



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 10:54 AM UTC

PDB ID : 2CV4 / pdb_00002cv4
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

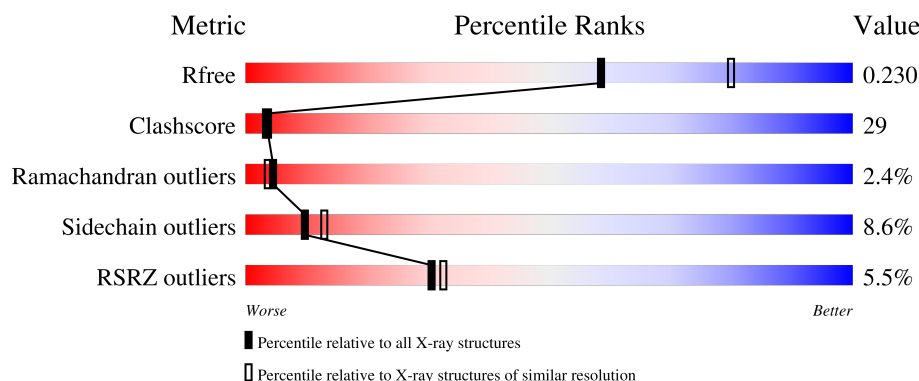
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	250	4% 58% 29% 8% • •
1	B	250	6% 58% 30% 8% • •
1	C	250	6% 56% 29% 10% • •
1	D	250	4% 51% 35% 8% • •
1	E	250	5% 57% 26% 10% • •

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Mol	Chain	Length	Quality of chain
1	F	250	
1	G	250	
1	H	250	
1	I	250	
1	J	250	

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	G	50	-	-	X	-
1	OCS	H	50	-	-	X	-
3	IPA	B	2005	-	-	X	-
3	IPA	D	2003	-	-	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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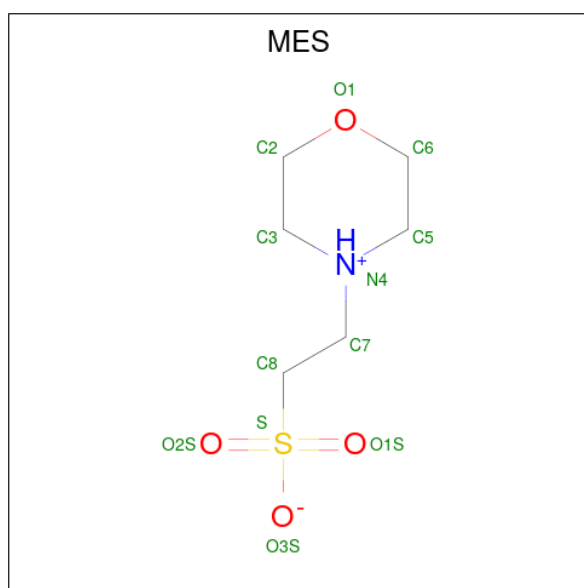
Chain	Residue	Modelled	Actual	Comment	Reference
B	140	MSE	MET	modified residue	UNP Q9Y9L0
B	145	MSE	MET	modified residue	UNP Q9Y9L0
B	200	MSE	MET	modified residue	UNP Q9Y9L0
C	1	MSE	MET	modified residue	UNP Q9Y9L0
C	15	MSE	MET	modified residue	UNP Q9Y9L0
C	50	OCS	CYS	modified residue	UNP Q9Y9L0
C	140	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 (CCD ID: 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 (CCD ID: IPA) (formula: C_3H_8O).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 4 3 1	0	0
3	D	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
3	H	1	Total C O 4 3 1	0	0
3	J	1	Total C O 4 3 1	0	0
3	J	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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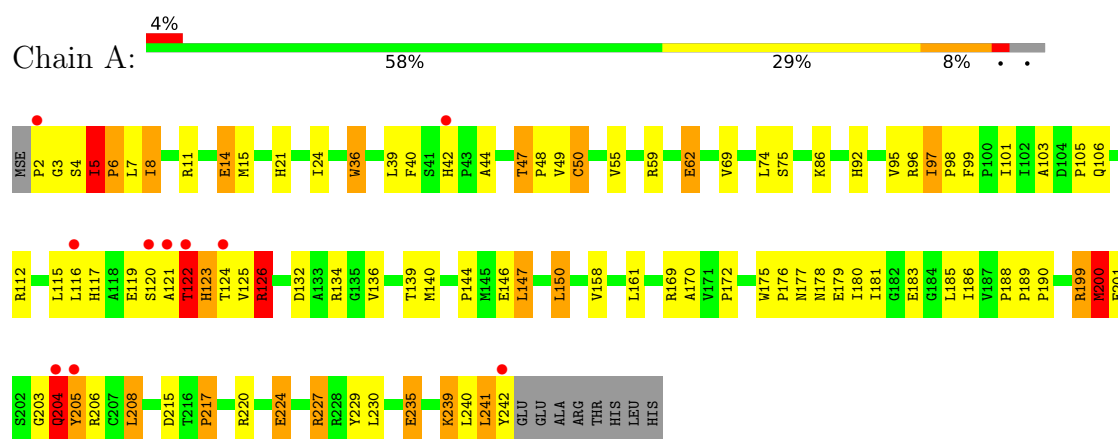
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	66	Total 66	O 66	0	0
4	E	70	Total 70	O 70	0	0
4	F	75	Total 75	O 75	0	0
4	G	85	Total 85	O 85	0	0
4	H	82	Total 82	O 82	0	0
4	I	82	Total 82	O 82	0	0
4	J	92	Total 92	O 92	0	0

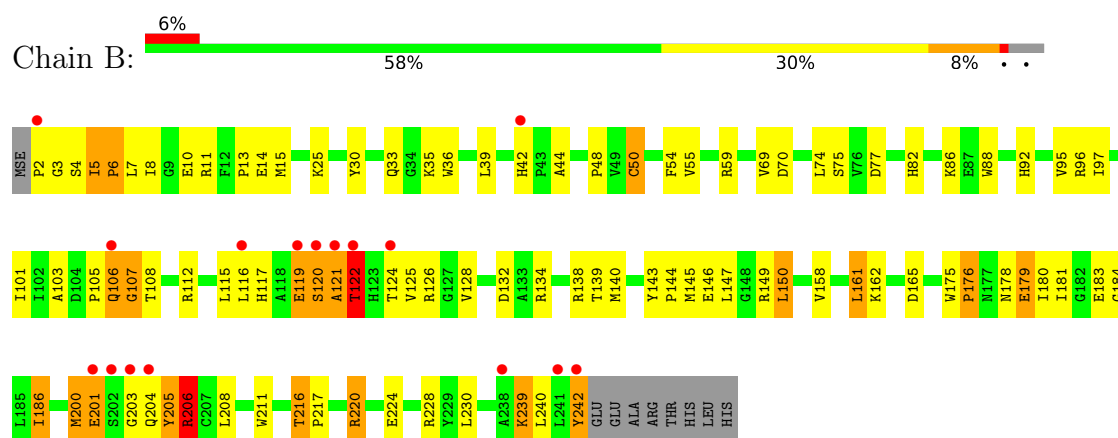
3 Residue-property plots [i](#)

