76
1:I:115:LEU:O	1:I:125:VAL:HG23	1.84	0.76
1:A:132:ASP:OD2	1:A:134:ARG:NH1	2.18	0.76
1:A:125:VAL:HG12	1:A:126:ARG:H	1.50	0.76
1:H:187:VAL:HG21	1:H:205:TYR:CE2	2.21	0.76
1:C:204:GLN:O	1:C:205:TYR:HD1	1.68	0.76
1:H:43:PRO:CB	1:H:123:HIS:HB3	2.17	0.75
1:D:106:GLN:HG2	1:E:122:THR:HA	1.67	0.75
1:C:124:THR:HG22	1:C:125:VAL:O	1.86	0.75
1:H:11:ARG:NH1	4:H:2079:HOH:O	2.17	0.75
1:A:49:VAL:HG12	1:A:126:ARG:HH21	1.51	0.75
1:J:50:OCS:OD2	1:J:126:ARG:NH2	2.19	0.75
1:G:201:GLU:HA	1:G:201:GLU:OE1	1.86	0.75
1:E:201:GLU:HG2	4:E:2067:HOH:O	1.84	0.75
1:H:115:LEU:HB3	1:H:124:THR:HG23	1.66	0.75
1:B:5:ILE:CD1	1:B:6:PRO:O	2.34	0.75
1:G:228:ARG:HH11	1:G:228:ARG:HG2	1.52	0.74
1:D:202:SER:O	1:D:204:GLN:CB	2.33	0.74
1:H:187:VAL:HG21	1:H:205:TYR:HE2	1.53	0.74
1:J:92:HIS:HE1	3:J:2002:IPA:H12	1.52	0.74
1:H:231:ARG:NH1	4:H:2049:HOH:O	2.19	0.74
1:A:177:ASN:OD1	1:A:227:ARG:NH1	2.20	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:242:TYR:HE2	1:D:206:ARG:NH1	1.85	0.74
1:F:42:HIS:HD2	1:F:50:OCS:OD2	1.70	0.74
1:A:92:HIS:CE1	3:J:2001:IPA:H12	2.22	0.74
1:I:187:VAL:HG21	1:I:205:TYR:CE2	2.22	0.74
1:J:145:MSE:HG2	4:J:2080:HOH:O	1.88	0.74
1:C:178:ASN:HD22	1:C:181:ILE:H	1.35	0.74
1:I:42:HIS:NE2	1:I:75:SER:HB2	2.02	0.73
1:J:204:GLN:CA	1:J:204:GLN:HE21	2.00	0.73
1:F:220:ARG:HH11	1:F:220:ARG:HB2	1.53	0.73
1:A:5:ILE:CG2	1:B:5:ILE:HG12	2.18	0.73
1:E:178:ASN:ND2	1:E:181:ILE:H	1.85	0.73
1:J:124:THR:HG22	1:J:125:VAL:O	1.88	0.73
1:F:117:HIS:CG	1:F:125:VAL:HG21	2.23	0.73
1:D:5:ILE:CG2	1:D:6:PRO:HD2	2.18	0.73
1:G:42:HIS:HD2	1:G:50:OCS:OD2	1.71	0.73
1:F:40:PHE:HD1	1:F:42:HIS:CE1	2.07	0.73
1:B:5:ILE:HD12	1:B:6:PRO:O	1.89	0.73
1:B:201:GLU:OE1	1:B:206:ARG:HA	1.89	0.72
1:E:117:HIS:CG	1:E:125:VAL:HG11	2.24	0.72
1:G:178:ASN:ND2	1:G:181:ILE:H	1.88	0.72
1:I:224:GLU:OE1	4:I:330:HOH:O	2.06	0.72
1:C:4:SER:HA	1:D:3:GLY:O	1.89	0.72
1:D:117:HIS:CG	1:D:125:VAL:HG11	2.25	0.72
1:C:242:TYR:C	1:C:242:TYR:CD1	2.63	0.72
1:E:202:SER:OG	1:E:203:GLY:N	2.23	0.72
1:C:150:LEU:HD22	4:C:282:HOH:O	1.89	0.72
1:F:106:GLN:HE22	1:G:107:GLY:N	1.86	0.72
1:C:4:SER:C	1:C:5:ILE:HD12	2.09	0.71
1:J:42:HIS:CD2	1:J:54:PHE:HE1	2.06	0.71
1:D:202:SER:C	1:D:204:GLN:N	2.28	0.71
1:J:205:TYR:HA	4:J:2093:HOH:O	1.89	0.71
1:C:132:ASP:OD2	1:C:134:ARG:NH1	2.23	0.71
1:D:5:ILE:HG13	1:D:114:GLY:HA3	1.71	0.71
1:F:122:THR:HA	1:G:106:GLN:HG3	1.72	0.71
1:G:222:ASP:OD2	4:G:2073:HOH:O	2.08	0.71
1:C:204:GLN:O	1:C:205:TYR:CD1	2.44	0.71
1:G:106:GLN:O	1:G:108:THR:N	2.22	0.71
1:A:161:LEU:HD21	1:B:144:PRO:HG3	1.71	0.70
1:E:205:TYR:O	1:E:206:ARG:C	2.29	0.70
1:F:4:SER:C	1:F:5:ILE:HD12	2.10	0.70
1:E:88:TRP:CD1	3:E:2006:IPA:H12	2.26	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:4:SER:HA	1:J:3:GLY:O	1.92	0.70
1:C:10:GLU:OE2	1:D:2:PRO:HB2	1.92	0.70
1:H:191:THR:H	1:H:195:GLN:NE2	1.89	0.70
1:A:49:VAL:HG12	1:A:126:ARG:NH2	2.06	0.70
1:C:203:GLY:C	1:C:204:GLN:O	2.27	0.70
1:J:62:GLU:OE1	1:J:66:ARG:NH2	2.25	0.70
1:C:201:GLU:N	1:C:201:GLU:OE1	2.25	0.69
1:H:117:HIS:CG	1:H:125:VAL:HG21	2.26	0.69
1:G:121:ALA:O	1:G:122:THR:CG2	2.35	0.69
1:J:203:GLY:O	1:J:204:GLN:HG2	1.92	0.69
1:I:117:HIS:HE1	1:J:140:MSE:CE	2.06	0.69
1:E:5:ILE:HD13	1:F:5:ILE:HB	1.74	0.69
1:G:204:GLN:O	1:G:205:TYR:CD1	2.46	0.69
1:G:43:PRO:HB2	1:G:123:HIS:HB3	1.74	0.69
1:J:117:HIS:CG	1:J:125:VAL:HG11	2.27	0.69
1:G:144:PRO:HD3	1:H:139:THR:OG1	1.93	0.69
1:H:42:HIS:HD2	1:H:50:OCS:OD2	1.75	0.69
1:A:115:LEU:O	1:A:125:VAL:HG23	1.93	0.69
1:I:201:GLU:OE1	1:I:207:CYS:N	2.23	0.69
1:F:50:OCS:OD2	1:F:126:ARG:NH2	2.26	0.69
1:A:178:ASN:ND2	1:A:181:ILE:H	1.90	0.69
1:J:74:LEU:HD23	1:J:75:SER:N	2.08	0.68
1:H:144:PRO:HG2	1:H:147:LEU:HB3	1.75	0.68
1:J:204:GLN:CA	1:J:204:GLN:NE2	2.54	0.68
1:G:3:GLY:HA3	1:H:7:LEU:HD21	1.75	0.68
1:G:203:GLY:O	1:G:205:TYR:N	2.26	0.68
1:D:239:LYS:HB3	1:D:239:LYS:NZ	2.08	0.68
1:C:144:PRO:HG2	1:C:147:LEU:HB3	1.74	0.68
1:E:199:ARG:C	1:E:201:GLU:N	2.45	0.68
1:B:204:GLN:C	1:B:205:TYR:HD2	1.97	0.68
1:D:20:ASP:OD1	1:D:101:ILE:HB	1.93	0.68
1:F:178:ASN:ND2	1:F:181:ILE:H	1.87	0.68
1:A:5:ILE:CG1	1:A:6:PRO:O	2.39	0.68
1:E:200:MSE:HG3	1:E:201:GLU:OE1	1.94	0.68
1:B:205:TYR:N	1:B:205:TYR:HD2	1.91	0.68
1:F:5:ILE:HG22	1:F:6:PRO:O	1.94	0.67
1:F:42:HIS:CE1	1:F:54:PHE:HE1	2.11	0.67
1:D:115:LEU:HB3	1:D:124:THR:HG23	1.77	0.67
1:I:204:GLN:HB2	1:I:205:TYR:CD1	2.30	0.67
1:G:48:PRO:HG3	1:H:211:TRP:O	1.94	0.67
1:B:228:ARG:HD2	4:B:2024:HOH:O	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:202:SER:C	1:E:204:GLN:H	1.98	0.67
1:G:204:GLN:C	1:G:205:TYR:CG	2.67	0.67
1:J:204:GLN:C	1:J:205:TYR:CG	2.68	0.67
1:C:69:VAL:HG21	1:C:158:VAL:HG11	1.75	0.67
1:F:69:VAL:HG21	1:F:158:VAL:HG11	1.77	0.67
1:E:20:ASP:OD2	1:E:86:LYS:NZ	2.28	0.66
1:I:117:HIS:HB2	1:I:125:VAL:HG22	1.74	0.66
1:I:178:ASN:ND2	1:I:180:ILE:H	1.93	0.66
1:H:40:PHE:HD1	1:H:42:HIS:CE1	2.12	0.66
1:D:178:ASN:ND2	1:D:181:ILE:H	1.89	0.66
1:F:220:ARG:NH1	1:F:220:ARG:HB2	2.10	0.66
1:C:220:ARG:HH11	1:C:220:ARG:HB2	1.60	0.66
1:C:126:ARG:HD3	1:C:149:ARG:CZ	2.25	0.66
1:A:190:PRO:HG3	1:A:199:ARG:HD2	1.77	0.66
1:A:69:VAL:HG21	1:A:158:VAL:HG11	1.77	0.65
1:H:116:LEU:HD21	1:I:106:GLN:OE1	1.96	0.65
1:J:4:SER:O	1:J:5:ILE:CD1	2.43	0.65
1:F:74:LEU:C	1:F:74:LEU:HD23	2.17	0.65
1:B:205:TYR:N	1:B:205:TYR:CD2	2.63	0.65
3:D:2003:IPA:C3	1:E:84:LYS:NZ	2.59	0.65
1:A:240:LEU:CB	1:A:242:TYR:CE2	2.76	0.65
1:E:188:PRO:O	1:E:199:ARG:NH1	2.29	0.65
1:C:222:ASP:OD2	4:C:301:HOH:O	2.13	0.65
1:F:205:TYR:O	1:F:206:ARG:C	2.35	0.65
1:I:204:GLN:HB2	1:I:205:TYR:HD1	1.62	0.65
1:D:5:ILE:HG22	1:D:6:PRO:HD2	1.79	0.65
1:I:153:GLU:OE1	1:J:150:LEU:HD12	1.97	0.65
1:A:48:PRO:HD2	4:A:1106:HOH:O	1.95	0.64
1:G:42:HIS:CD2	1:G:50:OCS:OD2	2.49	0.64
1:F:42:HIS:CE1	1:F:54:PHE:CE1	2.86	0.64
1:E:134:ARG:HD2	4:E:2013:HOH:O	1.97	0.64
1:G:40:PHE:HD1	1:G:42:HIS:CE1	2.10	0.64
1:D:59:ARG:HG3	1:D:59:ARG:HH11	1.61	0.64
1:A:126:ARG:CG	1:A:126:ARG:NH1	2.45	0.64
4:A:1018:HOH:O	1:B:150:LEU:HD22	1.97	0.64
1:B:115:LEU:HB3	1:B:124:THR:HG23	1.80	0.64
1:G:126:ARG:HB2	1:G:143:TYR:O	1.97	0.64
1:G:139:THR:OG1	1:H:144:PRO:HD3	1.98	0.64
1:E:39:LEU:C	1:E:39:LEU:HD23	2.18	0.64
1:J:5:ILE:HG22	1:J:6:PRO:O	1.97	0.64
1:C:93:ILE:HG22	1:C:95:VAL:HG12	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:178:ASN:ND2	1:I:181:ILE:H	1.93	0.64
1:G:59:ARG:HH11	1:G:59:ARG:HG3	1.63	0.64
1:H:84:LYS:NZ	3:H:2009:IPA:H32	2.13	0.64
1:G:124:THR:HG22	1:G:125:VAL:N	2.12	0.64
1:E:126:ARG:HD2	1:E:144:PRO:O	1.98	0.64
1:F:193:GLU:HB3	1:F:197:ARG:HH12	1.63	0.63
1:I:211:TRP:O	1:J:48:PRO:HG3	1.98	0.63
1:D:178:ASN:ND2	1:D:180:ILE:H	1.96	0.63
1:F:107:GLY:H	1:G:106:GLN:NE2	1.96	0.63
1:A:115:LEU:HB3	1:A:124:THR:HG23	1.78	0.63
1:B:117:HIS:CG	1:B:125:VAL:HG21	2.32	0.63
1:F:48:PRO:HD2	4:F:2029:HOH:O	1.98	0.63
1:D:220:ARG:O	1:D:224:GLU:HG2	1.98	0.63
1:D:243:GLU:CA	1:D:243:GLU:OE1	2.38	0.63
1:D:5:ILE:HG23	1:D:113:LEU:O	1.98	0.63
1:H:115:LEU:HB3	1:H:124:THR:CG2	2.28	0.63
1:G:117:HIS:CD2	1:G:125:VAL:HG21	2.34	0.62
1:J:166:SER:HA	4:J:2083:HOH:O	1.98	0.62
1:H:126:ARG:NH1	1:H:145:MSE:O	2.31	0.62
1:G:67:LEU:O	1:G:162:LYS:HE2	1.98	0.62
1:H:88:TRP:CD1	3:H:2004:IPA:H12	2.34	0.62
1:J:126:ARG:NH1	1:J:145:MSE:O	2.31	0.62
1:A:117:HIS:CD2	1:A:125:VAL:HG21	2.35	0.62
1:D:239:LYS:O	1:D:240:LEU:HB2	2.00	0.62
1:D:201:GLU:O	1:D:202:SER:HB2	1.98	0.62
3:B:2005:IPA:H32	1:C:84:LYS:NZ	2.14	0.62
1:H:42:HIS:CD2	1:H:50:OCS:OD2	2.52	0.62
1:D:4:SER:C	1:D:5:ILE:HD12	2.20	0.62
1:D:126:ARG:HH11	1:D:145:MSE:HA	1.65	0.62
1:C:188:PRO:O	1:C:199:ARG:NH2	2.32	0.62
1:F:42:HIS:CD2	1:F:50:OCS:OD2	2.52	0.61
1:C:42:HIS:CE1	1:C:75:SER:HB2	2.34	0.61
1:D:204:GLN:HG3	4:D:2054:HOH:O	2.00	0.61
1:C:242:TYR:CE2	1:D:206:ARG:NH1	2.56	0.61
1:B:59:ARG:HH11	1:B:59:ARG:HG3	1.65	0.61
1:E:204:GLN:HA	1:E:204:GLN:NE2	2.14	0.61
1:B:239:LYS:O	1:B:240:LEU:HB2	1.99	0.61
1:J:239:LYS:NZ	1:J:239:LYS:HB3	2.14	0.61
1:D:236:LYS:HE3	4:D:2025:HOH:O	2.00	0.61
1:A:5:ILE:CG2	1:B:5:ILE:CG1	2.79	0.61
1:I:126:ARG:NH1	1:I:145:MSE:O	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:OCS:OD2	1:B:126:ARG:NH2	2.34	0.61
1:A:106:GLN:OE1	1:J:116:LEU:HD21	2.01	0.61
1:F:124:THR:HG22	1:F:125:VAL:O	2.00	0.61
1:D:14:GLU:OE1	1:D:25:LYS:NZ	2.30	0.61
1:H:120:SER:C	1:H:122:THR:H	2.03	0.61
1:C:86:LYS:HE3	1:C:101:ILE:CD1	2.30	0.61
1:G:211:TRP:O	1:H:48:PRO:HG3	2.00	0.61
1:H:190:PRO:HG3	1:H:199:ARG:HD2	1.81	0.61
1:E:2:PRO:HA	1:F:5:ILE:O	2.00	0.61
1:G:204:GLN:O	1:G:205:TYR:CG	2.54	0.61
1:H:121:ALA:C	1:H:122:THR:HG22	2.21	0.61
1:I:242:TYR:CE1	1:J:206:ARG:HD2	2.36	0.61
1:C:146:GLU:N	1:C:146:GLU:OE1	2.26	0.61
1:B:75:SER:HB3	1:B:82:HIS:HE1	1.66	0.60
1:C:126:ARG:HD3	1:C:149:ARG:NH2	2.16	0.60
1:J:3:GLY:O	1:J:5:ILE:HD12	2.02	0.60
1:A:220:ARG:HB2	1:A:220:ARG:HH11	1.66	0.60
1:J:42:HIS:NE2	1:J:54:PHE:HE1	1.99	0.60
1:A:125:VAL:HG12	1:A:126:ARG:N	2.16	0.60
1:F:106:GLN:C	1:F:108:THR:H	2.04	0.60
1:E:200:MSE:O	1:E:201:GLU:OE1	2.20	0.60
1:I:106:GLN:O	1:I:108:THR:N	2.34	0.60
1:A:48:PRO:HG3	1:B:211:TRP:O	2.01	0.60
1:H:128:VAL:HG23	1:H:149:ARG:HH11	1.66	0.60
1:H:111:ARG:HE	1:H:116:LEU:HD22	1.66	0.60
1:B:70:ASP:OD1	4:B:2042:HOH:O	2.16	0.60
1:G:69:VAL:CG2	1:G:158:VAL:HG11	2.28	0.60
1:I:5:ILE:CG1	1:J:5:ILE:HD13	2.22	0.59
1:E:42:HIS:HE2	1:E:75:SER:HB2	1.64	0.59
1:D:126:ARG:NH1	1:D:145:MSE:O	2.35	0.59
1:B:201:GLU:O	1:B:201:GLU:HG3	2.01	0.59
1:B:42:HIS:NE2	1:B:54:PHE:HE1	1.99	0.59
1:C:11:ARG:NH2	4:C:279:HOH:O	2.21	0.59
1:B:5:ILE:HD13	1:B:6:PRO:O	2.01	0.59
1:H:75:SER:HB3	1:H:82:HIS:CE1	2.38	0.59
1:J:74:LEU:HD23	1:J:74:LEU:C	2.23	0.59
1:J:42:HIS:NE2	1:J:54:PHE:CE1	2.70	0.59
1:H:86:LYS:HE2	1:H:97:ILE:HG22	1.83	0.59
1:J:69:VAL:HG21	1:J:158:VAL:HG11	1.84	0.59
1:J:120:SER:HB3	1:J:122:THR:O	2.02	0.59
1:J:183:GLU:HG2	4:J:2039:HOH:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:7:LEU:HD21	1:D:3:GLY:HA3	1.83	0.59
1:D:5:ILE:HG23	1:D:6:PRO:HD2	1.82	0.59
1:A:139:THR:HG1	1:B:144:PRO:HD3	1.68	0.59
1:J:62:GLU:HG3	4:J:2065:HOH:O	2.02	0.59
1:C:86:LYS:HE3	1:C:101:ILE:HD11	1.85	0.59
1:G:197:ARG:HE	1:I:96:ARG:NH2	2.00	0.59
1:A:203:GLY:O	1:A:204:GLN:HB2	2.01	0.59
1:I:74:LEU:HD23	1:I:75:SER:N	2.18	0.59
1:H:106:GLN:HG3	1:I:122:THR:HA	1.83	0.59
1:A:204:GLN:HE21	1:A:204:GLN:CA	2.15	0.58
1:E:199:ARG:O	1:E:201:GLU:N	2.36	0.58
1:E:124:THR:HG22	1:E:125:VAL:O	2.02	0.58
1:E:239:LYS:HB3	1:E:239:LYS:NZ	2.18	0.58
1:H:5:ILE:N	1:H:5:ILE:HD12	2.17	0.58
1:G:178:ASN:ND2	1:G:180:ILE:H	2.01	0.58
1:J:239:LYS:HZ2	1:J:239:LYS:HB3	1.68	0.58
1:F:14:GLU:OE1	1:F:14:GLU:HA	2.01	0.58
1:J:178:ASN:ND2	1:J:180:ILE:H	2.02	0.58
1:C:220:ARG:HB2	1:C:220:ARG:NH1	2.18	0.58
1:H:50:OCS:HD2	1:H:126:ARG:NH2	2.00	0.58
1:J:92:HIS:HE1	3:J:2002:IPA:C1	2.15	0.58
1:H:132:ASP:OD2	1:H:134:ARG:NH1	2.36	0.58