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

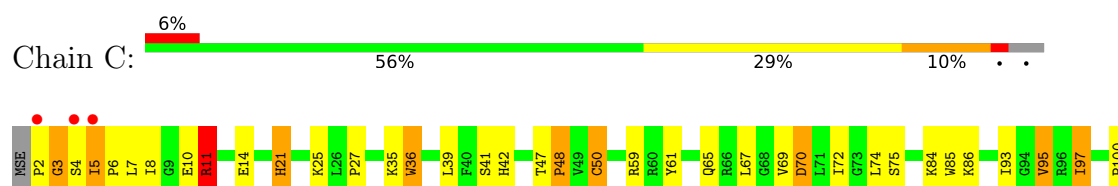
- Molecule 1: peroxiredoxin

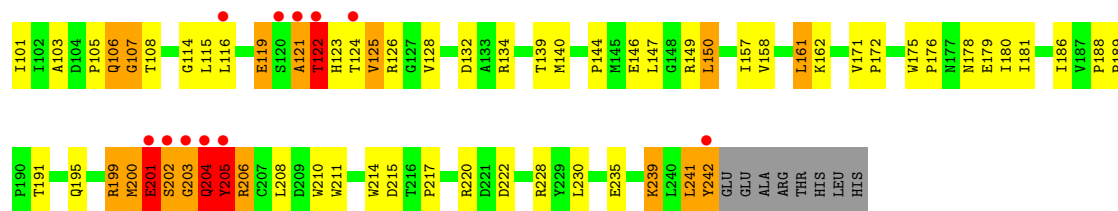


- Molecule 1: peroxiredoxin

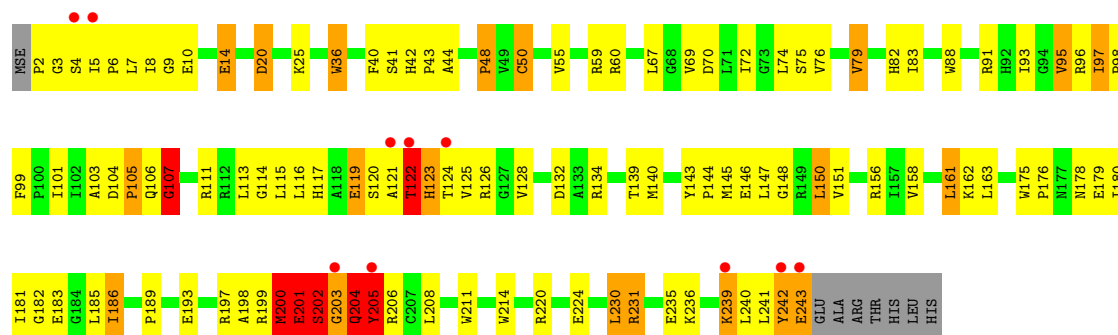


- Molecule 1: peroxiredoxin

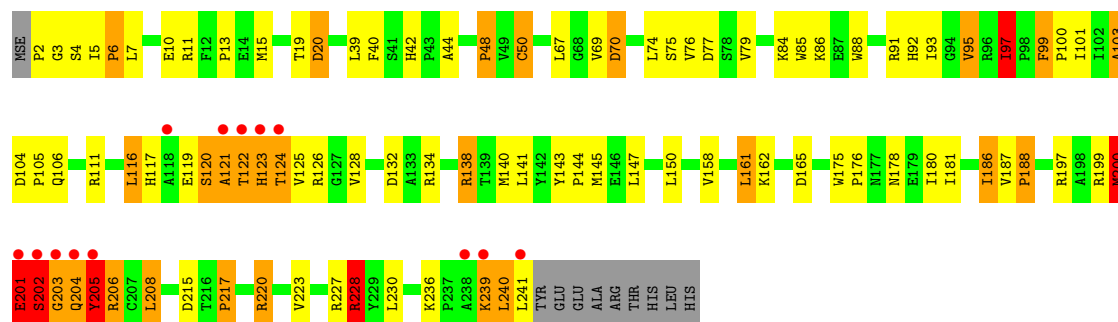




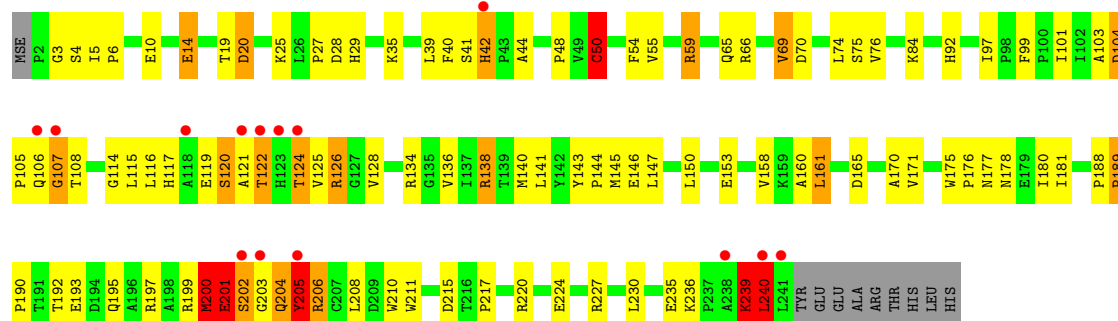
• Molecule 1: peroxiredoxin



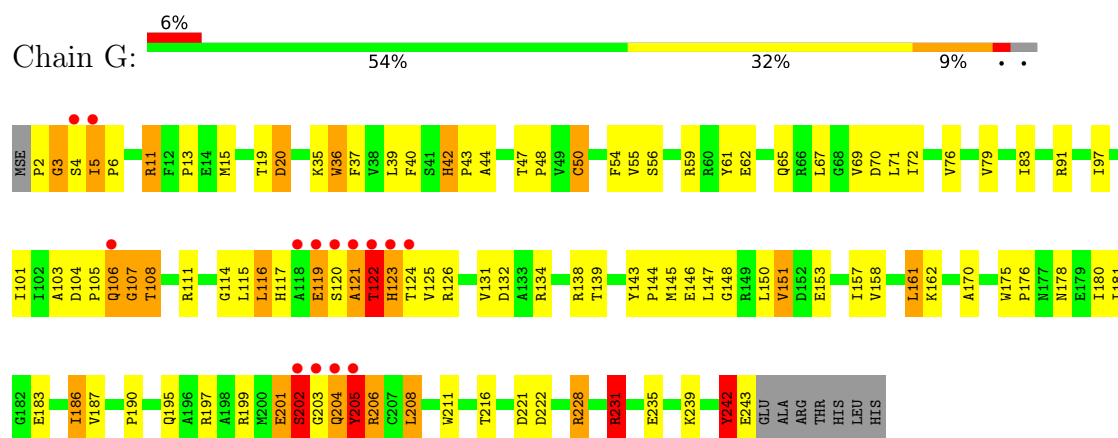
• Molecule 1: peroxiredoxin



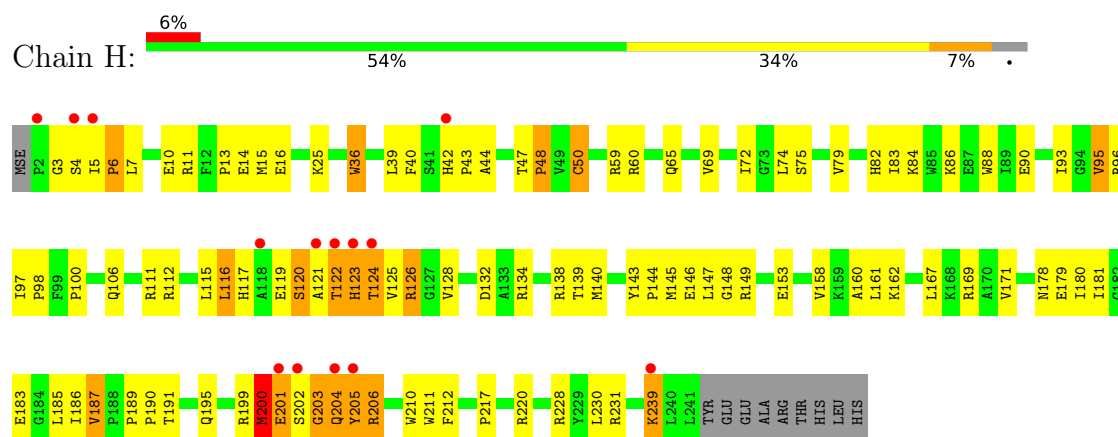
• Molecule 1: peroxiredoxin



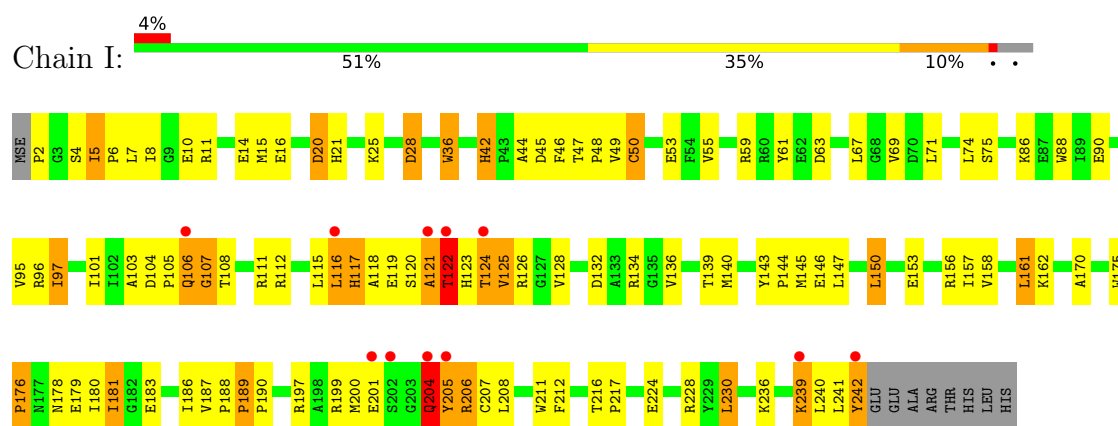
- Molecule 1: peroxiredoxin



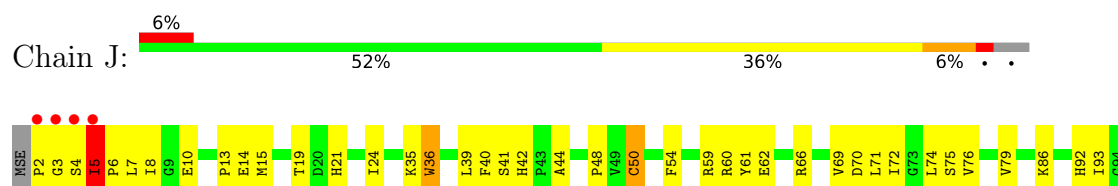
- Molecule 1: peroxiredoxin

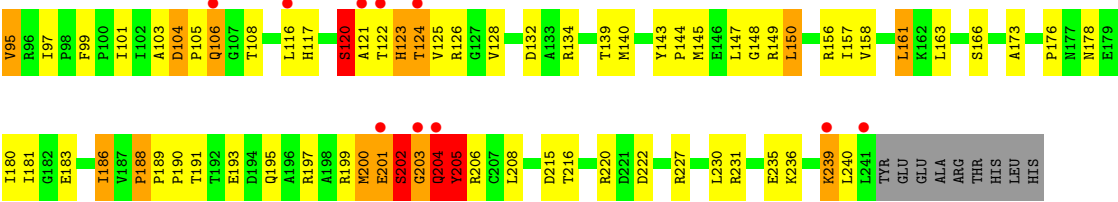


- Molecule 1: peroxiredoxin



- Molecule 1: peroxiredoxin





4 Data and refinement statistics

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) 93.5 (49.20-2.31)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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 (5.04%)	wwPDB-VP
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 , 55.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	1.00	0/1994	1.31	21/2703 (0.8%)
1	B	0.93	1/1994 (0.1%)	1.26	18/2703 (0.7%)
1	C	0.96	2/1994 (0.1%)	1.28	16/2703 (0.6%)
1	D	0.98	4/2003 (0.2%)	1.39	23/2715 (0.8%)
1	E	0.91	1/1981 (0.1%)	1.34	27/2685 (1.0%)
1	F	0.96	5/1981 (0.3%)	1.39	31/2685 (1.2%)
1	G	0.94	3/2003 (0.1%)	1.34	33/2715 (1.2%)
1	H	0.92	1/1981 (0.1%)	1.23	14/2685 (0.5%)
1	I	0.89	1/1994 (0.1%)	1.27	26/2703 (1.0%)
1	J	0.89	1/1981 (0.1%)	1.34	19/2685 (0.7%)
All	All	0.94	19/19906 (0.1%)	1.32	228/26982 (0.8%)

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 (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	202	SER	CA-C	-7.54	1.42	1.52
1	B	5	ILE	CA-CB	7.02	1.63	1.54
1	F	201	GLU	CA-C	-6.97	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	202	SER	N-CA	-6.07	1.38	1.46
1	J	5	ILE	CA-CB	5.76	1.61	1.54
1	F	202	SER	N-CA	-5.65	1.38	1.46
1	G	42	HIS	CA-C	-5.65	1.47	1.52
1	C	125	VAL	CA-C	5.58	1.59	1.52
1	H	189	PRO	CA-C	5.58	1.54	1.51
1	D	72	ILE	CA-CB	5.55	1.61	1.54
1	G	122	THR	CA-CB	5.54	1.62	1.53
1	F	240	LEU	CA-C	5.44	1.60	1.52
1	F	42	HIS	CA-C	-5.41	1.47	1.52
1	I	205	TYR	CA-C	-5.40	1.45	1.52
1	F	239	LYS	CA-C	5.39	1.59	1.52
1	D	122	THR	CA-CB	5.28	1.62	1.53
1	E	79	VAL	CA-CB	5.23	1.62	1.54
1	G	72	ILE	CA-CB	5.14	1.61	1.54
1	C	204	GLN	CA-C	5.07	1.59	1.52

All (228) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	203	GLY	N-CA-C	-19.14	88.28	115.27
1	D	121	ALA	N-CA-C	-13.45	92.78	110.53
1	D	200	MSE	N-CA-C	-13.27	91.78	110.50
1	J	202	SER	N-CA-C	-12.07	92.17	109.31
1	E	205	TYR	N-CA-C	11.69	128.82	108.02
1	F	201	GLU	N-CA-C	11.49	126.41	107.23
1	F	122	THR	N-CA-C	11.08	126.34	113.38
1	E	202	SER	N-CA-C	10.91	134.05	110.80
1	I	121	ALA	N-CA-C	-10.43	96.16	110.35
1	C	121	ALA	N-CA-C	-10.33	96.90	110.43
1	J	204	GLN	N-CA-C	9.83	131.74	110.80
1	F	188	PRO	CA-C-N	9.71	126.75	119.66
1	F	188	PRO	C-N-CA	9.71	126.75	119.66
1	H	205	TYR	N-CA-C	9.48	130.99	110.80
1	A	121	ALA	N-CA-C	-9.21	97.52	110.50
1	G	204	GLN	N-CA-C	-9.17	91.28	110.80
1	G	202	SER	N-CA-C	9.02	130.00	110.80
1	B	121	ALA	N-CA-C	-8.97	98.15	110.35
1	E	6	PRO	N-CA-C	-8.90	98.03	111.57
1	E	121	ALA	N-CA-C	-8.89	98.78	110.43
1	A	6	PRO	N-CA-C	-8.72	97.11	111.68
1	E	201	GLU	N-CA-C	8.66	120.75	108.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	205	TYR	N-CA-C	8.59	129.10	110.80
1	H	47	THR	CA-C-N	8.58	130.57	119.84
1	H	47	THR	C-N-CA	8.58	130.57	119.84
1	G	119	GLU	N-CA-C	-8.50	102.92	113.38
1	G	5	ILE	N-CA-CB	-8.49	99.33	111.21
1	J	203	GLY	CA-C-O	7.98	127.87	119.01
1	C	204	GLN	N-CA-C	-7.92	93.94	110.80
1	C	119	GLU	N-CA-C	-7.88	103.66	113.28
1	F	171	VAL	N-CA-C	7.86	116.69	107.73
1	H	203	GLY	N-CA-C	7.69	131.40	113.18
1	E	205	TYR	CB-CA-C	-7.66	99.05	110.62
1	D	204	GLN	N-CA-C	-7.65	98.82	111.37
1	G	47	THR	CA-C-N	7.65	129.40	119.84
1	G	47	THR	C-N-CA	7.65	129.40	119.84
1	I	104	ASP	CA-C-N	7.61	127.99	119.32
1	I	104	ASP	C-N-CA	7.61	127.99	119.32
1	G	106	GLN	N-CA-C	-7.49	96.21	108.41
1	I	119	GLU	N-CA-C	-7.46	104.32	113.50
1	D	205	TYR	N-CA-C	7.39	121.39	108.75
1	C	171	VAL	N-CA-C	7.25	115.89	107.77
1	F	202	SER	CB-CA-C	7.17	124.68	110.42
1	I	118	ALA	N-CA-C	7.14	121.96	112.25
1	C	47	THR	CA-C-N	7.13	128.75	119.84
1	C	47	THR	C-N-CA	7.13	128.75	119.84
1	E	99	PHE	CA-C-N	7.09	127.26	120.31
1	E	99	PHE	C-N-CA	7.09	127.26	120.31
1	F	121	ALA	N-CA-C	-7.07	101.17	110.43
1	J	208	LEU	N-CA-C	-7.04	104.84	113.50
1	I	208	LEU	N-CA-C	-7.02	104.86	113.50
1	J	21	HIS	N-CA-C	-7.02	104.37	114.12
1	A	229	TYR	N-CA-C	-7.00	103.58	111.14
1	G	3	GLY	CA-C-O	-6.99	114.83	121.19
1	D	202	SER	O-C-N	6.98	131.87	122.59
1	F	19	THR	CA-C-N	6.97	130.55	120.38
1	F	19	THR	C-N-CA	6.97	130.55	120.38
1	E	19	THR	CA-C-N	6.93	130.50	120.38
1	E	19	THR	C-N-CA	6.93	130.50	120.38
1	D	44	ALA	N-CA-C	6.92	119.04	108.52
1	B	119	GLU	N-CA-C	-6.85	104.89	113.18
1	G	186	ILE	N-CA-C	6.81	117.88	108.89
1	F	69	VAL	N-CA-C	6.78	117.66	108.17
1	D	241	LEU	N-CA-C	6.78	119.50	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	119	GLU	N-CA-C	-6.71	105.07	113.18
1	G	121	ALA	N-CA-C	-6.70	96.70	108.23
1	F	208	LEU	N-CA-C	-6.68	105.28	113.50
1	A	21	HIS	N-CA-C	-6.68	103.60	113.61
1	H	201	GLU	N-CA-CB	-6.68	98.71	110.39
1	A	47	THR	CA-C-N	6.66	128.16	119.84
1	A	47	THR	C-N-CA	6.66	128.16	119.84
1	I	216	THR	CA-C-N	6.62	127.19	120.04
1	I	216	THR	C-N-CA	6.62	127.19	120.04
1	A	97	ILE	CA-C-N	6.61	126.32	119.64
1	A	97	ILE	C-N-CA	6.61	126.32	119.64
1	C	203	GLY	N-CA-C	-6.53	100.71	110.71
1	G	122	THR	N-CA-CB	6.53	121.53	110.49
1	H	119	GLU	N-CA-C	-6.51	104.97	113.17
1	G	104	ASP	CA-C-N	6.50	127.02	119.47
1	G	104	ASP	C-N-CA	6.50	127.02	119.47
1	D	186	ILE	N-CA-C	6.50	117.94	108.58
1	C	11	ARG	N-CA-C	-6.49	100.87	110.48
1	B	44	ALA	N-CA-C	6.48	118.99	108.76
1	F	122	THR	CB-CA-C	-6.44	100.73	111.23
1	E	208	LEU	N-CA-C	-6.40	105.63	113.50
1	B	186	ILE	N-CA-C	6.37	117.87	109.21
1	B	77	ASP	N-CA-C	6.33	118.49	110.33
1	H	189	PRO	N-CA-C	6.32	116.54	110.47
1	E	119	GLU	N-CA-C	-6.32	105.57	113.28
1	D	104	ASP	CA-C-N	6.30	126.78	119.47
1	D	104	ASP	C-N-CA	6.30	126.78	119.47
1	B	208	LEU	N-CA-C	-6.28	105.44	113.23
1	F	203	GLY	N-CA-C	-6.27	98.32	113.18
1	A	44	ALA	N-CA-C	6.26	118.04	108.52
1	J	236	LYS	N-CA-C	-6.25	101.78	109.65
1	G	44	ALA	N-CA-C	6.23	117.99	108.52
1	D	202	SER	CA-CB-OG	-6.22	98.66	111.10
1	I	6	PRO	N-CA-C	-6.20	102.54	111.22
1	F	124	THR	N-CA-C	6.19	118.97	110.24
1	E	97	ILE	CA-C-N	6.19	125.89	119.64
1	E	97	ILE	C-N-CA	6.19	125.89	119.64
1	G	201	GLU	CA-C-N	6.19	133.36	121.54
1	G	201	GLU	C-N-CA	6.19	133.36	121.54
1	I	206	ARG	N-CA-C	-6.18	100.44	110.20
1	I	47	THR	CA-C-N	6.17	127.56	119.84
1	I	47	THR	C-N-CA	6.17	127.56	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	106	GLN	N-CA-C	-6.16	99.35	109.40
1	B	3	GLY	N-CA-C	6.16	120.14	110.96
1	D	79	VAL	CB-CA-C	-6.14	102.64	112.16
1	E	188	PRO	CA-C-N	6.13	126.70	120.38
1	E	188	PRO	C-N-CA	6.13	126.70	120.38
1	J	186	ILE	N-CA-C	6.13	117.41	108.58
1	A	4	SER	N-CA-C	6.13	119.70	107.62
1	I	44	ALA	N-CA-C	6.13	118.47	108.55
1	D	201	GLU	CA-C-O	6.12	129.27	120.51
1	E	228	ARG	N-CA-CB	6.10	119.70	110.30
1	B	216	THR	CA-C-N	6.08	126.98	120.47
1	B	216	THR	C-N-CA	6.08	126.98	120.47
1	I	205	TYR	N-CA-C	6.06	118.65	108.23
1	F	99	PHE	CA-C-N	6.05	126.02	120.03
1	F	99	PHE	C-N-CA	6.05	126.02	120.03
1	G	216	THR	CA-C-N	6.01	126.53	120.04
1	G	216	THR	C-N-CA	6.01	126.53	120.04
1	A	200	MSE	N-CA-C	6.00	118.44	108.13
1	H	44	ALA	N-CA-C	5.99	118.23	108.76
1	I	42	HIS	CA-C-N	5.98	125.69	119.05
1	I	42	HIS	C-N-CA	5.98	125.69	119.05
1	I	170	ALA	N-CA-C	-5.97	101.17	110.42
1	G	36	TRP	N-CA-C	-5.96	102.51	110.55
1	G	108	THR	N-CA-C	-5.94	104.50	110.97
1	A	5	ILE	N-CA-C	5.94	121.70	108.88
1	A	208	LEU	N-CA-C	-5.88	106.26	113.50
1	D	9	GLY	N-CA-C	-5.88	107.69	114.69
1	D	36	TRP	N-CA-C	-5.88	102.94	110.53
1	C	208	LEU	N-CA-C	-5.86	105.96	113.23
1	C	206	ARG	N-CA-C	-5.84	102.26	110.50
1	A	126	ARG	N-CA-CB	-5.82	103.66	110.35
1	I	16	GLU	N-CA-C	-5.82	100.21	109.76
1	B	6	PRO	N-CA-C	-5.80	102.35	111.34
1	G	242	TYR	N-CA-C	-5.77	104.99	111.28
1	E	91	ARG	N-CA-C	5.76	117.64	111.36
1	A	227	ARG	CA-C-N	-5.75	111.08	121.14
1	A	227	ARG	C-N-CA	-5.75	111.08	121.14
1	C	3	GLY	N-CA-C	5.75	120.10	110.56
1	J	216	THR	CA-C-N	5.75	126.25	120.04
1	J	216	THR	C-N-CA	5.75	126.25	120.04
1	F	236	LYS	CA-C-N	-5.73	114.03	119.76
1	F	236	LYS	C-N-CA	-5.73	114.03	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	170	ALA	N-CA-C	-5.72	101.55	110.42
1	D	107	GLY	N-CA-C	-5.69	99.70	113.18
1	G	235	GLU	N-CA-C	5.65	119.12	110.20
1	G	151	VAL	N-CA-C	5.64	116.38	110.62
1	I	189	PRO	N-CA-C	5.62	115.87	110.47
1	B	201	GLU	CA-C-N	-5.61	113.84	122.87
1	B	201	GLU	C-N-CA	-5.61	113.84	122.87
1	J	104	ASP	CA-C-N	5.61	125.72	119.32
1	J	104	ASP	C-N-CA	5.61	125.72	119.32
1	J	36	TRP	N-CA-C	-5.60	102.24	110.52
1	F	205	TYR	CB-CA-C	-5.59	99.30	110.42
1	C	106	GLN	N-CA-C	-5.56	99.22	108.34
1	H	187	VAL	CB-CA-C	-5.54	105.79	110.94
1	G	187	VAL	N-CA-C	-5.54	103.87	108.63
1	E	228	ARG	CA-CB-CG	5.51	125.13	114.10
1	C	36	TRP	N-CA-C	-5.50	103.12	110.55
1	G	35	LYS	N-CA-C	5.50	118.78	109.76
1	B	206	ARG	N-CA-C	-5.49	100.75	109.76
1	G	91	ARG	N-CA-C	5.49	117.34	111.36
1	G	208	LEU	N-CA-C	-5.45	106.76	113.41
1	F	204	GLN	N-CA-C	-5.44	105.44	111.36
1	E	186	ILE	N-CA-C	5.43	117.12	108.87
1	B	220	ARG	N-CA-C	-5.42	105.37	111.28
1	C	21	HIS	N-CA-C	-5.42	105.47	113.61
1	F	29	HIS	N-CA-C	5.42	118.68	111.75
1	J	106	GLN	N-CA-C	-5.41	100.88	109.59
1	E	104	ASP	CA-C-N	5.41	126.60	119.84
1	E	104	ASP	C-N-CA	5.41	126.60	119.84
1	F	104	ASP	CA-C-N	5.41	125.74	119.47
1	F	104	ASP	C-N-CA	5.41	125.74	119.47
1	F	126	ARG	N-CA-CB	-5.39	103.66	110.45
1	B	106	GLN	N-CA-C	-5.38	100.40	109.07
1	A	186	ILE	N-CA-C	5.37	115.98	108.89
1	J	44	ALA	N-CA-C	5.36	117.41	108.99
1	H	6	PRO	N-CA-C	-5.36	103.72	111.22
1	G	19	THR	CA-C-N	5.34	131.75	121.54
1	G	19	THR	C-N-CA	5.34	131.75	121.54
1	A	170	ALA	N-CA-C	-5.30	101.64	110.17
1	H	200	MSE	CA-C-N	5.29	131.66	121.18
1	H	200	MSE	C-N-CA	5.29	131.66	121.18
1	G	231	ARG	N-CA-C	-5.27	105.53	111.28
1	C	205	TYR	N-CA-CB	5.27	119.40	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	208	LEU	N-CA-C	-5.27	106.98	113.41
1	F	202	SER	CA-CB-OG	-5.26	100.58	111.10
1	I	2	PRO	N-CA-CB	5.24	108.76	103.00
1	I	181	ILE	N-CA-C	5.23	117.14	112.17
1	D	91	ARG	N-CA-C	5.23	117.06	111.36
1	J	124	THR	N-CA-C	5.22	117.46	110.35
1	D	105	PRO	CA-C-N	-5.21	114.46	121.71
1	D	105	PRO	C-N-CA	-5.21	114.46	121.71
1	E	44	ALA	N-CA-C	5.21	116.44	108.52
1	J	188	PRO	CA-C-N	5.21	123.46	119.66
1	J	188	PRO	C-N-CA	5.21	123.46	119.66
1	F	170	ALA	N-CA-C	-5.21	101.67	109.95
1	A	36	TRP	N-CA-C	-5.20	102.35	110.42
1	A	199	ARG	CA-CB-CG	-5.20	103.70	114.10
1	F	44	ALA	N-CA-C	5.20	116.97	108.76
1	B	33	GLN	N-CA-C	-5.19	106.34	113.30
1	G	206	ARG	N-CA-C	-5.17	102.63	110.28
1	B	2	PRO	N-CA-CB	5.17	108.68	103.00
1	B	48	PRO	N-CA-C	5.16	123.11	112.47
1	E	48	PRO	N-CA-C	5.16	120.86	113.47
1	F	189	PRO	CA-C-N	5.16	124.92	119.76
1	F	189	PRO	C-N-CA	5.16	124.92	119.76
1	I	97	ILE	CA-C-N	-5.16	114.95	120.47
1	I	97	ILE	C-N-CA	-5.16	114.95	120.47
1	E	103	ALA	N-CA-C	-5.12	100.06	108.41
1	I	204	GLN	CB-CA-C	-5.09	100.49	110.11
1	J	2	PRO	N-CA-CB	5.09	108.60	103.00
1	H	36	TRP	N-CA-C	-5.07	103.01	110.52
1	F	200	MSE	CA-C-N	-5.07	113.91	121.72
1	F	200	MSE	C-N-CA	-5.07	113.91	121.72
1	I	36	TRP	N-CA-C	-5.07	103.02	110.52
1	E	77	ASP	N-CA-C	5.05	116.63	110.41
1	H	171	VAL	N-CA-C	5.05	113.49	107.73
1	E	205	TYR	CA-CB-CG	5.02	122.94	113.90
1	D	189	PRO	CA-C-N	5.02	124.95	119.78
1	D	189	PRO	C-N-CA	5.02	124.95	119.78
1	C	201	GLU	CB-CA-C	-5.01	100.44	110.42
1	A	119	GLU	N-CA-C	-5.00	107.17	113.28

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

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	107	0
1	C	1953	0	1940	134	0
1	D	1962	0	1946	155	0
1	E	1941	0	1931	117	0
1	F	1941	0	1931	119	0
1	G	1962	0	1946	124	1
1	H	1941	0	1931	132	0
1	I	1953	0	1940	126	0
1	J	1941	0	1931	148	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	7	0
3	E	4	0	8	3	0
3	F	4	0	8	1	0
3	G	4	0	8	1	0
3	H	8	0	16	5	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	9	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	20374	0	19473	1130	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 29.