1:E:228:ARG:HB3	4:E:2074:HOH:O	2.03	0.58
4:E:2059:HOH:O	1:F:227:ARG:HG3	2.02	0.58
1:I:143:TYR:HD1	1:I:147:LEU:HD12	1.68	0.58
1:F:125:VAL:HG12	1:F:126:ARG:N	2.17	0.58
1:F:126:ARG:HB3	1:F:143:TYR:O	2.02	0.58
1:H:112:ARG:HG2	1:H:112:ARG:HH11	1.68	0.58
1:H:121:ALA:C	1:H:122:THR:CG2	2.72	0.58
1:D:42:HIS:HB2	1:D:50:OCS:OD2	2.04	0.58
1:I:161:LEU:HD11	1:J:144:PRO:HG3	1.86	0.58
1:A:204:GLN:HE21	1:A:204:GLN:HA	1.68	0.58
1:B:5:ILE:HD11	1:B:7:LEU:HD23	1.87	0.57
1:G:54:PHE:HE2	1:G:101:ILE:HD11	1.68	0.57
1:C:139:THR:OG1	1:D:144:PRO:HD3	2.03	0.57
1:J:203:GLY:O	1:J:204:GLN:CB	2.52	0.57
1:A:117:HIS:HB2	1:A:125:VAL:CG2	2.35	0.57
1:D:124:THR:HG22	1:D:125:VAL:O	2.04	0.57
1:I:20:ASP:OD1	1:I:101:ILE:HB	2.05	0.57
1:E:180:ILE:HD11	1:F:55:VAL:HG21	1.87	0.57
1:J:106:GLN:O	1:J:108:THR:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:236:LYS:HD2	1:J:227:ARG:HH12	1.68	0.57
1:C:48:PRO:HG3	1:D:211:TRP:O	2.05	0.57
1:F:119:GLU:O	1:F:120:SER:OG	2.21	0.57
1:D:240:LEU:O	1:D:243:GLU:HB2	2.05	0.57
1:F:39:LEU:C	1:F:39:LEU:HD23	2.25	0.57
1:H:204:GLN:NE2	4:H:2071:HOH:O	2.29	0.57
1:E:215:ASP:OD1	1:E:217:PRO:HD3	2.05	0.57
1:D:50:OCS:OD1	1:D:126:ARG:NH2	2.37	0.57
1:H:84:LYS:HZ3	3:H:2009:IPA:C3	2.17	0.57
1:C:8:ILE:HG13	1:C:140:MSE:HE2	1.85	0.57
1:G:11:ARG:HG3	4:G:2083:HOH:O	2.04	0.57
1:A:55:VAL:O	1:A:59:ARG:HG2	2.05	0.57
1:G:242:TYR:HE2	4:G:2050:HOH:O	1.88	0.57
1:D:41:SER:HB2	1:D:124:THR:HG21	1.85	0.57
1:C:178:ASN:ND2	1:C:180:ILE:H	2.01	0.57
1:H:106:GLN:CG	1:I:122:THR:HA	2.34	0.57
1:H:5:ILE:HG23	1:H:6:PRO:HD2	1.86	0.56
1:D:88:TRP:HD1	3:D:2003:IPA:H33	1.70	0.56
3:D:2003:IPA:C3	1:E:84:LYS:HZ1	2.14	0.56
1:C:2:PRO:HA	1:D:7:LEU:HG	1.88	0.56
1:C:139:THR:HG1	1:D:144:PRO:HD3	1.70	0.56
1:E:48:PRO:HG3	1:F:211:TRP:O	2.06	0.56
1:D:175:TRP:CG	1:D:176:PRO:HA	2.40	0.56
1:G:4:SER:C	1:G:5:ILE:CD1	2.65	0.56
1:E:202:SER:C	1:E:204:GLN:N	2.55	0.56
1:C:59:ARG:NH1	1:D:179:GLU:OE2	2.38	0.56
1:J:126:ARG:HB2	1:J:143:TYR:O	2.05	0.56
1:B:42:HIS:NE2	1:B:54:PHE:CE1	2.73	0.56
1:H:86:LYS:HE2	1:H:97:ILE:CG2	2.36	0.56
1:I:239:LYS:HB3	1:I:239:LYS:NZ	2.20	0.56
1:F:239:LYS:HB3	1:F:239:LYS:NZ	2.20	0.56
1:D:48:PRO:HD2	4:D:2026:HOH:O	2.03	0.56
1:A:235:GLU:HG3	4:A:1102:HOH:O	2.06	0.56
1:D:206:ARG:HD2	1:D:214:TRP:CH2	2.41	0.56
1:E:220:ARG:HH11	1:E:220:ARG:HB2	1.70	0.56
1:C:179:GLU:O	1:D:240:LEU:HA	2.06	0.56
1:B:204:GLN:C	1:B:205:TYR:CD2	2.79	0.56
1:C:7:LEU:HD22	1:D:117:HIS:CD2	2.40	0.56
1:F:14:GLU:OE1	1:F:27:PRO:CD	2.54	0.56
1:H:190:PRO:HG3	1:H:199:ARG:CD	2.35	0.56
1:G:54:PHE:HE2	1:G:101:ILE:CD1	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:115:LEU:HB3	1:C:124:THR:HG23	1.87	0.56
1:I:28:ASP:OD1	1:I:28:ASP:N	2.39	0.56
1:D:204:GLN:C	1:D:204:GLN:HE21	2.09	0.56
1:J:203:GLY:C	1:J:204:GLN:CG	2.74	0.56
1:I:178:ASN:HD21	1:I:180:ILE:HB	1.71	0.56
1:C:211:TRP:O	1:D:48:PRO:HG3	2.06	0.55
1:J:163:LEU:HD11	1:J:222:ASP:HB3	1.88	0.55
1:B:106:GLN:C	1:B:108:THR:H	2.08	0.55
1:D:88:TRP:CD1	3:D:2003:IPA:H33	2.40	0.55
1:F:74:LEU:HD23	1:F:75:SER:N	2.20	0.55
1:H:122:THR:O	1:H:123:HIS:O	2.25	0.55
1:D:126:ARG:NH1	1:D:145:MSE:HA	2.21	0.55
1:G:48:PRO:HB2	1:H:186:ILE:HG21	1.88	0.55
1:A:125:VAL:CG1	1:A:126:ARG:H	2.19	0.55
1:G:242:TYR:HB3	1:H:180:ILE:O	2.07	0.55
4:A:1118:HOH:O	1:B:242:TYR:HB2	2.06	0.55
1:H:206:ARG:HD2	1:H:206:ARG:H	1.72	0.55
1:D:106:GLN:CG	1:E:122:THR:HA	2.37	0.55
1:I:144:PRO:HG2	1:I:147:LEU:HB3	1.89	0.55
1:G:65:GLN:HG3	4:G:2059:HOH:O	2.06	0.55
1:A:204:GLN:O	1:A:215:ASP:HB3	2.06	0.55
1:B:178:ASN:ND2	1:B:180:ILE:H	2.05	0.55
1:G:144:PRO:HD3	1:H:139:THR:HG1	1.72	0.55
1:H:36:TRP:NE1	1:H:162:LYS:HE2	2.22	0.55
1:C:215:ASP:OD1	1:C:217:PRO:HD3	2.07	0.55
1:G:175:TRP:CG	1:G:176:PRO:HA	2.42	0.55
1:B:36:TRP:HB2	1:B:69:VAL:HG22	1.89	0.55
1:H:5:ILE:HG22	1:H:6:PRO:N	2.22	0.55
1:I:74:LEU:HD23	1:I:74:LEU:C	2.27	0.55
1:J:41:SER:HB2	1:J:124:THR:HG21	1.88	0.55
1:C:126:ARG:NH1	1:C:144:PRO:O	2.40	0.55
1:D:239:LYS:HB3	1:D:239:LYS:HZ3	1.69	0.54
1:F:115:LEU:O	1:F:125:VAL:HG23	2.07	0.54
1:A:224:GLU:OE1	1:A:224:GLU:HA	2.06	0.54
1:J:199:ARG:HD3	4:J:2071:HOH:O	2.07	0.54
1:A:201:GLU:OE1	1:A:206:ARG:CA	2.47	0.54
1:J:92:HIS:CE1	3:J:2002:IPA:H12	2.37	0.54
1:B:75:SER:HB3	1:B:82:HIS:CE1	2.42	0.54
1:J:93:ILE:HG22	1:J:95:VAL:HG12	1.89	0.54
1:G:115:LEU:HB3	1:G:124:THR:HG23	1.90	0.54
1:B:35:LYS:HD3	1:B:70:ASP:OD2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:HIS:CD2	1:B:54:PHE:HE1	2.25	0.54
1:F:65:GLN:NE2	1:F:70:ASP:OD1	2.38	0.54
1:I:117:HIS:HE1	1:J:140:MSE:HE1	1.71	0.54
1:E:201:GLU:O	1:E:202:SER:HB2	2.05	0.54
1:A:36:TRP:HB2	1:A:69:VAL:HG22	1.89	0.54
1:F:125:VAL:HG12	1:F:126:ARG:H	1.73	0.54
1:G:48:PRO:HD2	4:G:2046:HOH:O	2.07	0.54
1:B:55:VAL:O	1:B:59:ARG:HG2	2.08	0.54
1:I:20:ASP:OD2	1:I:86:LYS:NZ	2.36	0.54
1:A:150:LEU:HD22	4:A:1007:HOH:O	2.05	0.54
1:E:40:PHE:HZ	1:E:99:PHE:CE2	2.26	0.54
1:B:5:ILE:CD1	1:B:7:LEU:HD23	2.37	0.54
1:J:220:ARG:NH1	1:J:220:ARG:HB2	2.22	0.54
1:H:50:OCS:SG	1:H:126:ARG:NH2	2.80	0.54
1:E:93:ILE:HG22	1:E:95:VAL:HG12	1.89	0.54
1:F:215:ASP:OD1	1:F:217:PRO:HD3	2.06	0.54
1:G:143:TYR:HD1	1:G:147:LEU:HD12	1.73	0.54
1:B:126:ARG:NH1	1:B:145:MSE:O	2.41	0.54
1:H:14:GLU:OE2	1:H:25:LYS:HE2	2.07	0.54
1:J:203:GLY:O	1:J:204:GLN:CG	2.55	0.54
1:G:3:GLY:C	1:G:5:ILE:CD1	2.76	0.54
1:E:106:GLN:O	1:E:111:ARG:NH1	2.37	0.54
1:D:231:ARG:HH11	1:D:231:ARG:HG3	1.73	0.54
1:J:132:ASP:OD2	1:J:134:ARG:NH1	2.41	0.53
1:I:175:TRP:CG	1:I:176:PRO:HA	2.44	0.53
1:D:96:ARG:HH11	1:D:96:ARG:HG2	1.73	0.53
1:E:201:GLU:O	1:E:202:SER:CB	2.56	0.53
1:D:76:VAL:O	1:D:105:PRO:HA	2.08	0.53
1:C:42:HIS:HB2	1:C:50:OCS:OD2	2.08	0.53
1:H:115:LEU:O	1:H:125:VAL:HG23	2.08	0.53
1:J:150:LEU:CD2	4:J:2008:HOH:O	2.56	0.53
1:D:59:ARG:NH1	1:D:59:ARG:HG3	2.23	0.53
1:D:96:ARG:NH1	1:D:96:ARG:HG2	2.23	0.53
1:J:203:GLY:O	1:J:204:GLN:HB2	2.08	0.53
1:A:206:ARG:HD2	1:A:206:ARG:H	1.73	0.53
1:H:117:HIS:CD2	1:H:125:VAL:HG21	2.43	0.53
1:J:42:HIS:CD2	1:J:54:PHE:CE1	2.93	0.53
1:F:14:GLU:OE1	1:F:27:PRO:HD2	2.08	0.53
1:J:61:TYR:HD2	1:J:71:LEU:HD12	1.74	0.53
1:J:39:LEU:HD23	1:J:39:LEU:C	2.28	0.53
1:C:5:ILE:HG22	1:C:6:PRO:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:42:HIS:CE1	1:E:85:TRP:CZ3	2.91	0.53
1:B:39:LEU:HD23	1:B:39:LEU:C	2.29	0.53
1:B:105:PRO:HB2	1:C:122:THR:HB	1.90	0.53
1:B:178:ASN:HD22	1:B:181:ILE:N	1.97	0.53
1:F:14:GLU:OE1	1:F:14:GLU:CA	2.56	0.53
1:J:231:ARG:O	1:J:235:GLU:HG3	2.08	0.53
1:B:128:VAL:HG23	1:B:149:ARG:HH11	1.74	0.53
1:J:204:GLN:O	1:J:205:TYR:CB	2.54	0.53
1:I:178:ASN:HD22	1:I:181:ILE:N	2.02	0.53
1:C:228:ARG:HD2	4:C:314:HOH:O	2.09	0.53
1:E:227:ARG:HG2	4:F:2065:HOH:O	2.08	0.53
1:I:5:ILE:HD13	1:J:5:ILE:HG21	1.90	0.53
1:C:106:GLN:C	1:C:108:THR:H	2.04	0.53
1:B:201:GLU:O	1:B:201:GLU:CG	2.57	0.53
1:A:92:HIS:HE1	3:J:2001:IPA:C1	2.17	0.53
1:I:201:GLU:HA	1:I:205:TYR:O	2.09	0.53
1:I:7:LEU:HD12	1:I:10:GLU:OE2	2.09	0.53
1:F:144:PRO:HG2	1:F:147:LEU:CB	2.38	0.53
1:D:206:ARG:HD2	1:D:214:TRP:CZ2	2.44	0.53
1:E:2:PRO:N	1:F:10:GLU:OE2	2.41	0.53
1:C:186:ILE:HG21	1:D:48:PRO:HB2	1.91	0.53
1:A:144:PRO:HG3	1:B:161:LEU:HD11	1.89	0.53
1:J:103:ALA:C	1:J:105:PRO:HD3	2.29	0.52
1:H:3:GLY:O	1:H:5:ILE:CD1	2.57	0.52
1:C:41:SER:HA	1:C:74:LEU:O	2.08	0.52
1:H:199:ARG:O	1:H:200:MSE:CE	2.35	0.52
1:C:202:SER:HB3	1:C:205:TYR:HB2	1.90	0.52
1:C:186:ILE:HG21	1:D:48:PRO:CB	2.40	0.52
1:H:124:THR:HG22	1:H:125:VAL:N	2.23	0.52
1:G:59:ARG:NH1	1:H:179:GLU:OE2	2.42	0.52
1:H:84:LYS:HZ3	3:H:2009:IPA:H32	1.75	0.52
1:I:150:LEU:CD2	4:J:2025:HOH:O	2.57	0.52
1:I:48:PRO:HB2	1:J:186:ILE:HD13	1.91	0.52
1:H:126:ARG:HB2	1:H:143:TYR:O	2.09	0.52
1:D:5:ILE:CG2	1:D:6:PRO:CD	2.87	0.52
1:E:42:HIS:HB2	1:E:50:OCS:OD2	2.08	0.52
1:E:92:HIS:HE1	3:E:2006:IPA:O2	1.93	0.52
1:F:144:PRO:HG2	1:F:147:LEU:HB3	1.91	0.52
1:E:103:ALA:C	1:E:105:PRO:HD3	2.29	0.52
1:H:228:ARG:NH2	4:H:2084:HOH:O	2.39	0.52
1:A:240:LEU:CB	1:A:242:TYR:CD2	2.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:122:THR:HA	1:G:106:GLN:CG	2.38	0.52
1:C:144:PRO:HG3	1:D:161:LEU:HD11	1.91	0.52
1:B:143:TYR:HD1	1:B:147:LEU:HD12	1.73	0.52
1:I:134:ARG:HH21	1:I:136:VAL:CB	2.23	0.52
1:D:8:ILE:HG13	1:D:140:MSE:HE2	1.92	0.52
1:F:5:ILE:HG23	1:F:6:PRO:HD2	1.92	0.52
1:I:144:PRO:HG3	1:J:161:LEU:HD11	1.92	0.52
1:E:88:TRP:HD1	3:E:2006:IPA:H12	1.74	0.52
1:E:13:PRO:HB2	1:E:15:MSE:HE3	1.92	0.52
1:B:117:HIS:CD2	1:B:125:VAL:HG21	2.45	0.52
1:I:63:ASP:CG	1:I:228:ARG:HH22	2.13	0.52
1:H:143:TYR:CD1	1:H:147:LEU:HD12	2.45	0.52
1:H:178:ASN:ND2	1:H:180:ILE:H	2.08	0.52
1:B:124:THR:HG22	1:B:125:VAL:O	2.10	0.52
1:B:86:LYS:HE3	1:B:101:ILE:CD1	2.39	0.52
1:G:117:HIS:HB2	1:G:125:VAL:CG2	2.40	0.51
1:D:107:GLY:HA3	1:E:106:GLN:HE22	1.75	0.51
1:I:42:HIS:HB2	1:I:50:OCS:OD2	2.11	0.51
1:B:8:ILE:HG13	1:B:140:MSE:CE	2.36	0.51
1:E:239:LYS:HE2	1:E:241:LEU:HD23	1.92	0.51
1:F:138:ARG:NH2	1:F:165:ASP:OD1	2.43	0.51
1:A:5:ILE:HD11	1:A:140:MSE:HE1	1.92	0.51
1:A:106:GLN:CD	1:J:116:LEU:HD21	2.30	0.51
1:D:75:SER:HB3	1:D:82:HIS:CE1	2.45	0.51
1:J:193:GLU:OE1	4:J:2013:HOH:O	2.19	0.51
1:G:126:ARG:NH1	1:G:145:MSE:O	2.44	0.51
1:E:2:PRO:N	1:F:10:GLU:OE1	2.44	0.51
1:B:86:LYS:HE3	1:B:101:ILE:HD12	1.92	0.51
1:A:112:ARG:NH1	1:A:112:ARG:O	2.44	0.51
1:D:111:ARG:NH2	1:E:106:GLN:HE22	2.09	0.51
1:B:115:LEU:O	1:B:125:VAL:HG23	2.09	0.51
1:B:126:ARG:HB2	1:B:143:TYR:O	2.10	0.51
1:J:122:THR:OG1	1:J:123:HIS:CD2	2.64	0.51
1:H:153:GLU:OE1	1:H:153:GLU:HA	2.11	0.51
1:F:178:ASN:ND2	1:F:180:ILE:H	2.09	0.51
1:E:175:TRP:CE2	1:E:176:PRO:HB3	2.46	0.51
1:D:193:GLU:O	1:D:197:ARG:HG3	2.10	0.51
1:G:124:THR:CG2	1:G:125:VAL:N	2.74	0.51
1:H:206:ARG:H	1:H:206:ARG:CD	2.23	0.51
1:E:205:TYR:O	1:E:206:ARG:O	2.28	0.51
1:F:204:GLN:HB3	1:F:205:TYR:CE1	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:220:ARG:HH11	1:H:220:ARG:HB2	1.74	0.51
1:I:144:PRO:HD3	1:J:139:THR:OG1	2.11	0.51
1:D:242:TYR:C	1:D:242:TYR:CD2	2.84	0.51
1:F:134:ARG:HG3	1:F:136:VAL:HG23	1.93	0.51
1:J:200:MSE:HE2	1:J:200:MSE:H	1.76	0.51
1:J:4:SER:O	1:J:5:ILE:CG1	2.59	0.51
1:H:5:ILE:CG2	1:H:6:PRO:HD2	2.40	0.51
1:A:103:ALA:C	1:A:105:PRO:HD3	2.30	0.51
1:H:112:ARG:HG2	1:H:112:ARG:NH1	2.26	0.51
1:F:103:ALA:C	1:F:105:PRO:HD3	2.31	0.51
1:A:117:HIS:CB	1:A:125:VAL:HG21	2.40	0.51
1:B:74:LEU:HD23	1:B:75:SER:N	2.26	0.51
1:A:122:THR:HB	1:J:105:PRO:HB2	1.93	0.50
1:G:50:OCS:OD2	1:G:126:ARG:NH2	2.44	0.50
1:E:50:OCS:OD2	1:E:126:ARG:NH2	2.44	0.50
1:C:200:MSE:O	1:C:201:GLU:C	2.48	0.50
1:C:69:VAL:CG2	1:C:158:VAL:HG11	2.39	0.50
1:E:161:LEU:HD11	1:F:144:PRO:HG3	1.92	0.50
1:A:240:LEU:HB3	1:A:242:TYR:CD2	2.46	0.50
1:J:36:TRP:HB2	1:J:69:VAL:HG22	1.93	0.50
1:E:223:VAL:CG1	1:E:227:ARG:NH1	2.74	0.50
1:A:204:GLN:NE2	1:A:204:GLN:HA	2.25	0.50
1:A:204:GLN:O	1:A:205:TYR:HD2	1.95	0.50