All (1130) 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	1.16
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:G:4:SER:C	1:G:5:ILE:HD12	1.81	1.05
1:A:126:ARG:HG3	1:A:126:ARG:HH11	0.95	1.04
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: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:H:4:SER:C	1:H:5:ILE:HD12	1.88	0.99
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:OE1	1:D:243:GLU:HA	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:E:178:ASN:HD22	1:E:181:ILE:H	1.13	0.94
1:A:126:ARG:HH11	1:A:126:ARG:CG	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:HA	1:H:200:MSE:HE2	1.51	0.92
1:H:200:MSE:HA	1:H:200:MSE:CE	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:178:ASN:HD22	1:A:181:ILE:H	1.14	0.89
1:B:106:GLN:HE22	1:C:107:GLY: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
3:D:2003:IPA:H32	1:E:84:LYS:HZ1	1.37	0.88
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:A:92:HIS:HE1	3:J:2001:IPA:H12	1.40	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: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:E:199:ARG:C	1:E:201:GLU:H	1.83	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
1:A:5:ILE:HG21	1:B:5:ILE:HG12	1.58	0.85
1:A:49:VAL:CG1	1:A:126:ARG:NH2	2.39	0.85
1:J:4:SER:O	1:J:5:ILE:HD12	1.74	0.85
1:J:204:GLN:O	1:J:205:TYR:CD2	2.28	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
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:C:59:ARG:HD3	1:D:179:GLU:OE2	1.79	0.83
1:J:200:MSE:CE	1:J:203:GLY:HA3	2.08	0.83
1:C:3:GLY:O	1:D:4:SER:HA	1.79	0.83
1:H:69:VAL:HG21	1:H:158:VAL:HG11	1.59	0.83
1:E:42:HIS:CD2	1:E:75:SER:HB2	2.13	0.83
1:D:202:SER:C	1:D:204:GLN:N	2.28	0.83
3:D:2003:IPA:H32	1:E:84:LYS:NZ	1.94	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:69:VAL:HG21	1:D:158:VAL:HG11	1.61	0.82
1:D:106:GLN:O	1:E:106:GLN:NE2	2.12	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: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:C:2:PRO:N	1:D:10:GLU:OE2	2.15	0.80
1:C:42:HIS:NE2	1:C:75:SER:HB2	1.97	0.80
1:G:117:HIS:CG	1:G:125:VAL:HG21	2.17	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
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:G:2:PRO:HB2	1:H:10:GLU:OE2	1.82	0.79
1:I:242:TYR:CE2	4:I:321:HOH:O	2.36	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:H:40:PHE:CD1	1:H:42:HIS:HE1	2.00	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:E:42:HIS:HE1	1:E:85:TRP:CZ3	2.00	0.78
1:I:117:HIS:CE1	1:J:8:ILE:H	2.02	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:C:242:TYR:CD1	1:C:242:TYR:C	2.63	0.76
1:I:117:HIS:CB	1:I:125:VAL:HG21	2.15	0.76
1:C:4:SER:C	1:C:5:ILE:HD12	2.09	0.76
1:I:115:LEU:O	1:I:125:VAL:HG23	1.84	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:204:GLN:O	1:C:205:TYR:HD1	1.68	0.76
1:H:187:VAL:HG21	1:H:205:TYR:CE2	2.21	0.76
1:C:124:THR:HG22	1:C:125:VAL:O	1.86	0.75
1:D:106:GLN:HG2	1:E:122:THR:HA	1.67	0.75
1:H:11:ARG:NH1	4:H:2079:HOH:O	2.17	0.75
1:H:43:PRO:CB	1:H:123:HIS:HB3	2.17	0.75
1:A:49:VAL:HG12	1:A:126:ARG:HH21	1.51	0.75
1:G:201:GLU:OE1	1:G:201:GLU:HA	1.86	0.75
1:J:50:OCS:OD2	1:J:126:ARG:NH2	2.19	0.75
1:E:201:GLU:HG2	4:E:2067:HOH:O	1.84	0.75
1:E:205:TYR:O	1:E:206:ARG:C	2.29	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:F:4:SER:C	1:F:5:ILE:HD12	2.10	0.75
1:C:203:GLY:C	1:C:204:GLN:O	2.27	0.75
1:G:228:ARG:HG2	1:G:228:ARG:HH11	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:A:177:ASN:OD1	1:A:227:ARG:NH1	2.20	0.74
1:H:231:ARG:NH1	4:H:2049:HOH:O	2.19	0.74
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:F:220:ARG:HH11	1:F:220:ARG:HB2	1.53	0.73
1:J:204:GLN:HE21	1:J:204:GLN:CA	2.00	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:D:5:ILE:CG2	1:D:6:PRO:HD2	2.18	0.73
1:F:117:HIS:CG	1:F:125:VAL:HG21	2.23	0.73
1:F:40:PHE:HD1	1:F:42:HIS:CE1	2.07	0.73
1:G:42:HIS:HD2	1:G:50:OCS:OD2	1.71	0.73
1:B:204:GLN:C	1:B:205:TYR:HD2	1.97	0.73
1:B:5:ILE:HD12	1:B:6:PRO:O	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:199:ARG:C	1:E:201:GLU:N	2.45	0.72
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: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:E:202:SER:C	1:E:204:GLN:H	1.98	0.71
1:J:42:HIS:CD2	1:J:54:PHE:HE1	2.06	0.71
1:C:132:ASP:OD2	1:C:134:ARG:NH1	2.23	0.71
1:J:204:GLN:C	1:J:205:TYR:CG	2.68	0.71
1:J:205:TYR:HA	4:J:2093:HOH:O	1.89	0.71
1:D:5:ILE:HG13	1:D:114:GLY:HA3	1.71	0.71
1:H:84:LYS:HZ1	3:H:2009:IPA:H32	1.54	0.71
1:F:122:THR:HA	1:G:106:GLN:HG3	1.72	0.71
1:G:204:GLN:C	1:G:205:TYR:CG	2.67	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:88:TRP:CD1	3:E:2006:IPA:H12	2.26	0.70
1:C:10:GLU:OE2	1:D:2:PRO:HB2	1.92	0.70
1:I:4:SER:HA	1:J:3:GLY:O	1.92	0.70
1:A:49:VAL:HG12	1:A:126:ARG:NH2	2.06	0.70
1:H:191:THR:H	1:H:195:GLN:NE2	1.89	0.70
1:J:62:GLU:OE1	1:J:66:ARG:NH2	2.25	0.70
1:F:205:TYR:O	1:F:206:ARG:C	2.35	0.70
1:C:201:GLU:OE1	1:C:201:GLU:N	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: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:I:117:HIS:HE1	1:J:140:MSE:CE	2.06	0.69
1:G:43:PRO:HB2	1:G:123:HIS:HB3	1.74	0.69
1:G:144:PRO:HD3	1:H:139:THR:OG1	1.93	0.69
1:J:117:HIS:CG	1:J:125:VAL:HG11	2.27	0.69
1:G:4:SER:C	1:G:5:ILE:CD1	2.65	0.69
1:H:42:HIS:HD2	1:H:50:OCS:OD2	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:LEU:O	1:A:125:VAL:HG23	1.93	0.69
1:F:50:OCS:OD2	1:F:126:ARG:NH2	2.26	0.69
1:F:74:LEU:C	1:F:74:LEU:HD23	2.17	0.69
1:I:201:GLU:OE1	1:I:207:CYS:N	2.23	0.69
1:A:178:ASN:ND2	1:A:181:ILE:H	1.90	0.69
1:E:39:LEU:HD23	1:E:39:LEU:C	2.18	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: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:J:204:GLN:NE2	1:J:204:GLN:CA	2.54	0.68
1:C:144:PRO:HG2	1:C:147:LEU:HB3	1.74	0.68
1:D:239:LYS:NZ	1:D:239:LYS:HB3	2.08	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:HD2	1:B:205:TYR:N	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:E:202:SER:OG	1:E:203:GLY:N	2.23	0.67
1:B:228:ARG:HD2	4:B:2024:HOH:O	1.94	0.67
1:G:48:PRO:HG3	1:H:211:TRP:O	1.94	0.67
1:I:204:GLN:HB2	1:I:205:TYR:CD1	2.30	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:H:120:SER:C	1:H:122:THR:H	2.03	0.67
1:E:20:ASP:OD2	1:E:86:LYS:NZ	2.28	0.66
1:D:4:SER:C	1:D:5:ILE:HD12	2.20	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:HB2	1:F:220:ARG:NH1	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:H:121:ALA:C	1:H:122:THR:HG22	2.21	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:4:SER:O	1:J:5:ILE:CD1	2.43	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:C:222:ASP:OD2	4:C:301:HOH:O	2.13	0.65
1:E:188:PRO:O	1:E:199:ARG:NH1	2.29	0.65
1:F:106:GLN:C	1:F:108:THR:H	2.04	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:E:134:ARG:HD2	4:E:2013:HOH:O	1.97	0.64
1:F:42:HIS:CE1	1:F:54:PHE:CE1	2.86	0.64
1:G:42:HIS:CD2	1:G:50:OCS:OD2	2.49	0.64
1:D:59:ARG:HH11	1:D:59:ARG:HG3	1.61	0.64
1:G:40:PHE:HD1	1:G:42:HIS:CE1	2.10	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:C:93:ILE:HG22	1:C:95:VAL:HG12	1.79	0.64
1:J:5:ILE:HG22	1:J:6:PRO:O	1.97	0.64
1:J:74:LEU:HD23	1:J:74:LEU:C	2.23	0.64
1:G:59:ARG:HG3	1:G:59:ARG:HH11	1.63	0.64
1:H:84:LYS:NZ	3:H:2009:IPA:H32	2.13	0.64
1:I:178:ASN:ND2	1:I:181:ILE:H	1.93	0.64
1:E:126:ARG:HD2	1:E:144:PRO:O	1.98	0.64
1:G:124:THR:HG22	1:G:125:VAL:N	2.12	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:5:ILE:HG23	1:D:113:LEU:O	1.98	0.63
1:D:243:GLU:OE1	1:D:243:GLU:CA	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:121:ALA:C	1:H:122:THR:CG2	2.72	0.62
1:J:166:SER:HA	4:J:2083:HOH:O	1.98	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:H:126:ARG:NH1	1:H:145:MSE:O	2.31	0.62
1:J:126:ARG:NH1	1:J:145:MSE:O	2.31	0.62
1:C:106:GLN:C	1:C:108:THR:H	2.04	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
3:B:2005:IPA:H32	1:C:84:LYS:NZ	2.14	0.62
1:D:201:GLU:O	1:D:202:SER:HB2	1.98	0.62
1:F:39:LEU:C	1:F:39:LEU:HD23	2.25	0.62
1:H:42:HIS:CD2	1:H:50:OCS:OD2	2.52	0.62
1:C:188:PRO:O	1:C:199:ARG:NH2	2.32	0.62
1:D:126:ARG:HH11	1:D:145:MSE:HA	1.65	0.62
1:C:42:HIS:CE1	1:C:75:SER:HB2	2.34	0.61
1:F:42:HIS:CD2	1:F:50:OCS:OD2	2.52	0.61
1:B:59:ARG:HG3	1:B:59:ARG:HH11	1.65	0.61
1:C:242:TYR:CE2	1:D:206:ARG:NH1	2.56	0.61
1:D:204:GLN:HG3	4:D:2054:HOH:O	2.00	0.61
1:B:239:LYS:O	1:B:240:LEU:HB2	1.99	0.61
1:E:204:GLN:HA	1:E:204:GLN:NE2	2.14	0.61
1:J:239:LYS:HB3	1:J:239:LYS:NZ	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:B:50:OCS:OD2	1:B:126:ARG:NH2	2.34	0.61
1:I:126:ARG:NH1	1:I:145:MSE:O	2.33	0.61
1:A:106:GLN:OE1	1:J:116:LEU:HD21	2.01	0.61
1:D:14:GLU:OE1	1:D:25:LYS:NZ	2.30	0.61
1:F:124:THR:HG22	1:F:125:VAL:O	2.00	0.61
1:C:86:LYS:HE3	1:C:101:ILE:CD1	2.30	0.61
1:E:202:SER:C	1:E:204:GLN:N	2.55	0.61
1:G:211:TRP:O	1:H:48:PRO:HG3	2.00	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:190:PRO:HG3	1:H:199:ARG:HD2	1.81	0.61
1:C:146:GLU:OE1	1:C:146:GLU:N	2.26	0.61
1:I:242:TYR:CE1	1:J:206:ARG:HD2	2.36	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:A:220:ARG:HB2	1:A:220:ARG:HH11	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:GLN:C	1:B:205:TYR:CD2	2.79	0.60
1:J:3:GLY:O	1:J:5:ILE:HD12	2.02	0.60
1:D:204:GLN:HE21	1:D:204:GLN:C	2.09	0.60
1:J:42:HIS:NE2	1:J:54:PHE:HE1	1.99	0.60
1:J:203:GLY:C	1:J:204:GLN:CG	2.74	0.60
3:D:2003:IPA:C3	1:E:84:LYS:HZ1	2.10	0.60
1:A:48:PRO:HG3	1:B:211:TRP:O	2.01	0.60
1:A:125:VAL:HG12	1:A:126:ARG:N	2.16	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:B:106:GLN:C	1:B:108:THR:H	2.08	0.60
1:H:128:VAL:HG23	1:H:149:ARG:HH11	1.66	0.60
1:B:70:ASP:OD1	4:B:2042:HOH:O	2.16	0.60
1:H:111:ARG:HE	1:H:116:LEU:HD22	1.66	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:D:126:ARG:NH1	1:D:145:MSE:O	2.35	0.59
1:E:42:HIS:HE2	1:E:75:SER:HB2	1.64	0.59
1:B:42:HIS:NE2	1:B:54:PHE:HE1	1.99	0.59
1:B:201:GLU:O	1:B:201:GLU:HG3	2.01	0.59
1:C:11:ARG:NH2	4:C:279:HOH:O	2.21	0.59
1:I:74:LEU:C	1:I:74:LEU:HD23	2.27	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:H:86:LYS:HE2	1:H:97:ILE:HG22	1.83	0.59
1:J:42:HIS:NE2	1:J:54:PHE:CE1	2.70	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
1:C:7:LEU:HD21	1:D:3:GLY:HA3	1.83	0.59
1:C:86:LYS:HE3	1:C:101:ILE:HD11	1.85	0.59
1:D:5:ILE:HG23	1:D:6:PRO:HD2	1.82	0.59
1:G:197:ARG:HE	1:I:96:ARG:NH2	2.00	0.59
1:J:62:GLU:HG3	4:J:2065:HOH:O	2.02	0.59
1:A:203:GLY:O	1:A:204:GLN:HB2	2.01	0.59
1:H:106:GLN:HG3	1:I:122:THR:HA	1.83	0.59
1:I:74:LEU:HD23	1:I:75:SER:N	2.18	0.59
1:A:204:GLN:HE21	1:A:204:GLN:CA	2.15	0.58
1:E:124:THR:HG22	1:E:125:VAL:O	2.02	0.58
1:E:239:LYS:NZ	1:E:239:LYS:HB3	2.18	0.58
1:G:178:ASN:ND2	1:G:180:ILE:H	2.01	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:5:ILE:HD12	1:H:5:ILE:N	2.17	0.58
1:J:239:LYS:HB3	1:J:239:LYS:HZ2	1.68	0.58
1:E:143:TYR:OH	1:F:153:GLU:OE2	2.19	0.58
1:F:14:GLU:OE1	1:F:14:GLU:HA	2.01	0.58
1:C:220:ARG:HB2	1:C:220:ARG:NH1	2.18	0.58
1:G:3:GLY:C	1:G:5:ILE:CD1	2.76	0.58
1:J:178:ASN:ND2	1:J:180:ILE:H	2.02	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:H:132:ASP:OD2	1:H:134:ARG:NH1	2.36	0.58
1:J:92:HIS:HE1	3:J:2002:IPA:C1	2.15	0.58
1:I:143:TYR:HD1	1:I:147:LEU:HD12	1.68	0.58
1:J:39:LEU:HD23	1:J:39:LEU:C	2.28	0.58
1:E:199:ARG:O	1:E:201:GLU:N	2.36	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:HH11	1:H:112:ARG:HG2	1.68	0.58
1:C:242:TYR:C	1:C:242:TYR:HD1	2.11	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:B:39:LEU:C	1:B:39:LEU:HD23	2.29	0.57
1:C:139:THR:OG1	1:D:144:PRO:HD3	2.03	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:E:180:ILE:HD11	1:F:55:VAL:HG21	1.87	0.57
1:I:20:ASP:OD1	1:I:101:ILE:HB	2.05	0.57
1:J:203:GLY:O	1:J:204:GLN:CB	2.52	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:I:236:LYS:HD2	1:J:227:ARG:HH12	1.68	0.57
1:J:103:ALA:C	1:J:105:PRO:HD3	2.29	0.57
1:J:106:GLN:O	1:J:108:THR:N	2.37	0.57
1:D:240:LEU:O	1:D:243:GLU:HB2	2.05	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:C:8:ILE:HG13	1:C:140:MSE:HE2	1.85	0.57
1:D:50:OCS:OD1	1:D:126:ARG:NH2	2.37	0.57
1:E:103:ALA:C	1:E:105:PRO:HD3	2.29	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:178:ASN:ND2	1:C:180:ILE:H	2.01	0.57
1:D:41:SER:HB2	1:D:124:THR:HG21	1.85	0.57
1:G:242:TYR:HE2	4:G:2050:HOH:O	1.88	0.57
1:H:106:GLN:CG	1:I:122:THR:HA	2.34	0.57
1:D:88:TRP:HD1	3:D:2003:IPA:H33	1.70	0.56
1:H:5:ILE:HG23	1:H:6:PRO:HD2	1.86	0.56
1:C:2:PRO:HA	1:D:7:LEU:HG	1.88	0.56
1:D:175:TRP:CG	1:D:176:PRO:HA	2.40	0.56
1:E:48:PRO:HG3	1:F:211:TRP:O	2.06	0.56
1:A:106:GLN:CD	1:J:116:LEU:HD21	2.30	0.56
1:C:59:ARG:NH1	1:D:179:GLU:OE2	2.38	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:J:126:ARG:HB2	1:J:143:TYR:O	2.05	0.56
1:A:235:GLU:HG3	4:A:1102:HOH:O	2.06	0.56
1:D:48:PRO:HD2	4:D:2026:HOH:O	2.03	0.56
1:F:239:LYS:NZ	1:F:239:LYS:HB3	2.20	0.56
1:I:239:LYS:HB3	1:I:239:LYS:NZ	2.20	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:7:LEU:HD22	1:D:117:HIS:CD2	2.40	0.56
1:C:179:GLU:O	1:D:240:LEU:HA	2.06	0.56
1:F:14:GLU:OE1	1:F:27:PRO:CD	2.54	0.56
1:J:3:GLY:C	1:J:5:ILE:HD12	2.31	0.56
1:C:115:LEU:HB3	1:C:124:THR:HG23	1.87	0.56
1:G:54:PHE:HE2	1:G:101:ILE:CD1	2.19	0.56
1:H:190:PRO:HG3	1:H:199:ARG:CD	2.35	0.56
1:I:28:ASP:OD1	1:I:28:ASP:N	2.39	0.56
1:A:103:ALA:C	1:A:105:PRO:HD3	2.30	0.56
1:D:242:TYR:C	1:D:242:TYR:CD2	2.84	0.56
1:F:103:ALA:C	1:F:105:PRO:HD3	2.31	0.56
1:I:63:ASP:CG	1:I:228:ARG:HH22	2.13	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: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:C:200:MSE:O	1:C:201:GLU:C	2.48	0.55
1:D:126:ARG:NH1	1:D:145:MSE:HA	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:48:PRO:HB2	1:H:186:ILE:HG21	1.88	0.55
1:H:122:THR:O	1:H:123:HIS:O	2.25	0.55
1:A:125:VAL:CG1	1:A:126:ARG:H	2.19	0.55
4:A:1118:HOH:O	1:B:242:TYR:HB2	2.06	0.55
1:G:242:TYR:HB3	1:H:180:ILE:O	2.07	0.55
1:I:103:ALA:C	1:I:105:PRO:HD3	2.32	0.55
1:D:106:GLN:CG	1:E:122:THR:HA	2.37	0.55
1:G:65:GLN:HG3	4:G:2059:HOH:O	2.06	0.55
1:H:206:ARG:H	1:H:206:ARG:HD2	1.72	0.55
1:I:144:PRO:HG2	1:I:147:LEU:HB3	1.89	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: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:H:36:TRP:NE1	1:H:162:LYS:HE2	2.22	0.55
1:B:36:TRP:HB2	1:B:69:VAL:HG22	1.89	0.55
1:C:126:ARG:NH1	1:C:144:PRO:O	2.40	0.55
1:H:5:ILE:HG22	1:H:6:PRO:N	2.22	0.55
1:J:41:SER:HB2	1:J:124:THR:HG21	1.88	0.55
1:A:224:GLU:HA	1:A:224:GLU:OE1	2.06	0.54
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: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:B:75:SER:HB3	1:B:82:HIS:CE1	2.42	0.54
1:J:92:HIS:CE1	3:J:2002:IPA:H12	2.37	0.54
1:J:93:ILE:HG22	1:J:95:VAL:HG12	1.89	0.54
1:B:35:LYS:HD3	1:B:70:ASP:OD2	2.07	0.54
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:G:115:LEU:HB3	1:G:124:THR:HG23	1.90	0.54
1:A:36:TRP:HB2	1:A:69:VAL:HG22	1.89	0.54
1:E:201:GLU:O	1:E:202:SER:HB2	2.05	0.54
1:I:117:HIS:HE1	1:J:140:MSE:HE1	1.71	0.54
1:B:55:VAL:O	1:B:59:ARG:HG2	2.08	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: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:I:20:ASP:OD2	1:I:86:LYS:NZ	2.36	0.54
1:B:5:ILE:CD1	1:B:7:LEU:HD23	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:5:ILE:HD12	1:B:5:ILE:C	2.33	0.54
1:J:220:ARG:HB2	1:J:220:ARG:NH1	2.22	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:39:LEU:C	1:G:39:LEU:HD23	2.32	0.54
1:H:50:OCS:SG	1:H:126:ARG:NH2	2.80	0.54
1:B:126:ARG:NH1	1:B:145:MSE:O	2.41	0.54
1:G:143:TYR:HD1	1:G:147:LEU:HD12	1.73	0.54
1:H:14:GLU:OE2	1:H:25:LYS:HE2	2.07	0.54
1:D:231:ARG:HG3	1:D:231:ARG:HH11	1.73	0.54
1:E:106:GLN:O	1:E:111:ARG:NH1	2.37	0.54
1:J:203:GLY:O	1:J:204:GLN:CG	2.55	0.54
1:D:96:ARG:HG2	1:D:96:ARG:HH11	1.73	0.53
1:I:175:TRP:CG	1:I:176:PRO:HA	2.44	0.53
1:J:132:ASP:OD2	1:J:134:ARG:NH1	2.41	0.53
1:C:42:HIS:HB2	1:C:50:OCS:OD2	2.08	0.53
1:D:59:ARG:HG3	1:D:59:ARG:NH1	2.23	0.53
1:D:76:VAL:O	1:D:105:PRO:HA	2.08	0.53
1:D:96:ARG:HG2	1:D:96:ARG:NH1	2.23	0.53
1:E:201:GLU:O	1:E:202:SER:CB	2.56	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:A:206:ARG:H	1:A:206:ARG:HD2	1.73	0.53
1:F:14:GLU:OE1	1:F:27:PRO:HD2	2.08	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:J:61:TYR:HD2	1:J:71:LEU:HD12	1.74	0.53
1:J:203:GLY:O	1:J:204:GLN:HB2	2.08	0.53
1:C:5:ILE:HG22	1:C:6:PRO:O	2.08	0.53
1:E:42:HIS:CE1	1:E:85:TRP:CZ3	2.91	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:H:39:LEU:C	1:H:39:LEU:HD23	2.34	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:178:ASN:HD22	1:I:181:ILE:N	2.02	0.53
1:J:204:GLN:O	1:J:205:TYR:CB	2.54	0.53
1:A:92:HIS:HE1	3:J:2001:IPA:C1	2.17	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201:GLU:O	1:B:201:GLU:CG	2.57	0.53
1:F:144:PRO:HG2	1:F:147:LEU:CB	2.38	0.53
1:I:5:ILE:HD13	1:J:5:ILE:HG21	1.90	0.53
1:I:7:LEU:HD12	1:I:10:GLU:OE2	2.09	0.53
1:I:201:GLU:HA	1:I:205:TYR:O	2.09	0.53
1:A:144:PRO:HG3	1:B:161:LEU:HD11	1.89	0.53
1:C:186:ILE:HG21	1:D:48:PRO:HB2	1.91	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:41:SER:HA	1:C:74:LEU:O	2.08	0.52
1:H:3:GLY:O	1:H:5:ILE:CD1	2.57	0.52
1:I:106:GLN:C	1:I:108:THR:H	2.17	0.52
1:C:186:ILE:HG21	1:D:48:PRO:CB	2.40	0.52
1:C:202:SER:HB3	1:C:205:TYR:HB2	1.90	0.52
1:H:199:ARG:O	1:H:200:MSE:CE	2.35	0.52
1:G:59:ARG:NH1	1:H:179:GLU:OE2	2.42	0.52
1:H:124:THR:HG22	1:H:125:VAL:N	2.23	0.52
1:I:48:PRO:HB2	1:J:186:ILE:HD13	1.91	0.52
1:I:150:LEU:CD2	4:J:2025:HOH:O	2.57	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:H:126:ARG:HB2	1:H:143:TYR:O	2.09	0.52
1:H:228:ARG:NH2	4:H:2084:HOH:O	2.39	0.52
1:G:106:GLN:C	1:G:108:THR:H	2.16	0.52
1:A:240:LEU:CB	1:A:242:TYR:CD2	2.92	0.52
1:B:143:TYR:HD1	1:B:147:LEU:HD12	1.73	0.52
1:C:144:PRO:HG3	1:D:161:LEU:HD11	1.91	0.52
1:D:8:ILE:HG13	1:D:140:MSE:HE2	1.92	0.52
1:F:122:THR:HA	1:G:106:GLN:CG	2.38	0.52
1:I:134:ARG:HH21	1:I:136:VAL:CB	2.23	0.52
1:E:13:PRO:HB2	1:E:15:MSE:HE3	1.92	0.52
1:E:88:TRP:HD1	3:E:2006:IPA:H12	1.74	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:B:117:HIS:CD2	1:B:125:VAL:HG21	2.45	0.52
1:B:86:LYS:HE3	1:B:101:ILE:CD1	2.39	0.52
1:B:124:THR:HG22	1:B:125:VAL:O	2.10	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:ILE:HG13	1:B:140:MSE:CE	2.36	0.51
1:D:107:GLY:HA3	1:E:106:GLN:HE22	1.75	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:G:117:HIS:HB2	1:G:125:VAL:CG2	2.40	0.51
1:I:42:HIS:HB2	1:I:50:OCS:OD2	2.11	0.51
1:A:5:ILE:HD11	1:A:140:MSE:HE1	1.92	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:A:112:ARG:O	1:A:112:ARG:NH1	2.44	0.51
1:B:86:LYS:HE3	1:B:101:ILE:HD12	1.92	0.51
1:E:2:PRO:N	1:F:10:GLU:OE1	2.44	0.51
1:G:126:ARG:NH1	1:G:145:MSE:O	2.44	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:D:111:ARG:NH2	1:E:106:GLN:HE22	2.09	0.51
1:G:3:GLY:C	1:G:5:ILE:HD12	2.35	0.51
1:H:153:GLU:HA	1:H:153:GLU:OE1	2.11	0.51
1:J:122:THR:OG1	1:J:123:HIS:CD2	2.64	0.51
1:D:193:GLU:O	1:D:197:ARG:HG3	2.10	0.51
1:E:175:TRP:CE2	1:E:176:PRO:HB3	2.46	0.51
1:F:106:GLN:C	1:F:108:THR:N	2.67	0.51
1:F:178:ASN:ND2	1:F:180:ILE:H	2.09	0.51
1:D:198:ALA:C	1:D:200:MSE:O	2.54	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
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:H:220:ARG:HH11	1:H:220:ARG:HB2	1.74	0.51
1:F:134:ARG:HG3	1:F:136:VAL:HG23	1.93	0.51
1:I:144:PRO:HD3	1:J:139:THR:OG1	2.11	0.51
1:H:5:ILE:CG2	1:H:6:PRO:HD2	2.40	0.51
1:H:112:ARG:HG2	1:H:112:ARG:NH1	2.26	0.51
1:J:4:SER:O	1:J:5:ILE:CG1	2.59	0.51
1:J:200:MSE:HE2	1:J:200:MSE:H	1.76	0.51
1:A:139:THR:OG1	1:B:144:PRO:HD3	2.11	0.51
1:A:117:HIS:CB	1:A:125:VAL:HG21	2.40	0.51
1:B:74:LEU:C	1:B:74:LEU:HD23	2.35	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:E:4:SER:C	1:E:5:ILE:HD12	2.37	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:69:VAL:CG2	1:C:158:VAL:HG11	2.39	0.50
1:E:50:OCS:OD2	1:E:126:ARG:NH2	2.44	0.50
1:E:161:LEU:HD11	1:F:144:PRO:HG3	1.92	0.50
1:G:50:OCS:OD2	1:G:126:ARG:NH2	2.44	0.50
1:H:120:SER:C	1:H:122:THR:N	2.65	0.50
1:A:240:LEU:HB3	1:A:242:TYR:CD2	2.46	0.50
1:E:223:VAL:CG1	1:E:227:ARG:NH1	2.74	0.50
1:J:36:TRP:HB2	1:J:69:VAL:HG22	1.93	0.50
1:J:106:GLN:C	1:J:108:THR:H	2.18	0.50
1:A:204:GLN:HA	1:A:204:GLN:NE2	2.25	0.50