1:C:242:TYR:HD1	1:C:242:TYR:C	2.11	0.50
1:F:106:GLN:NE2	1:F:106:GLN:HA	2.27	0.50
1:H:178:ASN:ND2	1:H:181:ILE:H	2.01	0.50
1:D:60:ARG:HD2	1:D:151:VAL:CG1	2.41	0.50
1:J:190:PRO:HA	1:J:195:GLN:HE21	1.77	0.50
1:J:3:GLY:C	1:J:5:ILE:HD12	2.31	0.50
1:D:5:ILE:HG22	1:D:6:PRO:CD	2.41	0.50
1:C:35:LYS:HD3	1:C:70:ASP:OD2	2.12	0.50
1:I:117:HIS:CG	1:I:125:VAL:HG21	2.47	0.50
1:D:178:ASN:HD21	1:D:180:ILE:HB	1.77	0.50
1:H:120:SER:C	1:H:122:THR:N	2.65	0.50
1:E:20:ASP:HB2	1:E:101:ILE:H	1.76	0.50
1:G:79:VAL:O	1:G:83:ILE:HG13	2.11	0.50
1:E:138:ARG:NH2	1:E:165:ASP:OD2	2.44	0.50
1:F:92:HIS:ND1	4:F:2046:HOH:O	2.33	0.50
1:C:189:PRO:HG3	1:D:48:PRO:CD	2.42	0.50
1:B:112:ARG:HH11	1:B:112:ARG:HG2	1.76	0.50
1:G:143:TYR:CD1	1:G:147:LEU:HD12	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:126:ARG:HD2	1:J:144:PRO:O	2.12	0.50
1:I:128:VAL:O	1:I:140:MSE:HA	2.11	0.50
1:J:86:LYS:HE3	1:J:101:ILE:CD1	2.42	0.50
1:I:103:ALA:C	1:I:105:PRO:HD3	2.32	0.50
1:I:179:GLU:OE2	1:J:59:ARG:NH1	2.44	0.50
1:G:126:ARG:HH11	1:G:145:MSE:HA	1.77	0.50
1:H:187:VAL:CG2	1:H:205:TYR:CE2	2.83	0.50
1:I:45:ASP:O	1:I:46:PHE:HB2	2.10	0.50
1:A:2:PRO:N	1:B:10:GLU:OE1	2.45	0.49
1:F:138:ARG:NH2	1:F:165:ASP:OD2	2.45	0.49
1:G:231:ARG:HG3	1:G:231:ARG:HH11	1.77	0.49
1:F:117:HIS:N	4:F:2047:HOH:O	2.45	0.49
1:D:126:ARG:HB2	1:D:143:TYR:O	2.12	0.49
1:H:75:SER:HB3	1:H:82:HIS:HE1	1.74	0.49
1:E:143:TYR:OH	1:F:153:GLU:OE2	2.19	0.49
1:G:20:ASP:HB2	1:G:101:ILE:H	1.77	0.49
1:I:156:ARG:HD3	1:I:230:LEU:HD11	1.93	0.49
1:I:8:ILE:HG13	1:I:140:MSE:HE2	1.95	0.49
1:B:121:ALA:O	1:B:122:THR:O	2.31	0.49
1:C:61:TYR:O	1:C:65:GLN:HG2	2.12	0.49
1:H:122:THR:HG1	1:H:123:HIS:CD2	2.26	0.49
1:H:36:TRP:CD2	1:H:132:ASP:HA	2.48	0.49
1:A:86:LYS:HE3	1:A:101:ILE:HD11	1.94	0.49
1:G:147:LEU:HD13	1:G:148:GLY:O	2.13	0.49
1:G:5:ILE:HG22	1:G:6:PRO:O	2.12	0.49
1:C:7:LEU:HD13	1:D:117:HIS:HA	1.94	0.49
1:D:128:VAL:O	1:D:140:MSE:HA	2.12	0.49
1:A:86:LYS:HE3	1:A:101:ILE:CD1	2.42	0.49
1:G:39:LEU:HD23	1:G:39:LEU:C	2.32	0.49
1:A:240:LEU:HB3	1:A:242:TYR:HD2	1.78	0.49
1:A:134:ARG:HG3	1:A:136:VAL:HG23	1.94	0.49
1:A:139:THR:OG1	1:B:144:PRO:HD3	2.11	0.49
1:I:186:ILE:HG21	1:J:48:PRO:HB2	1.94	0.49
1:B:5:ILE:C	1:B:5:ILE:HD12	2.33	0.49
1:C:4:SER:O	1:C:5:ILE:HD12	2.12	0.49
1:D:144:PRO:HG2	1:D:147:LEU:HB3	1.95	0.49
1:A:150:LEU:CD2	4:A:1007:HOH:O	2.59	0.49
1:A:144:PRO:HG2	1:A:147:LEU:HB2	1.94	0.49
1:H:143:TYR:HD1	1:H:147:LEU:HD12	1.78	0.49
1:D:96:ARG:O	1:D:98:PRO:HD3	2.13	0.49
1:D:117:HIS:HB2	1:D:125:VAL:CG1	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:74:LEU:HD23	1:E:75:SER:N	2.28	0.49
3:B:2005:IPA:H32	1:C:84:LYS:HZ2	1.78	0.49
1:A:175:TRP:CG	1:A:176:PRO:HA	2.48	0.49
1:H:7:LEU:HA	1:H:140:MSE:HE1	1.95	0.48
1:J:178:ASN:HD22	1:J:181:ILE:N	1.92	0.48
1:D:42:HIS:NE2	1:D:75:SER:HB2	2.28	0.48
1:E:138:ARG:NH1	1:F:146:GLU:OE2	2.45	0.48
1:G:48:PRO:CB	1:H:186:ILE:HG21	2.44	0.48
1:G:37:PHE:CE1	1:G:131:VAL:HG11	2.48	0.48
1:B:5:ILE:O	1:B:5:ILE:HD12	2.13	0.48
1:C:239:LYS:NZ	1:C:239:LYS:HB3	2.28	0.48
1:D:4:SER:O	1:D:5:ILE:HG13	2.13	0.48
1:D:50:OCS:OD1	1:D:50:OCS:N	2.47	0.48
1:J:143:TYR:HD1	1:J:147:LEU:HD12	1.78	0.48
1:A:59:ARG:NH1	1:B:179:GLU:OE1	2.46	0.48
1:D:69:VAL:CG2	1:D:158:VAL:HG11	2.37	0.48
1:F:107:GLY:H	1:G:106:GLN:HE22	1.60	0.48
1:G:59:ARG:NH1	1:G:59:ARG:HG3	2.25	0.48
1:H:84:LYS:NZ	3:H:2009:IPA:C3	2.77	0.48
1:F:20:ASP:OD1	1:F:101:ILE:HB	2.13	0.48
1:G:146:GLU:HG3	4:H:2041:HOH:O	2.13	0.48
1:C:121:ALA:O	1:C:122:THR:O	2.31	0.48
1:I:86:LYS:HE3	1:I:101:ILE:CD1	2.44	0.48
1:G:199:ARG:O	1:G:201:GLU:N	2.44	0.48
1:H:39:LEU:HD23	1:H:39:LEU:C	2.34	0.48
1:I:117:HIS:CE1	1:J:140:MSE:HE1	2.48	0.48
1:D:117:HIS:N	4:D:2043:HOH:O	2.46	0.48
1:J:147:LEU:HD13	1:J:148:GLY:O	2.14	0.48
1:B:88:TRP:HD1	3:B:2005:IPA:H33	1.78	0.48
1:D:60:ARG:HH11	1:D:60:ARG:HG3	1.79	0.48
1:B:201:GLU:CB	1:B:205:TYR:O	2.55	0.48
1:C:241:LEU:H	1:C:241:LEU:HD23	1.77	0.48
1:C:5:ILE:HG13	1:C:114:GLY:HA3	1.95	0.48
1:I:126:ARG:HH11	1:I:126:ARG:HG3	1.79	0.48
1:J:157:ILE:O	1:J:161:LEU:HB2	2.13	0.48
1:A:239:LYS:HE2	1:A:241:LEU:HD12	1.95	0.48
1:D:156:ARG:HD3	1:D:230:LEU:HD11	1.96	0.48
1:H:144:PRO:HG2	1:H:147:LEU:CB	2.44	0.48
1:I:143:TYR:CD1	1:I:147:LEU:HD12	2.47	0.48
1:A:105:PRO:HB2	1:J:122:THR:HB	1.95	0.48
1:H:13:PRO:HB2	1:H:15:MSE:CE	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:106:GLN:C	1:I:108:THR:H	2.17	0.48
1:A:172:PRO:HG2	1:A:175:TRP:HB2	1.96	0.48
1:D:202:SER:O	1:D:204:GLN:CA	2.59	0.47
1:G:117:HIS:CD2	1:H:7:LEU:HD22	2.48	0.47
1:D:40:PHE:HZ	1:D:99:PHE:CE2	2.32	0.47
1:C:214:TRP:HZ2	1:D:242:TYR:CD1	2.32	0.47
1:D:79:VAL:O	1:D:83:ILE:HG13	2.14	0.47
1:D:67:LEU:O	1:D:162:LYS:HE2	2.14	0.47
1:A:200:MSE:HA	1:A:200:MSE:HE3	1.96	0.47
1:E:239:LYS:O	1:E:240:LEU:HB2	2.14	0.47
1:C:124:THR:CG2	1:C:125:VAL:N	2.77	0.47
1:C:42:HIS:CE1	1:C:85:TRP:CZ3	3.03	0.47
1:C:172:PRO:HG3	1:C:181:ILE:HD11	1.97	0.47
1:E:124:THR:CG2	1:E:125:VAL:N	2.78	0.47
1:H:13:PRO:HB2	1:H:15:MSE:HE3	1.97	0.47
1:I:14:GLU:HG2	1:I:25:LYS:HE2	1.96	0.47
1:F:125:VAL:HG22	4:F:2047:HOH:O	2.14	0.47
3:B:2005:IPA:C3	1:C:84:LYS:HZ1	2.27	0.47
1:C:48:PRO:CB	1:D:186:ILE:HG21	2.45	0.47
1:I:134:ARG:HH21	1:I:136:VAL:HB	1.79	0.47
1:H:146:GLU:N	1:H:146:GLU:OE1	2.40	0.47
1:I:59:ARG:NH1	1:I:241:LEU:HD11	2.30	0.47
1:A:117:HIS:HB2	1:A:125:VAL:HG22	1.97	0.47
1:H:4:SER:CA	1:H:5:ILE:HD12	2.45	0.47
1:B:178:ASN:HD21	1:B:180:ILE:HB	1.79	0.47
1:I:126:ARG:HH11	1:I:145:MSE:HA	1.79	0.47
1:J:117:HIS:HB2	1:J:125:VAL:CG1	2.45	0.47
1:F:204:GLN:HG3	4:F:2058:HOH:O	2.15	0.47
1:F:192:THR:OG1	1:F:195:GLN:HG3	2.15	0.47
1:I:183:GLU:HG2	4:I:311:HOH:O	2.15	0.47
1:A:40:PHE:HZ	1:A:99:PHE:CE2	2.33	0.47
1:I:5:ILE:HD11	1:J:5:ILE:HG12	1.96	0.47
1:F:14:GLU:OE1	1:F:27:PRO:HD3	2.14	0.47
1:C:214:TRP:CZ2	1:D:242:TYR:CD1	3.02	0.47
1:G:132:ASP:OD2	1:G:134:ARG:NH1	2.48	0.47
1:J:200:MSE:HE3	1:J:202:SER:O	2.15	0.47
1:G:117:HIS:CB	1:G:125:VAL:HG21	2.44	0.47
1:H:84:LYS:HZ1	3:H:2009:IPA:H32	1.80	0.47
1:J:120:SER:O	1:J:122:THR:O	2.32	0.47
1:I:55:VAL:O	1:I:59:ARG:HG2	2.15	0.47
1:H:167:LEU:HD13	1:H:217:PRO:HG2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:178:ASN:HD22	1:F:181:ILE:N	1.91	0.47
1:G:5:ILE:HG13	1:G:114:GLY:HA3	1.97	0.47
1:D:93:ILE:HG22	1:D:95:VAL:HG12	1.97	0.47
1:D:214:TRP:CD1	1:D:214:TRP:N	2.82	0.46
1:D:76:VAL:HG12	1:D:76:VAL:O	2.15	0.46
1:C:201:GLU:HB2	1:C:202:SER:H	1.17	0.46
1:I:199:ARG:HD2	4:I:271:HOH:O	2.15	0.46
1:E:141:LEU:HD22	1:F:141:LEU:HD22	1.97	0.46
1:G:3:GLY:C	1:G:5:ILE:HD12	2.35	0.46
1:F:106:GLN:C	1:F:108:THR:N	2.67	0.46
1:D:147:LEU:HD13	1:D:148:GLY:O	2.15	0.46
1:A:240:LEU:HB2	1:A:242:TYR:CD2	2.47	0.46
1:G:124:THR:HG22	1:G:125:VAL:O	2.16	0.46
1:B:14:GLU:CG	1:B:25:LYS:HE2	2.45	0.46
1:B:146:GLU:N	1:B:146:GLU:OE1	2.47	0.46
1:J:215:ASP:N	1:J:215:ASP:OD1	2.48	0.46
1:F:84:LYS:HD2	1:F:84:LYS:HA	1.76	0.46
1:D:198:ALA:C	1:D:200:MSE:O	2.54	0.46
1:H:183:GLU:HG2	4:H:2053:HOH:O	2.15	0.46
1:C:150:LEU:CD2	4:C:282:HOH:O	2.57	0.46
1:A:48:PRO:HB2	1:B:186:ILE:HG21	1.96	0.46
1:E:147:LEU:HD21	1:F:160:ALA:HB3	1.97	0.46
1:G:144:PRO:HB3	4:H:2030:HOH:O	2.14	0.46
1:B:92:HIS:HE1	3:B:2005:IPA:O2	1.98	0.46
1:F:107:GLY:N	1:G:106:GLN:HE22	2.13	0.46
1:B:74:LEU:C	1:B:74:LEU:HD23	2.35	0.46
1:A:169:ARG:HB3	1:A:185:LEU:HB3	1.97	0.46
1:J:60:ARG:HH11	1:J:60:ARG:HG3	1.80	0.46
1:E:4:SER:C	1:E:5:ILE:HD12	2.37	0.46
1:F:5:ILE:HG22	1:F:6:PRO:N	2.30	0.46
1:B:106:GLN:HG2	1:C:122:THR:HA	1.96	0.46
1:I:36:TRP:HB2	1:I:69:VAL:HG22	1.96	0.46
1:E:121:ALA:O	1:E:122:THR:O	2.33	0.46
1:F:204:GLN:C	1:F:205:TYR:CG	2.89	0.46
1:C:86:LYS:HE2	1:C:97:ILE:CG2	2.46	0.46
1:H:220:ARG:NH1	1:H:220:ARG:HB2	2.31	0.46
1:J:59:ARG:HH11	1:J:59:ARG:HG3	1.81	0.46
1:C:178:ASN:HD21	1:C:180:ILE:HB	1.81	0.46
1:E:7:LEU:HB2	1:E:10:GLU:HG3	1.98	0.46
1:A:178:ASN:HD21	1:A:180:ILE:HB	1.80	0.46
1:F:125:VAL:CG2	4:F:2047:HOH:O	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:74:LEU:C	1:C:74:LEU:HD23	2.37	0.46
1:B:42:HIS:CE1	1:B:54:PHE:HE1	2.33	0.46
1:J:128:VAL:O	1:J:140:MSE:HA	2.16	0.45
1:G:4:SER:N	1:G:5:ILE:CD1	2.76	0.45
1:D:143:TYR:HD1	1:D:147:LEU:HD12	1.81	0.45
3:B:2005:IPA:H32	1:C:84:LYS:HZ1	1.81	0.45
1:J:190:PRO:HA	1:J:195:GLN:NE2	2.30	0.45
1:I:201:GLU:OE1	1:I:206:ARG:CA	2.57	0.45
1:E:187:VAL:HG21	1:E:205:TYR:CE1	2.51	0.45
1:F:128:VAL:O	1:F:140:MSE:HA	2.17	0.45
1:B:103:ALA:C	1:B:105:PRO:HD3	2.36	0.45
1:A:183:GLU:OE2	1:A:227:ARG:NH2	2.49	0.45
1:C:36:TRP:CD2	1:C:132:ASP:HA	2.52	0.45
1:I:236:LYS:HD2	1:J:227:ARG:NH1	2.31	0.45
1:I:14:GLU:CG	1:I:25:LYS:HE2	2.47	0.45
1:G:208:LEU:HA	1:G:208:LEU:HD23	1.82	0.45
1:F:117:HIS:CD2	1:F:125:VAL:HG21	2.51	0.45
1:F:126:ARG:HG2	1:F:143:TYR:HB2	1.99	0.45
1:H:132:ASP:C	1:H:132:ASP:OD1	2.51	0.45
1:C:189:PRO:HG3	1:D:48:PRO:CG	2.47	0.45
1:C:21:HIS:CG	1:C:100:PRO:HB3	2.51	0.45
1:D:43:PRO:O	1:D:123:HIS:ND1	2.47	0.45
1:I:15:MSE:HE2	1:I:112:ARG:HG2	1.98	0.45
1:I:117:HIS:ND1	1:J:7:LEU:HB3	2.31	0.45
1:G:111:ARG:HG2	1:G:116:LEU:HD22	1.99	0.45
1:E:122:THR:O	1:E:123:HIS:O	2.35	0.45
1:I:126:ARG:HB2	1:I:143:TYR:O	2.16	0.45
1:D:7:LEU:HB2	1:D:10:GLU:HG3	1.99	0.45
1:G:106:GLN:C	1:G:108:THR:H	2.16	0.45
1:D:97:ILE:HD13	1:D:97:ILE:N	2.31	0.45
1:F:5:ILE:CG2	1:F:6:PRO:N	2.80	0.45
1:C:124:THR:HG22	1:C:125:VAL:N	2.30	0.45
1:I:188:PRO:HA	1:I:189:PRO:HD3	1.88	0.45
1:A:215:ASP:OD1	1:A:217:PRO:HD3	2.17	0.45
1:C:93:ILE:HD13	1:D:180:ILE:HD13	1.97	0.45
1:F:3:GLY:O	1:F:5:ILE:HD12	2.16	0.45
1:E:197:ARG:O	1:E:201:GLU:HB2	2.17	0.45
1:I:201:GLU:HG3	1:I:205:TYR:O	2.16	0.45
1:F:115:LEU:HB3	1:F:124:THR:HG23	1.99	0.45
1:B:183:GLU:HG2	4:B:2072:HOH:O	2.17	0.45
1:G:221:ASP:OD2	4:G:2074:HOH:O	2.21	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:LEU:HA	1:A:208:LEU:HD23	1.80	0.45
1:D:204:GLN:HB3	1:D:205:TYR:CD1	2.52	0.45
1:A:117:HIS:HB2	1:A:125:VAL:HG21	1.98	0.45
1:G:178:ASN:HD21	1:G:180:ILE:HB	1.82	0.45
1:H:121:ALA:O	1:H:122:THR:CG2	2.57	0.45
1:A:220:ARG:HB2	1:A:220:ARG:NH1	2.31	0.45
1:B:175:TRP:CG	1:B:176:PRO:HA	2.52	0.45
1:G:62:GLU:HG2	4:G:2033:HOH:O	2.17	0.45
1:B:106:GLN:C	1:B:108:THR:N	2.69	0.45
1:H:147:LEU:HD13	1:H:148:GLY:O	2.16	0.45
1:J:203:GLY:C	1:J:204:GLN:HG2	2.36	0.44
1:H:50:OCS:OD1	1:H:126:ARG:NH2	2.50	0.44
1:I:90:GLU:OE2	1:I:96:ARG:NE	2.50	0.44
1:J:106:GLN:C	1:J:108:THR:H	2.18	0.44
1:A:42:HIS:HD1	1:A:50:OCS:CB	2.31	0.44
1:G:115:LEU:O	1:G:125:VAL:HG23	2.16	0.44
1:C:242:TYR:OH	1:D:206:ARG:NH1	2.50	0.44
1:E:126:ARG:HH11	1:E:145:MSE:HA	1.81	0.44
1:I:42:HIS:CE1	1:I:75:SER:CB	2.96	0.44
1:D:231:ARG:O	1:D:235:GLU:HG3	2.17	0.44
1:J:188:PRO:HA	1:J:189:PRO:HD3	1.80	0.44
1:D:146:GLU:OE1	1:D:146:GLU:N	2.44	0.44
1:C:106:GLN:C	1:C:108:THR:N	2.64	0.44
1:B:143:TYR:HD1	1:B:147:LEU:CD1	2.30	0.44
1:C:175:TRP:CD1	1:C:176:PRO:HA	2.53	0.44