1:A:204:GLN:O	1:A:205:TYR:HD2	1.95	0.50
1:C:74:LEU:HD23	1:C:74:LEU:C	2.37	0.50
1:D:60:ARG:HD2	1:D:151:VAL:CG1	2.41	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:J:190:PRO:HA	1:J:195:GLN:HE21	1.77	0.50
1:C:35:LYS:HD3	1:C:70:ASP:OD2	2.12	0.50
1:D:5:ILE:HG22	1:D:6:PRO:CD	2.41	0.50
1:B:103:ALA:C	1:B:105:PRO:HD3	2.36	0.50
1:D:178:ASN:HD21	1:D:180:ILE:HB	1.77	0.50
1:E:20:ASP:HB2	1:E:101:ILE:H	1.76	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:G:79:VAL:O	1:G:83:ILE:HG13	2.11	0.50
1:G:144:PRO:HD3	1:H:139:THR:HG1	1.76	0.50
1:I:117:HIS:CG	1:I:125:VAL:HG21	2.47	0.50
1:B:112:ARG:HG2	1:B:112:ARG:HH11	1.76	0.50
1:C:189:PRO:HG3	1:D:48:PRO:CD	2.42	0.50
1:H:132:ASP:C	1:H:132:ASP:OD1	2.51	0.50
1:F:204:GLN:C	1:F:205:TYR:CG	2.89	0.50
1:G:143:TYR:CD1	1:G:147:LEU:HD12	2.47	0.50
1:I:128:VAL:O	1:I:140:MSE:HA	2.11	0.50
1:I:179:GLU:OE2	1:J:59:ARG:NH1	2.44	0.50
1:J:86:LYS:HE3	1:J:101:ILE:CD1	2.42	0.50
1:J:126:ARG:HD2	1:J:144:PRO:O	2.12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:126:ARG:HB2	1:D:143:TYR:O	2.12	0.49
1:F:117:HIS:N	4:F:2047:HOH:O	2.45	0.49
1:H:75:SER:HB3	1:H:82:HIS:HE1	1.74	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:G:20:ASP:HB2	1:G:101:ILE:H	1.77	0.49
1:I:8:ILE:HG13	1:I:140:MSE:HE2	1.95	0.49
1:I:156:ARG:HD3	1:I:230:LEU:HD11	1.93	0.49
1:A:86:LYS:HE3	1:A:101:ILE:HD11	1.94	0.49
1:B:106:GLN:C	1:B:108:THR:N	2.69	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:CD1	2.42	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:G:5:ILE:HG22	1:G:6:PRO:O	2.12	0.49
1:G:147:LEU:HD13	1:G:148:GLY:O	2.13	0.49
1:J:203:GLY:C	1:J:204:GLN:HG2	2.36	0.49
1:A:134:ARG:HG3	1:A:136:VAL:HG23	1.94	0.49
1:A:240:LEU:HB3	1:A:242:TYR:HD2	1.78	0.49
1:I:186:ILE:HG21	1:J:48:PRO:HB2	1.94	0.49
1:C:4:SER:O	1:C:5:ILE:HD12	2.12	0.49
1:C:106:GLN:C	1:C:108:THR:N	2.64	0.49
1:D:144:PRO:HG2	1:D:147:LEU:HB3	1.95	0.49
1:A:144:PRO:HG2	1:A:147:LEU:HB2	1.94	0.49
1:A:150:LEU:CD2	4:A:1007:HOH:O	2.59	0.49
1:D:96:ARG:O	1:D:98:PRO:HD3	2.13	0.49
1:H:143:TYR:HD1	1:H:147:LEU:HD12	1.78	0.49
1:A:175:TRP:CG	1:A:176:PRO:HA	2.48	0.49
3:B:2005:IPA:H32	1:C:84:LYS:HZ1	1.78	0.49
1:C:59:ARG:HD3	1:D:179:GLU:CD	2.38	0.49
1:D:117:HIS:HB2	1:D:125:VAL:CG1	2.43	0.49
1:E:74:LEU:HD23	1:E:75:SER:N	2.28	0.49
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: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:G:37:PHE:CE1	1:G:131:VAL:HG11	2.48	0.48
1:G:48:PRO:CB	1:H:186:ILE:HG21	2.44	0.48
1:B:5:ILE:HD12	1:B:5:ILE:O	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:50:OCS:OD1	1:D:50:OCS:N	2.47	0.48
1:E:74:LEU:HD23	1:E:74:LEU:C	2.38	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:20:ASP:OD1	1:F:101:ILE:HB	2.13	0.48
1:F:107:GLY:H	1:G:106:GLN:HE22	1.60	0.48
1:G:59:ARG:HG3	1:G:59:ARG:NH1	2.25	0.48
1:G:146:GLU:HG3	4:H:2041:HOH:O	2.13	0.48
1:H:84:LYS:NZ	3:H:2009:IPA:C3	2.77	0.48
1:C:121:ALA:O	1:C:122:THR:O	2.31	0.48
1:G:199:ARG:O	1:G:201:GLU:N	2.44	0.48
1:I:86:LYS:HE3	1:I:101:ILE:CD1	2.44	0.48
1:J:202:SER:C	1:J:204:GLN:H	1.81	0.48
1:B:88:TRP:HD1	3:B:2005:IPA:H33	1.78	0.48
1:D:60:ARG:HG3	1:D:60:ARG:HH11	1.79	0.48
1:D:117:HIS:N	4:D:2043:HOH:O	2.46	0.48
1:G:50:OCS:HD2	1:G:126:ARG:NH2	2.10	0.48
1:I:117:HIS:CE1	1:J:140:MSE:HE1	2.48	0.48
1:J:147:LEU:HD13	1:J:148:GLY:O	2.14	0.48
1:A:239:LYS:HE2	1:A:241:LEU:HD12	1.95	0.48
1:B:201:GLU:CB	1:B:205:TYR:O	2.55	0.48
1:C:5:ILE:HG13	1:C:114:GLY:HA3	1.95	0.48
1:C:241:LEU:HD23	1:C:241:LEU:H	1.77	0.48
1:D:74:LEU:C	1:D:74:LEU:HD23	2.39	0.48
1:D:156:ARG:HD3	1:D:230:LEU:HD11	1.96	0.48
1:G:199:ARG:C	1:G:201:GLU:H	2.22	0.48
1:I:126:ARG:HG3	1:I:126:ARG:HH11	1.79	0.48
1:J:157:ILE:O	1:J:161:LEU:HB2	2.13	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
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:172:PRO:HG2	1:A:175:TRP:HB2	1.96	0.48
1:D:40:PHE:HZ	1:D:99:PHE:CE2	2.32	0.47
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:C:214:TRP:HZ2	1:D:242:TYR:CD1	2.32	0.47
1:D:67:LEU:O	1:D:162:LYS:HE2	2.14	0.47
1:D:79:VAL:O	1:D:83:ILE:HG13	2.14	0.47
1:A:200:MSE:HE3	1:A:200:MSE:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:239:LYS:O	1:E:240:LEU:HB2	2.14	0.47
1:H:4:SER:C	1:H:5:ILE:CD1	2.75	0.47
1:J:4:SER:C	1:J:5:ILE:HD12	2.38	0.47
1:C:42:HIS:CE1	1:C:85:TRP:CZ3	3.03	0.47
1:C:124:THR:CG2	1:C:125:VAL:N	2.77	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
3:B:2005:IPA:C3	1:C:84:LYS:HZ3	2.27	0.47
1:C:48:PRO:CB	1:D:186:ILE:HG21	2.45	0.47
1:F:125:VAL:HG22	4:F:2047:HOH:O	2.14	0.47
1:H:146:GLU:OE1	1:H:146:GLU:N	2.40	0.47
1:I:59:ARG:NH1	1:I:241:LEU:HD11	2.30	0.47
1:I:134:ARG:HH21	1:I:136:VAL:HB	1.79	0.47
1:A:40:PHE:HZ	1:A:99:PHE:CE2	2.33	0.47
1:A:117:HIS:HB2	1:A:125:VAL:HG22	1.97	0.47
1:B:178:ASN:HD21	1:B:180:ILE:HB	1.79	0.47
1:F:192:THR:OG1	1:F:195:GLN:HG3	2.15	0.47
1:F:204:GLN:HG3	4:F:2058:HOH:O	2.15	0.47
1:I:126:ARG:HH11	1:I:145:MSE:HA	1.79	0.47
1:I:183:GLU:HG2	4:I:311:HOH:O	2.15	0.47
1:J:117:HIS:HB2	1:J:125:VAL:CG1	2.45	0.47
1:C:139:THR:HG1	1:D:144:PRO:HD3	1.79	0.47
1:C:214:TRP:CZ2	1:D:242:TYR:CD1	3.02	0.47
1:F:14:GLU:OE1	1:F:27:PRO:HD3	2.14	0.47
1:G:132:ASP:OD2	1:G:134:ARG:NH1	2.48	0.47
1:H:205:TYR:O	1:H:206:ARG:C	2.57	0.47
1:I:5:ILE:HD11	1:J:5:ILE:HG12	1.96	0.47
1:G:117:HIS:CB	1:G:125:VAL:HG21	2.44	0.47
1:H:167:LEU:HD13	1:H:217:PRO:HG2	1.97	0.47
1:I:55:VAL:O	1:I:59:ARG:HG2	2.15	0.47
1:J:120:SER:O	1:J:122:THR:O	2.32	0.47
1:J:200:MSE:HE3	1:J:202:SER:O	2.15	0.47
1:D:93:ILE:HG22	1:D:95:VAL:HG12	1.97	0.47
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:J:202:SER:C	1:J:204:GLN:N	2.46	0.47
1:A:39:LEU:C	1:A:39:LEU:HD23	2.40	0.46
1:C:201:GLU:HB2	1:C:202:SER:H	1.17	0.46
1:D:76:VAL:O	1:D:76:VAL:HG12	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:214:TRP:N	1:D:214:TRP:CD1	2.82	0.46
1:E:141:LEU:HD22	1:F:141:LEU:HD22	1.97	0.46
1:I:199:ARG:HD2	4:I:271:HOH:O	2.15	0.46
1:C:3:GLY:C	1:C:5:ILE:HD12	2.39	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:B:14:GLU:CG	1:B:25:LYS:HE2	2.45	0.46
1:B:146:GLU:OE1	1:B:146:GLU:N	2.47	0.46
1:F:84:LYS:HA	1:F:84:LYS:HD2	1.76	0.46
1:G:124:THR:HG22	1:G:125:VAL:O	2.16	0.46
1:J:215:ASP:OD1	1:J:215:ASP:N	2.48	0.46
1:H:183:GLU:HG2	4:H:2053:HOH:O	2.15	0.46
1:A:48:PRO:HB2	1:B:186:ILE:HG21	1.96	0.46
1:C:39:LEU:C	1:C:39:LEU:HD23	2.41	0.46
1:C:150:LEU:CD2	4:C:282:HOH:O	2.57	0.46
1:B:92:HIS:HE1	3:B:2005:IPA:O2	1.98	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:A:169:ARG:HB3	1:A:185:LEU:HB3	1.97	0.46
1:F:107:GLY:N	1:G:106:GLN:HE22	2.13	0.46
1:J:60:ARG:HG3	1:J:60:ARG:HH11	1.80	0.46
1:B:106:GLN:HG2	1:C:122:THR:HA	1.96	0.46
1:C:86:LYS:HE2	1:C:97:ILE:CG2	2.46	0.46
1:E:121:ALA:O	1:E:122:THR:O	2.33	0.46
1:F:5:ILE:HG22	1:F:6:PRO:N	2.30	0.46
1:H:220:ARG:HB2	1:H:220:ARG:NH1	2.31	0.46
1:I:36:TRP:HB2	1:I:69:VAL:HG22	1.96	0.46
1:J:59:ARG:HG3	1:J:59:ARG:HH11	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:B:42:HIS:CE1	1:B:54:PHE:HE1	2.33	0.46
1:F:125:VAL:CG2	4:F:2047:HOH:O	2.63	0.46
3:B:2005:IPA:H32	1:C:84:LYS:HZ3	1.81	0.45
1:D:103:ALA:C	1:D:105:PRO:HD3	2.41	0.45
1:D:143:TYR:HD1	1:D:147:LEU:HD12	1.81	0.45
1:J:128:VAL:O	1:J:140:MSE:HA	2.16	0.45
1:J:190:PRO:HA	1:J:195:GLN:NE2	2.30	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:I:201:GLU:OE1	1:I:206:ARG:CA	2.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:200:MSE:O	1:J:201:GLU:C	2.60	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:C:103:ALA:C	1:C:105:PRO:HD3	2.41	0.45
1:G:208:LEU:HD23	1:G:208:LEU:HA	1.82	0.45
1:I:14:GLU:CG	1:I:25:LYS:HE2	2.47	0.45
1:I:236:LYS:HD2	1:J:227:ARG:NH1	2.31	0.45
1:C:21:HIS:CG	1:C:100:PRO:HB3	2.51	0.45
1:C:189:PRO:HG3	1:D:48:PRO:CG	2.47	0.45
1:D:43:PRO:O	1:D:123:HIS:ND1	2.47	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:I:15:MSE:HE2	1:I:112:ARG:HG2	1.98	0.45
1:D:7:LEU:HB2	1:D:10:GLU:HG3	1.99	0.45
1:D:97:ILE:HD13	1:D:97:ILE:N	2.31	0.45
1:E:122:THR:O	1:E:123:HIS:O	2.35	0.45
1:G:111:ARG:HG2	1:G:116:LEU:HD22	1.99	0.45
1:I:117:HIS:ND1	1:J:7:LEU:HB3	2.31	0.45
1:I:126:ARG:HB2	1:I:143:TYR:O	2.16	0.45
1:C:124:THR:HG22	1:C:125:VAL:N	2.30	0.45
1:F:5:ILE:CG2	1:F:6:PRO:N	2.80	0.45
1:F:199:ARG:C	1:F:201:GLU:N	2.74	0.45
1:I:188:PRO:HA	1:I:189:PRO:HD3	1.88	0.45
1:A:208:LEU:HD23	1:A:208:LEU:HA	1.80	0.45
1:A:215:ASP:OD1	1:A:217:PRO:HD3	2.17	0.45
1:B:183:GLU:HG2	4:B:2072:HOH:O	2.17	0.45
1:C:93:ILE:HD13	1:D:180:ILE:HD13	1.97	0.45
1:E:197:ARG:O	1:E:201:GLU:HB2	2.17	0.45
1:F:3:GLY:O	1:F:5:ILE:HD12	2.16	0.45
1:F:115:LEU:HB3	1:F:124:THR:HG23	1.99	0.45
1:G:221:ASP:OD2	4:G:2074:HOH:O	2.21	0.45
1:I:201:GLU:HG3	1:I:205:TYR:O	2.16	0.45
1:A:117:HIS:HB2	1:A:125:VAL:HG21	1.98	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:D:204:GLN:HB3	1:D:205:TYR:CD1	2.52	0.45
1:F:84:LYS:HZ2	3:G:2008:IPA:H32	1.82	0.45
1:G:62:GLU:HG2	4:G:2033:HOH:O	2.17	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:H:74:LEU:C	1:H:74:LEU:HD23	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:147:LEU:HD13	1:H:148:GLY:O	2.16	0.45
1:A:42:HIS:HD1	1:A:50:OCS:CB	2.31	0.44
1:D:199:ARG:C	1:D:200:MSE:O	2.50	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:C:242:TYR:OH	1:D:206:ARG:NH1	2.50	0.44
1:D:146:GLU:OE1	1:D:146:GLU:N	2.44	0.44
1:D:231:ARG:O	1:D:235:GLU:HG3	2.17	0.44
1:E:126:ARG:HH11	1:E:145:MSE:HA	1.81	0.44
1:G:115:LEU:O	1:G:125:VAL:HG23	2.16	0.44
1:I:42:HIS:CE1	1:I:75:SER:CB	2.96	0.44
1:J:188:PRO:HA	1:J:189:PRO:HD3	1.80	0.44
1:A:3:GLY:O	1:B:4:SER:HA	2.16	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:E:2:PRO:N	1:F:10:GLU:CD	2.75	0.44
1:G:203:GLY:C	1:G:205:TYR:N	2.74	0.44
1:J:205:TYR:O	1:J:206:ARG:C	2.60	0.44
1:A:7:LEU:HD22	1:B:117:HIS:CD2	2.51	0.44
1:C:242:TYR:CD2	1:D:214:TRP:CZ2	3.05	0.44
1:E:20:ASP:OD2	1:E:86:LYS:CE	2.66	0.44
1:F:189:PRO:HA	1:F:190:PRO:HD3	1.81	0.44
1:G:55:VAL:O	1:G:59:ARG:HG2	2.18	0.44
1:I:36:TRP:CD2	1:I:132:ASP:HA	2.53	0.44
1:I:117:HIS:ND1	1:J:8:ILE:N	2.64	0.44
1:A:122:THR:O	1:A:123:HIS:HB2	2.17	0.44
1:B:119:GLU:O	1:B:120:SER:OG	2.27	0.44
1:J:220:ARG:HB2	1:J:220:ARG:HH11	1.82	0.44