1:A:3:GLY:O	1:B:4:SER:HA	2.16	0.44
1:I:117:HIS:ND1	1:J:8:ILE:N	2.64	0.44
1:C:242:TYR:CD2	1:D:214:TRP:CZ2	3.05	0.44
1:I:36:TRP:CD2	1:I:132:ASP:HA	2.53	0.44
1:E:20:ASP:OD2	1:E:86:LYS:CE	2.66	0.44
1:A:7:LEU:HD22	1:B:117:HIS:CD2	2.51	0.44
1:G:55:VAL:O	1:G:59:ARG:HG2	2.18	0.44
1:F:189:PRO:HA	1:F:190:PRO:HD3	1.81	0.44
1:A:122:THR:O	1:A:123:HIS:HB2	2.17	0.44
1:J:220:ARG:HH11	1:J:220:ARG:HB2	1.82	0.44
1:B:119:GLU:O	1:B:120:SER:OG	2.27	0.44
1:B:106:GLN:CG	1:C:122:THR:HA	2.48	0.44
3:D:2003:IPA:C3	1:E:84:LYS:HZ3	2.30	0.44
1:F:92:HIS:NE2	3:F:2007:IPA:H33	2.33	0.44
1:J:13:PRO:HB2	1:J:15:MSE:HE3	1.99	0.44
1:I:199:ARG:CD	4:I:271:HOH:O	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:13:PRO:HB2	1:G:15:MSE:HE3	2.00	0.44
1:I:67:LEU:O	1:I:162:LYS:HE2	2.18	0.44
1:J:72:ILE:HG23	1:J:72:ILE:O	2.18	0.44
1:B:138:ARG:NH2	1:B:165:ASP:OD1	2.50	0.44
1:I:50:OCS:OD2	1:I:126:ARG:NH2	2.50	0.44
1:I:49:VAL:HG12	1:I:126:ARG:NH2	2.33	0.44
1:I:63:ASP:OD2	1:I:228:ARG:NH2	2.50	0.44
1:J:14:GLU:O	1:J:15:MSE:HB3	2.18	0.44
1:J:202:SER:C	1:J:204:GLN:N	2.46	0.44
1:H:5:ILE:CG2	1:H:6:PRO:CD	2.95	0.44
1:E:42:HIS:HD2	1:E:74:LEU:O	2.01	0.44
1:B:128:VAL:O	1:B:140:MSE:HA	2.18	0.44
1:C:175:TRP:CG	1:C:176:PRO:HA	2.53	0.44
1:A:199:ARG:O	1:A:200:MSE:HE3	2.17	0.43
1:G:175:TRP:CD1	1:G:176:PRO:HA	2.53	0.43
1:E:175:TRP:CG	1:E:176:PRO:HA	2.53	0.43
1:H:60:ARG:HG3	1:H:60:ARG:HH11	1.82	0.43
1:G:117:HIS:HB2	1:G:125:VAL:HG22	1.98	0.43
1:G:42:HIS:CE1	1:G:54:PHE:HE1	2.36	0.43
1:E:117:HIS:CD2	1:E:125:VAL:HG11	2.52	0.43
1:E:86:LYS:HE2	1:E:97:ILE:HG22	1.99	0.43
1:B:184:GLY:HA2	1:B:216:THR:HG22	2.00	0.43
4:C:302:HOH:O	1:D:150:LEU:CD2	2.65	0.43
1:J:202:SER:C	1:J:204:GLN:H	1.81	0.43
1:J:3:GLY:O	1:J:5:ILE:CD1	2.66	0.43
1:H:4:SER:C	1:H:5:ILE:CD1	2.75	0.43
1:E:86:LYS:HE2	1:E:97:ILE:CG2	2.48	0.43
1:C:48:PRO:HB2	1:D:186:ILE:HG21	2.00	0.43
1:G:36:TRP:CD2	1:G:132:ASP:HA	2.54	0.43
1:B:107:GLY:H	1:C:106:GLN:NE2	2.16	0.43
1:B:143:TYR:CD1	1:B:147:LEU:HD12	2.50	0.43
1:H:220:ARG:NH2	4:H:2083:HOH:O	2.47	0.43
1:G:54:PHE:CE2	1:G:101:ILE:CD1	3.01	0.43
1:D:4:SER:N	1:D:5:ILE:HD12	2.33	0.43
1:D:74:LEU:HD23	1:D:74:LEU:C	2.39	0.43
1:E:74:LEU:HD23	1:E:74:LEU:C	2.38	0.43
1:I:20:ASP:HB3	1:I:21:HIS:CD2	2.54	0.43
1:G:199:ARG:C	1:G:201:GLU:H	2.22	0.43
1:C:210:TRP:CZ3	1:C:211:TRP:HB3	2.53	0.43
1:I:48:PRO:CG	1:J:189:PRO:HG3	2.48	0.43
1:H:239:LYS:HB3	1:H:239:LYS:NZ	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:THR:CG2	1:A:125:VAL:N	2.81	0.43
3:D:2003:IPA:H11	4:E:2052:HOH:O	2.18	0.43
1:D:119:GLU:OE2	1:D:145:MSE:HB2	2.18	0.43
1:J:50:OCS:SG	1:J:126:ARG:NH2	2.91	0.43
1:A:144:PRO:HG2	1:A:147:LEU:CB	2.48	0.43
1:G:54:PHE:CE2	1:G:101:ILE:HD11	2.50	0.43
1:E:3:GLY:O	1:E:5:ILE:HD12	2.19	0.43
1:H:205:TYR:O	1:H:206:ARG:C	2.57	0.43
1:D:75:SER:HB3	1:D:82:HIS:HE1	1.82	0.43
1:E:99:PHE:HB2	1:E:100:PRO:HD2	2.01	0.43
1:A:74:LEU:HD23	1:A:75:SER:N	2.33	0.43
1:E:204:GLN:CA	1:E:204:GLN:NE2	2.78	0.43
1:H:210:TRP:CZ3	1:H:211:TRP:HB3	2.54	0.43
1:J:163:LEU:HD23	1:J:163:LEU:HA	1.76	0.43
1:I:53:GLU:HG2	1:J:173:ALA:HB2	2.00	0.43
1:G:125:VAL:HG12	1:G:126:ARG:N	2.34	0.43
1:F:117:HIS:CB	1:F:125:VAL:HG21	2.47	0.43
1:H:124:THR:CG2	1:H:125:VAL:N	2.82	0.43
3:H:2009:IPA:H33	1:I:88:TRP:HD1	1.84	0.43
1:I:117:HIS:CE1	1:J:140:MSE:CE	2.95	0.43
1:J:5:ILE:CG2	1:J:6:PRO:O	2.65	0.43
1:D:117:HIS:CD2	1:D:125:VAL:HG11	2.54	0.43
1:B:139:THR:HG22	1:B:140:MSE:N	2.34	0.43
1:A:122:THR:HA	1:J:106:GLN:HG2	2.01	0.43
1:I:156:ARG:HD2	1:I:175:TRP:O	2.19	0.43
1:I:150:LEU:HD22	4:J:2025:HOH:O	2.17	0.43
1:I:48:PRO:HD2	4:I:274:HOH:O	2.18	0.43
1:J:35:LYS:HD3	1:J:70:ASP:OD2	2.19	0.43
1:I:61:TYR:HD2	1:I:71:LEU:HD12	1.83	0.43
1:H:190:PRO:HB3	1:H:195:GLN:HB3	2.02	0.42
1:J:4:SER:C	1:J:5:ILE:HD12	2.38	0.42
1:E:200:MSE:CG	1:E:201:GLU:OE1	2.64	0.42
1:B:200:MSE:HE3	1:B:200:MSE:O	2.19	0.42
1:J:104:ASP:N	1:J:105:PRO:HD3	2.34	0.42
1:H:72:ILE:HG13	1:H:100:PRO:HG2	2.01	0.42
1:A:124:THR:HG22	1:A:125:VAL:N	2.34	0.42
1:D:117:HIS:HB2	1:D:125:VAL:HG11	2.01	0.42
1:D:185:LEU:HA	1:D:185:LEU:HD23	1.65	0.42
1:A:96:ARG:NH2	1:I:197:ARG:HE	2.17	0.42
1:J:128:VAL:HG23	1:J:149:ARG:HH11	1.84	0.42
1:J:7:LEU:HB2	1:J:10:GLU:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:36:TRP:CD2	1:B:132:ASP:HA	2.54	0.42
1:F:41:SER:HB2	1:F:124:THR:HG21	2.01	0.42
1:C:4:SER:HA	1:D:4:SER:HA	2.01	0.42
1:E:106:GLN:HE21	1:E:106:GLN:CA	2.30	0.42
1:E:186:ILE:HG21	1:F:48:PRO:HG2	2.01	0.42
1:H:90:GLU:OE2	1:H:96:ARG:NE	2.36	0.42
1:J:200:MSE:O	1:J:201:GLU:O	2.38	0.42
1:F:125:VAL:CG1	1:F:126:ARG:H	2.32	0.42
1:C:74:LEU:HD23	1:C:75:SER:N	2.34	0.42
1:E:117:HIS:HB2	1:E:125:VAL:CG1	2.48	0.42
1:F:161:LEU:HD12	1:F:161:LEU:HA	1.82	0.42
1:J:76:VAL:O	1:J:76:VAL:HG12	2.19	0.42
1:G:107:GLY:O	1:G:111:ARG:HG3	2.20	0.42
1:E:5:ILE:HB	1:F:5:ILE:HD13	2.01	0.42
1:C:3:GLY:C	1:C:5:ILE:HD12	2.39	0.42
1:A:47:THR:HA	1:A:48:PRO:HD3	1.81	0.42
1:J:191:THR:H	1:J:195:GLN:NE2	2.17	0.42
1:C:70:ASP:OD1	4:C:284:HOH:O	2.21	0.42
1:G:190:PRO:HB3	1:G:195:GLN:HB3	2.02	0.42
1:I:107:GLY:O	1:I:111:ARG:N	2.31	0.42
1:F:117:HIS:HB2	4:F:2047:HOH:O	2.19	0.42
1:F:125:VAL:CG1	1:F:126:ARG:N	2.81	0.42
1:E:126:ARG:HG3	1:E:126:ARG:HH11	1.83	0.42
1:I:146:GLU:OE1	1:I:146:GLU:N	2.45	0.42
1:F:126:ARG:NH1	1:F:145:MSE:O	2.52	0.42
1:H:16:GLU:HG2	1:H:25:LYS:HG3	2.01	0.42
1:B:96:ARG:NH2	1:D:197:ARG:HE	2.18	0.42
1:F:76:VAL:CG1	1:G:105:PRO:O	2.68	0.42
1:E:84:LYS:HD2	1:E:84:LYS:HA	1.90	0.42
1:D:55:VAL:O	1:D:59:ARG:HG2	2.19	0.42
1:F:239:LYS:O	1:F:240:LEU:HB2	2.20	0.42
1:I:134:ARG:HB2	1:I:134:ARG:HE	1.73	0.42
1:H:191:THR:H	1:H:195:GLN:HE22	1.64	0.42
1:B:59:ARG:NH1	1:B:59:ARG:HG3	2.32	0.42
1:E:223:VAL:HG12	1:E:227:ARG:NH1	2.34	0.42
1:B:120:SER:HA	4:B:2064:HOH:O	2.20	0.42
1:A:146:GLU:OE1	1:A:146:GLU:N	2.45	0.42
1:C:59:ARG:HH11	1:D:179:GLU:CG	2.33	0.42
1:C:128:VAL:O	1:C:140:MSE:HA	2.20	0.42
1:E:76:VAL:O	1:E:105:PRO:HA	2.18	0.42
1:D:198:ALA:O	1:D:200:MSE:O	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:147:LEU:HD21	1:H:160:ALA:HB3	2.02	0.41
1:D:117:HIS:CB	1:D:125:VAL:HG11	2.50	0.41
1:D:163:LEU:HA	1:D:163:LEU:HD23	1.85	0.41
1:A:8:ILE:HG13	1:A:140:MSE:HE2	2.02	0.41
1:B:200:MSE:CE	1:B:200:MSE:O	2.68	0.41
1:C:241:LEU:N	1:C:241:LEU:HD23	2.35	0.41
1:D:20:ASP:HB2	1:D:101:ILE:H	1.84	0.41
1:H:111:ARG:HE	1:H:116:LEU:CD2	2.31	0.41
1:J:156:ARG:HD3	1:J:230:LEU:HD11	2.02	0.41
1:J:19:THR:HG21	1:J:24:ILE:HD12	2.02	0.41
1:C:116:LEU:HD12	1:C:116:LEU:HA	1.76	0.41
1:G:153:GLU:O	1:G:157:ILE:HG13	2.20	0.41
1:D:105:PRO:HB2	1:E:122:THR:HB	2.02	0.41
1:I:157:ILE:O	1:I:161:LEU:HB2	2.20	0.41
1:C:14:GLU:CG	1:C:25:LYS:HE2	2.50	0.41
1:C:39:LEU:C	1:C:39:LEU:HD23	2.41	0.41
1:G:56:SER:OG	1:G:151:VAL:HG21	2.19	0.41
1:A:206:ARG:HH11	1:A:215:ASP:HA	1.86	0.41
1:F:106:GLN:HE21	1:F:106:GLN:HA	1.85	0.41
1:H:122:THR:O	1:H:123:HIS:HB2	2.19	0.41
1:G:186:ILE:HD13	1:H:48:PRO:HB2	2.03	0.41
1:I:48:PRO:HG3	1:J:189:PRO:HG3	2.02	0.41
1:C:214:TRP:CD1	1:C:214:TRP:N	2.88	0.41
1:C:157:ILE:O	1:C:161:LEU:HB2	2.21	0.41
1:A:39:LEU:HD23	1:A:39:LEU:C	2.40	0.41
1:H:128:VAL:O	1:H:140:MSE:HA	2.20	0.41
1:H:178:ASN:HD21	1:H:180:ILE:HB	1.84	0.41
1:C:119:GLU:OE1	1:D:8:ILE:HG21	2.20	0.41
1:F:104:ASP:N	1:F:105:PRO:HD3	2.36	0.41
1:D:36:TRP:CD2	1:D:132:ASP:HA	2.55	0.41
1:D:199:ARG:HD2	4:D:2053:HOH:O	2.20	0.41
1:D:4:SER:CA	1:D:5:ILE:HD12	2.51	0.41
1:E:144:PRO:HG2	1:E:147:LEU:CB	2.50	0.41
1:I:144:PRO:HD3	1:J:139:THR:HG1	1.86	0.41
1:E:117:HIS:CB	1:E:125:VAL:HG11	2.51	0.41
1:I:189:PRO:HA	1:I:190:PRO:HD3	1.92	0.41
1:B:220:ARG:O	1:B:224:GLU:HG3	2.20	0.41
1:B:7:LEU:HB2	1:B:10:GLU:HG3	2.02	0.41
1:C:201:GLU:O	1:C:202:SER:CB	2.68	0.41
1:I:7:LEU:HB3	1:J:117:HIS:CG	2.56	0.41
1:E:48:PRO:HD3	1:F:189:PRO:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:125:VAL:H	1:I:125:VAL:HG23	1.42	0.41
1:A:125:VAL:CG1	1:A:126:ARG:N	2.81	0.41
1:H:5:ILE:CG2	1:H:6:PRO:N	2.84	0.41
1:C:59:ARG:HH11	1:D:179:GLU:HG2	1.86	0.41
1:E:42:HIS:HE2	1:E:75:SER:CB	2.30	0.41
1:D:103:ALA:C	1:D:105:PRO:HD3	2.41	0.41
1:B:139:THR:CG2	1:B:140:MSE:N	2.84	0.41
1:C:144:PRO:HD3	1:D:139:THR:OG1	2.21	0.41
1:A:188:PRO:HA	1:A:189:PRO:HD3	1.81	0.41
1:C:86:LYS:HE2	1:C:97:ILE:HG22	2.03	0.41
1:J:193:GLU:HB3	1:J:197:ARG:HH12	1.86	0.41
1:A:42:HIS:HD1	1:A:50:OCS:HB2	1.85	0.41
1:A:14:GLU:O	1:A:15:MSE:HB3	2.21	0.41
1:E:70:ASP:OD1	4:E:2021:HOH:O	2.21	0.41
1:H:93:ILE:HG22	1:H:95:VAL:HG12	2.01	0.41
1:C:191:THR:H	1:C:195:GLN:NE2	2.19	0.41
1:I:116:LEU:HA	1:I:116:LEU:HD12	1.80	0.41
1:J:200:MSE:O	1:J:201:GLU:C	2.60	0.41
1:I:178:ASN:ND2	1:I:180:ILE:N	2.65	0.41
1:C:42:HIS:CD2	1:C:75:SER:HB2	2.54	0.41
1:J:117:HIS:CB	1:J:125:VAL:HG11	2.51	0.41
1:J:150:LEU:HD23	4:J:2008:HOH:O	2.19	0.41
1:I:189:PRO:HG3	1:J:48:PRO:HD3	2.03	0.41
1:E:176:PRO:HG2	1:E:227:ARG:HG3	2.03	0.41
1:B:13:PRO:HB2	1:B:15:MSE:HE3	2.03	0.41
1:E:208:LEU:HD23	1:E:208:LEU:HA	1.91	0.41
1:C:103:ALA:C	1:C:105:PRO:HD3	2.41	0.41
1:F:3:GLY:O	1:F:5:ILE:CD1	2.69	0.40
1:F:39:LEU:HD23	1:F:40:PHE:N	2.36	0.40
1:I:139:THR:OG1	1:J:144:PRO:HD3	2.21	0.40
1:F:20:ASP:HB2	1:F:101:ILE:H	1.85	0.40
1:G:161:LEU:HA	1:G:161:LEU:HD12	1.90	0.40
1:G:76:VAL:O	1:G:76:VAL:HG12	2.21	0.40
1:G:117:HIS:CG	1:H:7:LEU:HB3	2.56	0.40
1:C:93:ILE:HG22	1:C:95:VAL:CG1	2.49	0.40
1:F:5:ILE:HG13	1:F:114:GLY:HA3	2.03	0.40
1:C:59:ARG:NH1	1:D:179:GLU:HG2	2.36	0.40
1:C:41:SER:HB2	1:C:124:THR:HG21	2.03	0.40
1:D:144:PRO:HG2	1:D:147:LEU:CB	2.51	0.40
1:D:143:TYR:CD1	1:D:147:LEU:HD12	2.57	0.40
1:A:179:GLU:O	1:B:240:LEU:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:239:LYS:O	1:J:240:LEU:HB2	2.22	0.40
1:E:236:LYS:HA	1:F:177:ASN:OD1	2.20	0.40
1:J:40:PHE:HZ	1:J:99:PHE:CE2	2.40	0.40
1:G:61:TYR:HD2	1:G:71:LEU:HD12	1.86	0.40
1:I:124:THR:HG22	1:I:125:VAL:O	2.22	0.40
1:G:119:GLU:OE2	1:G:145:MSE:HB2	2.22	0.40
1:D:41:SER:HA	1:D:74:LEU:O	2.21	0.40
1:A:36:TRP:CD2	1:A:132:ASP:HA	2.57	0.40
1:E:239:LYS:HB3	1:E:239:LYS:HZ3	1.86	0.40
1:J:40:PHE:N	1:J:40:PHE:CD2	2.88	0.40
1:B:36:TRP:CD1	1:B:162:LYS:HE3	2.57	0.40
4:A:1048:HOH:O	3:J:2001:IPA:H11	2.22	0.40
1:F:107:GLY:HA3	1:G:106:GLN:HE22	1.86	0.40
1:A:189:PRO:HA	1:A:190:PRO:HD3	1.84	0.40
1:B:125:VAL:HG12	1:B:126:ARG:N	2.36	0.40
1:G:231:ARG:HG3	1:G:231:ARG:NH1	2.37	0.40
1:F:175:TRP:CD1	1:F:176:PRO:HA	2.56	0.40
1:E:67:LEU:O	1:E:162:LYS:HE2	2.21	0.40
1:F:199:ARG:C	1:F:201:GLU:N	2.74	0.40
1:C:72:ILE:O	1:C:72:ILE:HG23	2.22	0.40
1:E:116:LEU:HA	1:E:116:LEU:HD12	1.95	0.40
1:E:128:VAL:O	1:E:140:MSE:HA	2.22	0.40
1:C:67:LEU:O	1:C:162:LYS:HE2	2.22	0.40
1:F:59:ARG:HE	1:F:59:ARG:HB3	1.52	0.40
1:H:185:LEU:HD23	1:H:185:LEU:HA	1.81	0.40
1:H:79:VAL:O	1:H:83:ILE:HG13	2.22	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:231:ARG:NH2	4:B:2033:HOH:O[1_544]	2.09	0.11

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	238/250 (95%)	221 (93%)	13 (6%)	4 (2%)	11	10
1	B	238/250 (95%)	222 (93%)	12 (5%)	4 (2%)	11	10
1	C	238/250 (95%)	223 (94%)	7 (3%)	8 (3%)	5	2
1	D	239/250 (96%)	222 (93%)	8 (3%)	9 (4%)	4	2
1	E	237/250 (95%)	222 (94%)	8 (3%)	7 (3%)	5	3
1	F	237/250 (95%)	224 (94%)	8 (3%)	5 (2%)	9	7
1	G	239/250 (96%)	222 (93%)	11 (5%)	6 (2%)	7	5
1	H	237/250 (95%)	223 (94%)	9 (4%)	5 (2%)	9	7
1	I	238/250 (95%)	223 (94%)	11 (5%)	4 (2%)	11	10
1	J	237/250 (95%)	214 (90%)	18 (8%)	5 (2%)	9	7
All	All	2378/2500 (95%)	2216 (93%)	105 (4%)	57 (2%)	7	5

All (57) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	204	GLN
1	C	107	GLY
1	C	201	GLU
1	C	202	SER
1	C	205	TYR
1	D	202	SER
1	D	203	GLY
1	E	202	SER
1	E	203	GLY
1	F	107	GLY
1	G	122	THR
1	J	201	GLU
1	J	204	GLN
1	A	120	SER
1	B	107	GLY
1	B	122	THR
1	B	203	GLY
1	C	122	THR
1	C	204	GLN
1	D	201	GLU
1	E	120	SER
1	E	122	THR