1:B:106:GLN:CG	1:C:122:THR:HA	2.48	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:B:138:ARG:NH2	1:B:165:ASP:OD1	2.50	0.44
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:I:199:ARG:CD	4:I:271:HOH:O	2.65	0.44
1:I:49:VAL:HG12	1:I:126:ARG:NH2	2.33	0.44
1:I:50:OCS:OD2	1:I:126:ARG:NH2	2.50	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:42:HIS:HD2	1:E:74:LEU:O	2.01	0.44
1:G:242:TYR:CD1	1:G:242:TYR:C	2.95	0.44
1:H:5:ILE:CG2	1:H:6:PRO:CD	2.95	0.44
1:J:147:LEU:HD13	1:J:147:LEU:C	2.42	0.44
1:A:199:ARG:O	1:A:200:MSE:HE3	2.17	0.43
1:E:175:TRP:CG	1:E:176:PRO:HA	2.53	0.43
1:G:103:ALA:C	1:G:105:PRO:HD3	2.43	0.43
1:G:175:TRP:CD1	1:G:176:PRO:HA	2.53	0.43
1:H:42:HIS:CD2	1:H:50:OCS:HD2	2.36	0.43
1:H:60:ARG:HG3	1:H:60:ARG:HH11	1.82	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:E:86:LYS:HE2	1:E:97:ILE:HG22	1.99	0.43
1:E:117:HIS:CD2	1:E:125:VAL:HG11	2.52	0.43
1:G:42:HIS:CE1	1:G:54:PHE:HE1	2.36	0.43
1:G:117:HIS:HB2	1:G:125:VAL:HG22	1.98	0.43
1:H:4:SER:CA	1:H:5:ILE:HD12	2.45	0.43
1:C:48:PRO:HB2	1:D:186:ILE:HG21	2.00	0.43
1:E:86:LYS:HE2	1:E:97:ILE:CG2	2.48	0.43
1:E:200:MSE:C	1:E:201:GLU:OE1	2.61	0.43
1:F:138:ARG:NH2	1:F:165:ASP:CG	2.76	0.43
1:G:36:TRP:CD2	1:G:132:ASP:HA	2.54	0.43
1:I:121:ALA:C	1:I:122:THR:HG23	2.42	0.43
1:J:3:GLY:O	1:J:5:ILE:CD1	2.66	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:E:39:LEU:C	1:E:39:LEU:CD2	2.90	0.43
1:H:220:ARG:NH2	4:H:2083:HOH:O	2.47	0.43
1:C:210:TRP:CZ3	1:C:211:TRP:HB3	2.53	0.43
1:D:4:SER:N	1:D:5:ILE:HD12	2.33	0.43
1:G:54:PHE:CE2	1:G:101:ILE:CD1	3.01	0.43
1:H:199:ARG:C	1:H:200:MSE:HE3	2.30	0.43
1:H:239:LYS:NZ	1:H:239:LYS:HB3	2.33	0.43
1:I:20:ASP:HB3	1:I:21:HIS:CD2	2.54	0.43
1:I:48:PRO:CG	1:J:189:PRO:HG3	2.48	0.43
1:A:144:PRO:HG2	1:A:147:LEU:CB	2.48	0.43
1:D:119:GLU:OE2	1:D:145:MSE:HB2	2.18	0.43
3:D:2003:IPA:H11	4:E:2052:HOH:O	2.18	0.43
1:F:235:GLU:CD	4:F:2081:HOH:O	2.62	0.43
1:J:50:OCS:SG	1:J:126:ARG:NH2	2.91	0.43
1:A:74:LEU:HD23	1:A:75:SER:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:75:SER:HB3	1:D:82:HIS:HE1	1.82	0.43
1:E:3:GLY:O	1:E:5:ILE:HD12	2.19	0.43
1:E:99:PHE:HB2	1:E:100:PRO:HD2	2.01	0.43
1:G:54:PHE:CE2	1:G:101:ILE:HD11	2.50	0.43
1:J:74:LEU:C	1:J:74:LEU:CD2	2.92	0.43
1:H:210:TRP:CZ3	1:H:211:TRP:HB3	2.54	0.43
1:I:53:GLU:HG2	1:J:173:ALA:HB2	2.00	0.43
1:J:163:LEU:HA	1:J:163:LEU:HD23	1.76	0.43
1:F:117:HIS:CB	1:F:125:VAL:HG21	2.47	0.43
1:G:125:VAL:HG12	1:G:126:ARG:N	2.34	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:A:122:THR:HA	1:J:106:GLN:HG2	2.01	0.43
1:B:139:THR:HG22	1:B:140:MSE:N	2.34	0.43
1:D:117:HIS:CD2	1:D:125:VAL:HG11	2.54	0.43
1:F:74:LEU:C	1:F:74:LEU:CD2	2.89	0.43
1:I:48:PRO:HD2	4:I:274:HOH:O	2.18	0.43
1:I:61:TYR:HD2	1:I:71:LEU:HD12	1.83	0.43
1:I:117:HIS:CE1	1:J:140:MSE:CE	2.95	0.43
1:I:150:LEU:HD22	4:J:2025:HOH:O	2.17	0.43
1:I:156:ARG:HD2	1:I:175:TRP:O	2.19	0.43
1:J:5:ILE:CG2	1:J:6:PRO:O	2.65	0.43
1:J:35:LYS:HD3	1:J:70:ASP:OD2	2.19	0.43
1:B:200:MSE:HE3	1:B:200:MSE:O	2.19	0.42
1:E:200:MSE:CG	1:E:201:GLU:OE1	2.64	0.42
1:H:72:ILE:HG13	1:H:100:PRO:HG2	2.01	0.42
1:H:190:PRO:HB3	1:H:195:GLN:HB3	2.02	0.42
1:I:107:GLY:O	1:I:108:THR:C	2.62	0.42
1:J:104:ASP:N	1:J:105:PRO:HD3	2.34	0.42
1:A:96:ARG:NH2	1:I:197:ARG:HE	2.17	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:HD23	1:D:185:LEU:HA	1.65	0.42
1:J:72:ILE:O	1:J:72:ILE:HG23	2.18	0.42
1:B:36:TRP:CD2	1:B:132:ASP:HA	2.54	0.42
1:C:4:SER:HA	1:D:4:SER:HA	2.01	0.42
1:E:106:GLN:CA	1:E:106:GLN:HE21	2.30	0.42
1:E:120:SER:C	1:E:121:ALA:O	2.57	0.42
1:E:186:ILE:HG21	1:F:48:PRO:HG2	2.01	0.42
1:F:41:SER:HB2	1:F:124:THR:HG21	2.01	0.42
1:G:211:TRP:H	1:G:211:TRP:CD1	2.36	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:90:GLU:OE2	1:H:96:ARG:NE	2.36	0.42
1:J:7:LEU:HB2	1:J:10:GLU:HG3	2.01	0.42
1:J:128:VAL:HG23	1:J:149:ARG:HH11	1.84	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:25:LYS:HD3	1:F:28:ASP:CG	2.43	0.42
1:F:125:VAL:CG1	1:F:126:ARG:H	2.32	0.42
1:F:161:LEU:HD12	1:F:161:LEU:HA	1.82	0.42
1:J:200:MSE:O	1:J:201:GLU:O	2.38	0.42
1:A:47:THR:HA	1:A:48:PRO:HD3	1.81	0.42
1:C:70:ASP:OD1	4:C:284:HOH:O	2.21	0.42
1:E:5:ILE:HB	1:F:5:ILE:HD13	2.01	0.42
1:G:107:GLY:O	1:G:111:ARG:HG3	2.20	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:J:191:THR:H	1:J:195:GLN:NE2	2.17	0.42
1:E:126:ARG:HH11	1:E:126:ARG:HG3	1.83	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:I:146:GLU:OE1	1:I:146:GLU:N	2.45	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: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:D:55:VAL:O	1:D:59:ARG:HG2	2.19	0.42
1:E:84:LYS:HD2	1:E:84:LYS:HA	1.90	0.42
1:F:239:LYS:O	1:F:240:LEU:HB2	2.20	0.42
1:H:212:PHE:CD1	1:H:212:PHE:C	2.98	0.42
1:I:74:LEU:C	1:I:74:LEU:CD2	2.93	0.42
1:I:134:ARG:HE	1:I:134:ARG:HB2	1.73	0.42
1:J:76:VAL:O	1:J:76:VAL:HG12	2.19	0.42
1:A:124:THR:CG2	1:A:125:VAL:N	2.81	0.42
1:A:146:GLU:OE1	1:A:146:GLU:N	2.45	0.42
1:B:59:ARG:HG3	1:B:59:ARG:NH1	2.32	0.42
1:B:120:SER:HA	4:B:2064:HOH:O	2.20	0.42
1:E:223:VAL:HG12	1:E:227:ARG:NH1	2.34	0.42
1:H:191:THR:H	1:H:195:GLN:HE22	1.64	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:D:198:ALA:O	1:D:200:MSE:O	2.37	0.42
1:E:76:VAL:O	1:E:105:PRO:HA	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:117:HIS:CB	1:D:125:VAL:HG11	2.50	0.41
1:D:163:LEU:HD23	1:D:163:LEU:HA	1.85	0.41
1:G:147:LEU:HD21	1:H:160:ALA:HB3	2.02	0.41
1:I:212:PHE:C	1:I:212:PHE:CD1	2.98	0.41
1:A:8:ILE:HG13	1:A:140:MSE:HE2	2.02	0.41
1:A:144:PRO:HB2	1:A:146:GLU:CD	2.45	0.41
1:B:200:MSE:O	1:B:200:MSE:CE	2.68	0.41
1:C:116:LEU:HA	1:C:116:LEU:HD12	1.76	0.41
1:C:241:LEU:HD23	1:C:241:LEU:N	2.35	0.41
1:D:20:ASP:HB2	1:D:101:ILE:H	1.84	0.41
1:G:153:GLU:O	1:G:157:ILE:HG13	2.20	0.41
1:H:111:ARG:HE	1:H:116:LEU:CD2	2.31	0.41
1:J:19:THR:HG21	1:J:24:ILE:HD12	2.02	0.41
1:J:156:ARG:HD3	1:J:230:LEU:HD11	2.02	0.41
1:C:14:GLU:CG	1:C:25:LYS:HE2	2.50	0.41
1:D:105:PRO:HB2	1:E:122:THR:HB	2.02	0.41
1:E:132:ASP:C	1:E:132:ASP:OD1	2.64	0.41
1:G:56:SER:OG	1:G:151:VAL:HG21	2.19	0.41
1:I:157:ILE:O	1:I:161:LEU:HB2	2.20	0.41
1:A:206:ARG:HH11	1:A:215:ASP:HA	1.86	0.41
1:C:157:ILE:O	1:C:161:LEU:HB2	2.21	0.41
1:C:214:TRP:CD1	1:C:214:TRP:N	2.88	0.41
1:F:106:GLN:HA	1:F:106:GLN:HE21	1.85	0.41
1:G:186:ILE:HD13	1:H:48:PRO:HB2	2.03	0.41
1:H:122:THR:O	1:H:123:HIS:HB2	2.19	0.41
1:I:48:PRO:HG3	1:J:189:PRO:HG3	2.02	0.41
1:C:119:GLU:OE1	1:D:8:ILE:HG21	2.20	0.41
1:D:36:TRP:CD2	1:D:132:ASP:HA	2.55	0.41
1:F:104:ASP:N	1:F:105:PRO:HD3	2.36	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:D:199:ARG:HD2	4:D:2053:HOH:O	2.20	0.41
1:H:138:ARG:C	1:H:139:THR:HG1	2.26	0.41
1:A:146:GLU:CD	1:A:146:GLU:H	2.27	0.41
1:B:220:ARG:O	1:B:224:GLU:HG3	2.20	0.41
1:D:4:SER:CA	1:D:5:ILE:HD12	2.51	0.41
1:E:117:HIS:CB	1:E:125:VAL:HG11	2.51	0.41
1:E:144:PRO:HG2	1:E:147:LEU:CB	2.50	0.41
1:I:189:PRO:HA	1:I:190:PRO:HD3	1.92	0.41
1:J:106:GLN:C	1:J:108:THR:N	2.79	0.41
1:B:7:LEU:HB2	1:B:10:GLU:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:201:GLU:O	1:C:202:SER:CB	2.68	0.41
1:D:203:GLY:O	1:D:204:GLN:C	2.63	0.41
1:E:48:PRO:HD3	1:F:189:PRO:HG3	2.02	0.41
1:G:199:ARG:C	1:G:201:GLU:N	2.78	0.41
1:I:7:LEU:HB3	1:J:117:HIS:CG	2.56	0.41
1:A:14:GLU:O	1:A:15:MSE:HB3	2.21	0.41
1:A:42:HIS:HD1	1:A:50:OCS:HB2	1.85	0.41
1:A:188:PRO:HA	1:A:189:PRO:HD3	1.81	0.41
1:B:139:THR:CG2	1:B:140:MSE:N	2.84	0.41
1:C:2:PRO:C	1:D:7:LEU:HD11	2.46	0.41
1:C:59:ARG:HH11	1:D:179:GLU:HG2	1.86	0.41
1:C:86:LYS:HE2	1:C:97:ILE:HG22	2.03	0.41
1:C:144:PRO:HD3	1:D:139:THR:OG1	2.21	0.41
1:C:191:THR:H	1:C:195:GLN:NE2	2.19	0.41
1:C:201:GLU:N	1:C:201:GLU:CD	2.77	0.41
1:E:42:HIS:HE2	1:E:75:SER:CB	2.30	0.41
1:E:70:ASP:OD1	4:E:2021:HOH:O	2.21	0.41
1:H:5:ILE:CG2	1:H:6:PRO:N	2.84	0.41
1:H:93:ILE:HG22	1:H:95:VAL:HG12	2.01	0.41
1:I:116:LEU:HD12	1:I:116:LEU:HA	1.80	0.41
1:I:120:SER:C	1:I:121:ALA:O	2.59	0.41
1:I:125:VAL:HG23	1:I:125:VAL:H	1.42	0.41
1:J:193:GLU:HB3	1:J:197:ARG:HH12	1.86	0.41
1:B:13:PRO:HB2	1:B:15:MSE:HE3	2.03	0.41
1:C:42:HIS:CD2	1:C:75:SER:HB2	2.54	0.41
1:E:176:PRO:HG2	1:E:227:ARG:HG3	2.03	0.41
1:E:208:LEU:HD23	1:E:208:LEU:HA	1.91	0.41
1:I:178:ASN:ND2	1:I:180:ILE:N	2.65	0.41
1:I:189:PRO:HG3	1:J:48:PRO:HD3	2.03	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:F:3:GLY:O	1:F:5:ILE:CD1	2.69	0.40
1:F:20:ASP:HB2	1:F:101:ILE:H	1.85	0.40
1:F:39:LEU:HD23	1:F:40:PHE:N	2.36	0.40
1:G:76:VAL:O	1:G:76:VAL:HG12	2.21	0.40
1:G:161:LEU:HD12	1:G:161:LEU:HA	1.90	0.40
1:I:139:THR:OG1	1:J:144:PRO:HD3	2.21	0.40
1:I:212:PHE:C	1:I:212:PHE:HD1	2.29	0.40
1:A:179:GLU:O	1:B:240:LEU:HA	2.21	0.40
1:C:41:SER:HB2	1:C:124:THR:HG21	2.03	0.40
1:C:59:ARG:NH1	1:D:179:GLU:HG2	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:93:ILE:HG22	1:C:95:VAL:CG1	2.49	0.40
1:D:143:TYR:CD1	1:D:147:LEU:HD12	2.57	0.40
1:D:144:PRO:HG2	1:D:147:LEU:CB	2.51	0.40
1:E:236:LYS:HA	1:F:177:ASN:OD1	2.20	0.40
1:F:5:ILE:HG13	1:F:114:GLY:HA3	2.03	0.40
1:G:61:TYR:HD2	1:G:71:LEU:HD12	1.86	0.40
1:G:117:HIS:CG	1:H:7:LEU:HB3	2.56	0.40
1:J:40:PHE:HZ	1:J:99:PHE:CE2	2.40	0.40
1:J:239:LYS:O	1:J:240:LEU:HB2	2.22	0.40
1:A:36:TRP:CD2	1:A:132:ASP:HA	2.57	0.40
1:D:41:SER:HA	1:D:74:LEU:O	2.21	0.40
1:G:119:GLU:OE2	1:G:145:MSE:HB2	2.22	0.40
1:I:124:THR:HG22	1:I:125:VAL:O	2.22	0.40
1:J:40:PHE:CD2	1:J:40:PHE:N	2.88	0.40
1:A:189:PRO:HA	1:A:190:PRO:HD3	1.84	0.40
4:A:1048:HOH:O	3:J:2001:IPA:H11	2.22	0.40
1:B:36:TRP:CD1	1:B:162:LYS:HE3	2.57	0.40
1:B:125:VAL:HG12	1:B:126:ARG:N	2.36	0.40
1:C:72:ILE:O	1:C:72:ILE:HG23	2.22	0.40
1:E:67:LEU:O	1:E:162:LYS:HE2	2.21	0.40
1:E:116:LEU:HD12	1:E:116:LEU:HA	1.95	0.40
1:F:107:GLY:HA3	1:G:106:GLN:HE22	1.86	0.40
1:F:175:TRP:CD1	1:F:176:PRO:HA	2.56	0.40
1:G:4:SER:C	1:G:5:ILE:CG1	2.94	0.40
1:G:231:ARG:HG3	1:G:231:ARG:NH1	2.37	0.40
1:C:67:LEU:O	1:C:162:LYS:HE2	2.22	0.40
1:E:128:VAL:O	1:E:140:MSE:HA	2.22	0.40
1:F:39:LEU:C	1:F:39:LEU:CD2	2.93	0.40
1:F:59:ARG:HE	1:F:59:ARG:HB3	1.52	0.40
1:H:79:VAL:O	1:H:83:ILE:HG13	2.22	0.40
1:H:185:LEU:HD23	1:H:185:LEU:HA	1.81	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