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Mol	Chain	Res	Type
1	E	123	HIS
1	E	206	ARG
1	F	120	SER
1	G	107	GLY
1	G	120	SER
1	G	202	SER
1	H	120	SER
1	H	203	GLY
1	I	107	GLY
1	A	122	THR
1	B	120	SER
1	D	120	SER
1	D	122	THR
1	D	123	HIS
1	E	200	MSE
1	F	202	SER
1	F	206	ARG
1	G	123	HIS
1	H	124	THR
1	I	122	THR
1	I	240	LEU
1	A	123	HIS
1	C	48	PRO
1	H	123	HIS
1	J	123	HIS
1	C	123	HIS
1	G	205	TYR
1	I	123	HIS
1	J	205	TYR
1	D	107	GLY
1	F	240	LEU
1	J	120	SER
1	H	48	PRO
1	D	182	GLY
1	D	48	PRO

5.3.2 Protein sidechains (i)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	207/210 (99%)	184 (89%)	23 (11%)	8 8
1	B	207/210 (99%)	187 (90%)	20 (10%)	10 12
1	C	207/210 (99%)	188 (91%)	19 (9%)	11 13
1	D	208/210 (99%)	191 (92%)	17 (8%)	14 17
1	E	206/210 (98%)	189 (92%)	17 (8%)	14 17
1	F	206/210 (98%)	189 (92%)	17 (8%)	14 17
1	G	208/210 (99%)	193 (93%)	15 (7%)	18 22
1	H	206/210 (98%)	190 (92%)	16 (8%)	16 19
1	I	207/210 (99%)	188 (91%)	19 (9%)	11 13
1	J	206/210 (98%)	190 (92%)	16 (8%)	16 19
All	All	2068/2100 (98%)	1889 (91%)	179 (9%)	13 15

All (179) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	11	ARG
1	A	14	GLU
1	A	24	ILE
1	A	28	ASP
1	A	62	GLU
1	A	95	VAL
1	A	97	ILE
1	A	98	PRO
1	A	122	THR
1	A	126	ARG
1	A	147	LEU
1	A	150	LEU
1	A	200	MSE
1	A	204	GLN
1	A	205	TYR
1	A	206	ARG
1	A	212	PHE
1	A	217	PRO
1	A	230	LEU
1	A	235	GLU
1	A	239	LYS
1	A	241	LEU

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Mol	Chain	Res	Type
1	B	11	ARG
1	B	28	ASP
1	B	70	ASP
1	B	95	VAL
1	B	97	ILE
1	B	116	LEU
1	B	122	THR
1	B	134	ARG
1	B	150	LEU
1	B	161	LEU
1	B	176	PRO
1	B	179	GLU
1	B	200	MSE
1	B	201	GLU
1	B	205	TYR
1	B	206	ARG
1	B	212	PHE
1	B	217	PRO
1	B	230	LEU
1	B	242	TYR
1	C	11	ARG
1	C	27	PRO
1	C	28	ASP
1	C	70	ASP
1	C	95	VAL
1	C	97	ILE
1	C	122	THR
1	C	150	LEU
1	C	161	LEU
1	C	199	ARG
1	C	200	MSE
1	C	201	GLU
1	C	206	ARG
1	C	212	PHE
1	C	230	LEU
1	C	235	GLU
1	C	239	LYS
1	C	241	LEU
1	C	242	TYR
1	D	11	ARG
1	D	14	GLU
1	D	20	ASP

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Mol	Chain	Res	Type
1	D	28	ASP
1	D	70	ASP
1	D	95	VAL
1	D	122	THR
1	D	134	ARG
1	D	150	LEU
1	D	161	LEU
1	D	183	GLU
1	D	201	GLU
1	D	204	GLN
1	D	205	TYR
1	D	212	PHE
1	D	242	TYR
1	D	243	GLU
1	E	20	ASP
1	E	28	ASP
1	E	42	HIS
1	E	70	ASP
1	E	97	ILE
1	E	150	LEU
1	E	161	LEU
1	E	199	ARG
1	E	200	MSE
1	E	201	GLU
1	E	205	TYR
1	E	212	PHE
1	E	217	PRO
1	E	220	ARG
1	E	224	GLU
1	E	228	ARG
1	E	230	LEU
1	F	14	GLU
1	F	20	ASP
1	F	28	ASP
1	F	35	LYS
1	F	59	ARG
1	F	66	ARG
1	F	97	ILE
1	F	126	ARG
1	F	138	ARG
1	F	150	LEU
1	F	161	LEU

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Mol	Chain	Res	Type
1	F	200	MSE
1	F	201	GLU
1	F	205	TYR
1	F	212	PHE
1	F	224	GLU
1	F	230	LEU
1	G	11	ARG
1	G	20	ASP
1	G	28	ASP
1	G	70	ASP
1	G	97	ILE
1	G	126	ARG
1	G	150	LEU
1	G	161	LEU
1	G	202	SER
1	G	205	TYR
1	G	206	ARG
1	G	212	PHE
1	G	228	ARG
1	G	239	LYS
1	G	242	TYR
1	H	28	ASP
1	H	59	ARG
1	H	70	ASP
1	H	95	VAL
1	H	98	PRO
1	H	122	THR
1	H	126	ARG
1	H	161	LEU
1	H	200	MSE
1	H	201	GLU
1	H	202	SER
1	H	204	GLN
1	H	206	ARG
1	H	212	PHE
1	H	230	LEU
1	H	239	LYS
1	I	11	ARG
1	I	20	ASP
1	I	28	ASP
1	I	70	ASP
1	I	95	VAL

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Mol	Chain	Res	Type
1	I	97	ILE
1	I	117	HIS
1	I	122	THR
1	I	150	LEU
1	I	176	PRO
1	I	200	MSE
1	I	202	SER
1	I	204	GLN
1	I	212	PHE
1	I	217	PRO
1	I	230	LEU
1	I	239	LYS
1	I	241	LEU
1	I	242	TYR
1	J	5	ILE
1	J	11	ARG
1	J	28	ASP
1	J	70	ASP
1	J	79	VAL
1	J	95	VAL
1	J	120	SER
1	J	150	LEU
1	J	161	LEU
1	J	176	PRO
1	J	200	MSE
1	J	202	SER
1	J	204	GLN
1	J	205	TYR
1	J	212	PHE
1	J	239	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	HIS
1	A	178	ASN
1	A	195	GLN
1	A	204	GLN
1	B	92	HIS
1	B	106	GLN
1	B	178	ASN
1	B	195	GLN

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Mol	Chain	Res	Type
1	B	204	GLN
1	C	106	GLN
1	C	178	ASN
1	C	195	GLN
1	C	204	GLN
1	D	42	HIS
1	D	65	GLN
1	D	92	HIS
1	D	106	GLN
1	D	178	ASN
1	D	195	GLN
1	D	204	GLN
1	E	21	HIS
1	E	42	HIS
1	E	92	HIS
1	E	106	GLN
1	E	178	ASN
1	E	195	GLN
1	E	204	GLN
1	F	42	HIS
1	F	106	GLN
1	F	178	ASN
1	F	195	GLN
1	F	204	GLN
1	G	42	HIS
1	G	92	HIS
1	G	106	GLN
1	G	178	ASN
1	G	195	GLN
1	G	204	GLN
1	H	42	HIS
1	H	106	GLN
1	H	123	HIS
1	H	178	ASN
1	H	195	GLN
1	H	204	GLN
1	I	42	HIS
1	I	65	GLN
1	I	117	HIS
1	I	178	ASN
1	I	195	GLN
1	J	92	HIS

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Mol	Chain	Res	Type
1	J	123	HIS
1	J	178	ASN
1	J	195	GLN
1	J	204	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

10 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	OCS	A	50	1	7,8,9	2.06	2 (28%)	7,11,13	1.69	2 (28%)
1	OCS	B	50	1	7,8,9	2.13	2 (28%)	7,11,13	1.66	2 (28%)
1	OCS	C	50	1	7,8,9	4.81	4 (57%)	7,11,13	2.18	2 (28%)
1	OCS	D	50	1	7,8,9	1.79	2 (28%)	7,11,13	2.38	2 (28%)
1	OCS	E	50	1	7,8,9	2.57	3 (42%)	7,11,13	3.33	5 (71%)
1	OCS	F	50	1	7,8,9	2.20	3 (42%)	7,11,13	3.20	4 (57%)
1	OCS	G	50	1	7,8,9	2.12	3 (42%)	7,11,13	2.61	4 (57%)
1	OCS	H	50	1	7,8,9	3.57	4 (57%)	7,11,13	2.38	2 (28%)
1	OCS	I	50	1	7,8,9	3.55	4 (57%)	7,11,13	2.35	4 (57%)
1	OCS	J	50	1	7,8,9	2.88	3 (42%)	7,11,13	1.68	2 (28%)

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
1	OCS	A	50	1	-	0/4/7/9	0/0/0/0
1	OCS	B	50	1	-	0/4/7/9	0/0/0/0
1	OCS	C	50	1	-	0/4/7/9	0/0/0/0
1	OCS	D	50	1	-	0/4/7/9	0/0/0/0
1	OCS	E	50	1	-	0/4/7/9	0/0/0/0
1	OCS	F	50	1	-	0/4/7/9	0/0/0/0
1	OCS	G	50	1	-	0/4/7/9	0/0/0/0
1	OCS	H	50	1	-	0/4/7/9	0/0/0/0
1	OCS	I	50	1	-	0/4/7/9	0/0/0/0
1	OCS	J	50	1	-	0/4/7/9	0/0/0/0

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	50	OCS	OD2-SG	2.00	1.51	1.46
1	H	50	OCS	OD3-SG	2.09	1.51	1.45
1	G	50	OCS	OD1-SG	2.30	1.52	1.45
1	F	50	OCS	OD3-SG	2.30	1.52	1.45
1	D	50	OCS	CB-SG	2.51	1.81	1.77
1	F	50	OCS	OD1-SG	2.52	1.53	1.45
1	B	50	OCS	OD1-SG	2.77	1.53	1.45
1	I	50	OCS	OD3-SG	2.89	1.54	1.45
1	D	50	OCS	OD1-SG	2.96	1.54	1.45
1	E	50	OCS	OD2-SG	3.33	1.55	1.46
1	J	50	OCS	OD2-SG	3.43	1.55	1.46
1	I	50	OCS	OD2-SG	3.64	1.55	1.46
1	H	50	OCS	OD2-SG	3.67	1.55	1.46
1	A	50	OCS	OD1-SG	3.74	1.56	1.45
1	E	50	OCS	CB-SG	3.76	1.83	1.77
1	A	50	OCS	CB-SG	3.83	1.83	1.77
1	E	50	OCS	OD1-SG	4.03	1.57	1.45
1	G	50	OCS	CB-SG	4.13	1.84	1.77
1	F	50	OCS	CB-SG	4.25	1.84	1.77
1	H	50	OCS	OD1-SG	4.38	1.58	1.45
1	C	50	OCS	OD3-SG	4.39	1.58	1.45
1	J	50	OCS	OD1-SG	4.42	1.59	1.45
1	B	50	OCS	CB-SG	4.53	1.84	1.77
1	J	50	OCS	CB-SG	4.62	1.84	1.77
1	C	50	OCS	OD1-SG	5.54	1.62	1.45
1	I	50	OCS	CB-SG	5.61	1.86	1.77
1	I	50	OCS	OD1-SG	5.77	1.63	1.45
1	C	50	OCS	OD2-SG	6.88	1.64	1.46
1	H	50	OCS	CB-SG	7.12	1.88	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	50	OCS	CB-SG	7.91	1.89	1.77

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	50	OCS	OD1-SG-CB	-4.88	102.83	106.94
1	C	50	OCS	OD3-SG-CB	-4.10	103.49	106.94
1	G	50	OCS	OD1-SG-CB	-3.69	103.83	106.94
1	D	50	OCS	OD1-SG-CB	-3.38	104.09	106.94
1	B	50	OCS	O-C-CA	-2.93	117.85	125.49
1	F	50	OCS	CB-CA-C	-2.93	103.44	111.46
1	J	50	OCS	CB-CA-C	-2.91	103.49	111.46
1	I	50	OCS	CB-CA-C	-2.88	103.57	111.46
1	E	50	OCS	O-C-CA	-2.81	118.16	125.49
1	G	50	OCS	O-C-CA	-2.76	118.29	125.49
1	A	50	OCS	OD1-SG-CB	-2.67	104.69	106.94
1	A	50	OCS	CB-CA-C	-2.57	104.41	111.46
1	E	50	OCS	CB-CA-C	-2.17	105.51	111.46
1	E	50	OCS	OD1-SG-CB	-2.15	105.13	106.94
1	I	50	OCS	O-C-CA	-2.14	119.91	125.49
1	F	50	OCS	O-C-CA	-2.07	120.09	125.49
1	J	50	OCS	OD3-SG-CB	2.02	108.65	106.94
1	G	50	OCS	OD2-SG-OD1	2.21	116.76	111.61
1	E	50	OCS	OD2-SG-OD1	2.41	117.21	111.61
1	F	50	OCS	OD2-SG-OD3	2.44	117.28	111.61
1	B	50	OCS	OD2-SG-OD1	2.58	117.62	111.61
1	H	50	OCS	OD2-SG-OD3	2.84	118.22	111.61
1	I	50	OCS	OD3-SG-CB	3.20	109.64	106.94
1	C	50	OCS	OD2-SG-OD3	3.24	119.14	111.61
1	I	50	OCS	OD2-SG-OD1	3.50	119.75	111.61
1	G	50	OCS	OD3-SG-CB	4.18	110.47	106.94
1	D	50	OCS	OD3-SG-CB	4.41	110.66	106.94
1	F	50	OCS	OD3-SG-CB	7.06	112.89	106.94
1	E	50	OCS	OD3-SG-CB	7.13	112.95	106.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	50	OCS	2	0
1	B	50	OCS	1	0
1	C	50	OCS	1	0
1	D	50	OCS	3	0
1	E	50	OCS	2	0
1	F	50	OCS	3	0
1	G	50	OCS	3	0
1	H	50	OCS	6	0
1	I	50	OCS	2	0
1	J	50	OCS	2	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

11 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	MES	A	1001	-	11,12,12	0.74	0	14,16,16	0.77	0
3	IPA	B	2005	-	3,3,3	0.61	0	3,3,3	1.43	1 (33%)
3	IPA	D	2003	-	3,3,3	0.30	0	3,3,3	1.70	1 (33%)
3	IPA	E	2006	-	3,3,3	0.60	0	3,3,3	1.62	1 (33%)
2	MES	F	1002	-	11,12,12	1.16	0	14,16,16	1.39	2 (14%)
3	IPA	F	2007	-	3,3,3	0.77	0	3,3,3	1.37	1 (33%)
3	IPA	G	2008	-	3,3,3	0.35	0	3,3,3	1.70	1 (33%)
3	IPA	H	2004	-	3,3,3	0.49	0	3,3,3	1.71	1 (33%)
3	IPA	H	2009	-	3,3,3	0.61	0	3,3,3	1.60	1 (33%)
3	IPA	J	2001	-	3,3,3	0.46	0	3,3,3	1.57	1 (33%)
3	IPA	J	2002	-	3,3,3	0.42	0	3,3,3	1.39	1 (33%)

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
2	MES	A	1001	-	-	0/6/14/14	0/1/1/1
3	IPA	B	2005	-	-	0/0/0/0	0/0/0/0
3	IPA	D	2003	-	-	0/0/0/0	0/0/0/0
3	IPA	E	2006	-	-	0/0/0/0	0/0/0/0
2	MES	F	1002	-	-	0/6/14/14	0/1/1/1
3	IPA	F	2007	-	-	0/0/0/0	0/0/0/0
3	IPA	G	2008	-	-	0/0/0/0	0/0/0/0
3	IPA	H	2004	-	-	0/0/0/0	0/0/0/0
3	IPA	H	2009	-	-	0/0/0/0	0/0/0/0
3	IPA	J	2001	-	-	0/0/0/0	0/0/0/0
3	IPA	J	2002	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	1002	MES	O1S-S-C8	-4.28	103.25	106.91
3	G	2008	IPA	C3-C2-C1	-2.91	89.98	113.70
3	D	2003	IPA	C3-C2-C1	-2.83	90.62	113.70
3	H	2004	IPA	C3-C2-C1	-2.80	90.83	113.70
3	E	2006	IPA	C3-C2-C1	-2.75	91.27	113.70
3	H	2009	IPA	C3-C2-C1	-2.73	91.41	113.70
3	J	2001	IPA	C3-C2-C1	-2.68	91.82	113.70
3	B	2005	IPA	C3-C2-C1	-2.44	93.80	113.70
3	J	2002	IPA	C3-C2-C1	-2.37	94.33	113.70
3	F	2007	IPA	C3-C2-C1	-2.35	94.54	113.70
2	F	1002	MES	O2S-S-C8	2.39	108.94	106.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	MES	1	0
3	B	2005	IPA	6	0
3	D	2003	IPA	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	2006	IPA	3	0
3	F	2007	IPA	1	0
3	H	2004	IPA	1	0
3	H	2009	IPA	6	0
3	J	2001	IPA	4	0
3	J	2002	IPA	3	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	236/250 (94%)	-0.35	10 (4%) 40 49	15, 27, 63, 101	0
1	B	236/250 (94%)	-0.33	7 (2%) 54 63	14, 27, 65, 98	0
1	C	236/250 (94%)	-0.29	7 (2%) 54 63	17, 28, 68, 111	0
1	D	237/250 (94%)	-0.18	12 (5%) 32 41	18, 31, 70, 102	0
1	E	235/250 (94%)	-0.21	9 (3%) 44 53	18, 33, 69, 107	0
1	F	235/250 (94%)	-0.32	11 (4%) 35 44	17, 29, 74, 100	0
1	G	237/250 (94%)	-0.21	11 (4%) 36 45	18, 31, 76, 106	0
1	H	235/250 (94%)	-0.27	11 (4%) 35 44	18, 29, 76, 102	0
1	I	236/250 (94%)	-0.18	8 (3%) 49 58	17, 32, 70, 112	0
1	J	235/250 (94%)	-0.20	10 (4%) 39 48	17, 33, 70, 109	0
All	All	2358/2500 (94%)	-0.25	96 (4%) 41 50	14, 30, 71, 112	0

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	202	SER	11.0
1	B	204	GLN	7.2
1	A	204	GLN	7.0
1	I	204	GLN	6.5
1	G	4	SER	6.4
1	A	242	TYR	6.4
1	J	201	GLU	5.8
1	C	201	GLU	5.5
1	J	204	GLN	5.4
1	E	203	GLY	5.4
1	E	238	ALA	5.4
1	D	5	ILE	5.4
1	H	202	SER	5.3

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Mol	Chain	Res	Type	RSRZ
1	E	239	LYS	5.3
1	I	242	TYR	5.2
1	E	205	TYR	4.9
1	E	204	GLN	4.7
1	C	204	GLN	4.5
1	J	203	GLY	4.4
1	G	121	ALA	4.3
1	H	5	ILE	4.3
1	H	204	GLN	4.2
1	J	239	LYS	3.9
1	A	201	GLU	3.8
1	B	239	LYS	3.8
1	G	118	ALA	3.8
1	F	106	GLN	3.6
1	F	202	SER	3.6
1	I	202	SER	3.5
1	D	242	TYR	3.5
1	C	122	THR	3.5
1	D	4	SER	3.5
1	A	202	SER	3.4
1	G	204	GLN	3.4
1	I	205	TYR	3.4
1	H	205	TYR	3.4
1	I	201	GLU	3.4
1	G	5	ILE	3.3
1	D	204	GLN	3.3
1	I	203	GLY	3.2
1	A	203	GLY	3.2
1	F	238	ALA	3.2
1	C	4	SER	3.1
1	E	202	SER	3.1
1	B	202	SER	3.1
1	D	238	ALA	3.0
1	F	239	LYS	3.0
1	F	204	GLN	2.9
1	G	120	SER	2.9
1	E	201	GLU	2.9
1	C	5	ILE	2.9
1	A	220	ARG	2.8
1	G	203	GLY	2.8
1	G	201	GLU	2.8
1	A	198	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	120	SER	2.7
1	H	201	GLU	2.7
1	C	202	SER	2.6
1	E	2	PRO	2.6
1	F	4	SER	2.6
1	A	205	TYR	2.6
1	F	201	GLU	2.5
1	A	122	THR	2.5
1	H	241	LEU	2.5
1	B	203	GLY	2.5
1	H	4	SER	2.5
1	D	121	ALA	2.5
1	F	205	TYR	2.5
1	G	122	THR	2.4
1	J	238	ALA	2.4
1	I	239	LYS	2.4
1	D	203	GLY	2.4
1	H	122	THR	2.4
1	D	239	LYS	2.4
1	D	32	SER	2.3
1	A	206	ARG	2.3
1	J	5	ILE	2.3
1	F	241	LEU	2.3
1	D	201	GLU	2.3
1	J	205	TYR	2.3
1	B	242	TYR	2.2
1	B	238	ALA	2.2
1	C	203	GLY	2.2
1	H	203	GLY	2.2
1	I	122	THR	2.2
1	D	2	PRO	2.2
1	J	122	THR	2.2
1	D	243	GLU	2.2
1	F	2	PRO	2.2
1	F	118	ALA	2.2
1	E	241	LEU	2.1
1	G	2	PRO	2.1
1	J	106	GLN	2.1
1	J	220	ARG	2.0
1	H	239	LYS	2.0
1	H	124	THR	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
1	OCS	H	50	9/10	0.98	0.10	-	24,27,30,40	0
1	OCS	E	50	9/10	0.99	0.09	-	22,27,37,42	0
1	OCS	J	50	9/10	0.98	0.11	-	23,28,36,38	0
1	OCS	I	50	9/10	0.97	0.14	-	27,29,37,37	0
1	OCS	C	50	9/10	0.98	0.12	-	24,25,34,36	0
1	OCS	B	50	9/10	0.98	0.09	-	23,25,33,34	0
1	OCS	G	50	9/10	0.98	0.09	-	23,27,37,47	0
1	OCS	D	50	9/10	0.99	0.10	-	16,26,38,43	0
1	OCS	A	50	9/10	0.98	0.09	-	20,24,36,41	0
1	OCS	F	50	9/10	0.98	0.09	-	20,23,35,36	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	MES	F	1002	12/12	0.89	0.17	4.27	70,75,82,84	0
3	IPA	E	2006	4/4	0.85	0.20	2.61	52,57,61,62	0
3	IPA	F	2007	4/4	0.81	0.21	2.48	39,40,43,45	0
3	IPA	J	2002	4/4	0.94	0.16	1.61	38,39,39,41	0
3	IPA	H	2004	4/4	0.83	0.19	1.33	55,61,61,63	0
2	MES	A	1001	12/12	0.94	0.15	0.88	41,51,65,66	0
3	IPA	G	2008	4/4	0.97	0.12	0.12	31,34,42,46	0
3	IPA	D	2003	4/4	0.95	0.11	-0.28	33,38,40,44	0
3	IPA	B	2005	4/4	0.93	0.10	-0.42	40,42,46,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	IPA	H	2009	4/4	0.96	0.11	-0.58	38,46,47,53	0
3	IPA	J	2001	4/4	0.96	0.10	-0.88	32,38,40,42	0

6.5 Other polymers (i)

There are no such residues in this entry.