5.3.1 Protein backbone

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

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

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

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
1	D	48	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	207/210 (99%)	185 (89%)	22 (11%)	6	8
1	B	207/210 (99%)	190 (92%)	17 (8%)	10	14
1	C	207/210 (99%)	189 (91%)	18 (9%)	9	12
1	D	208/210 (99%)	188 (90%)	20 (10%)	8	10
1	E	206/210 (98%)	186 (90%)	20 (10%)	8	10
1	F	206/210 (98%)	190 (92%)	16 (8%)	11	16
1	G	208/210 (99%)	191 (92%)	17 (8%)	10	14
1	H	206/210 (98%)	192 (93%)	14 (7%)	14	20
1	I	207/210 (99%)	187 (90%)	20 (10%)	8	10
1	J	206/210 (98%)	193 (94%)	13 (6%)	16	23
All	All	2068/2100 (98%)	1891 (91%)	177 (9%)	10	13

All (177) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	8	ILE
1	A	11	ARG
1	A	14	GLU
1	A	24	ILE
1	A	62	GLU
1	A	95	VAL
1	A	97	ILE
1	A	98	PRO
1	A	116	LEU
1	A	122	THR
1	A	126	ARG

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Mol	Chain	Res	Type
1	A	147	LEU
1	A	150	LEU
1	A	200	MSE
1	A	204	GLN
1	A	217	PRO
1	A	224	GLU
1	A	230	LEU
1	A	235	GLU
1	A	239	LYS
1	A	241	LEU
1	B	11	ARG
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	205	TYR
1	B	206	ARG
1	B	217	PRO
1	B	230	LEU
1	B	239	LYS
1	B	242	TYR
1	C	5	ILE
1	C	11	ARG
1	C	27	PRO
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	230	LEU
1	C	235	GLU

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Mol	Chain	Res	Type
1	C	239	LYS
1	C	241	LEU
1	C	242	TYR
1	D	14	GLU
1	D	20	ASP
1	D	70	ASP
1	D	95	VAL
1	D	97	ILE
1	D	116	LEU
1	D	122	THR
1	D	134	ARG
1	D	150	LEU
1	D	161	LEU
1	D	183	GLU
1	D	200	MSE
1	D	201	GLU
1	D	204	GLN
1	D	205	TYR
1	D	230	LEU
1	D	231	ARG
1	D	239	LYS
1	D	242	TYR
1	D	243	GLU
1	E	11	ARG
1	E	20	ASP
1	E	70	ASP
1	E	95	VAL
1	E	97	ILE
1	E	116	LEU
1	E	124	THR
1	E	138	ARG
1	E	150	LEU
1	E	161	LEU
1	E	200	MSE
1	E	201	GLU
1	E	204	GLN
1	E	205	TYR
1	E	217	PRO
1	E	220	ARG
1	E	228	ARG
1	E	230	LEU
1	E	239	LYS

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Mol	Chain	Res	Type
1	E	240	LEU
1	F	14	GLU
1	F	20	ASP
1	F	35	LYS
1	F	59	ARG
1	F	66	ARG
1	F	97	ILE
1	F	116	LEU
1	F	138	ARG
1	F	150	LEU
1	F	161	LEU
1	F	200	MSE
1	F	201	GLU
1	F	205	TYR
1	F	224	GLU
1	F	230	LEU
1	F	239	LYS
1	G	11	ARG
1	G	20	ASP
1	G	70	ASP
1	G	97	ILE
1	G	116	LEU
1	G	122	THR
1	G	138	ARG
1	G	150	LEU
1	G	161	LEU
1	G	202	SER
1	G	205	TYR
1	G	206	ARG
1	G	228	ARG
1	G	231	ARG
1	G	239	LYS
1	G	242	TYR
1	G	243	GLU
1	H	59	ARG
1	H	95	VAL
1	H	98	PRO
1	H	116	LEU
1	H	122	THR
1	H	126	ARG
1	H	161	LEU
1	H	200	MSE

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Mol	Chain	Res	Type
1	H	201	GLU
1	H	202	SER
1	H	204	GLN
1	H	206	ARG
1	H	230	LEU
1	H	239	LYS
1	I	5	ILE
1	I	11	ARG
1	I	20	ASP
1	I	28	ASP
1	I	95	VAL
1	I	97	ILE
1	I	116	LEU
1	I	117	HIS
1	I	122	THR
1	I	124	THR
1	I	125	VAL
1	I	150	LEU
1	I	161	LEU
1	I	176	PRO
1	I	200	MSE
1	I	204	GLN
1	I	217	PRO
1	I	230	LEU
1	I	239	LYS
1	I	242	TYR
1	J	5	ILE
1	J	79	VAL
1	J	95	VAL
1	J	97	ILE
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	239	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	HIS
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	123	HIS
1	B	178	ASN
1	B	195	GLN
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	92	HIS
1	D	106	GLN
1	D	178	ASN
1	D	195	GLN
1	D	204	GLN
1	E	42	HIS
1	E	92	HIS
1	E	106	GLN
1	E	123	HIS
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	29	HIS
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	29	HIS
1	H	42	HIS
1	H	92	HIS

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Mol	Chain	Res	Type
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	92	HIS
1	I	117	HIS
1	I	123	HIS
1	I	178	ASN
1	I	195	GLN
1	J	33	GLN
1	J	92	HIS
1	J	106	GLN
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	D	50	1	6,8,9	2.39	2 (33%)	7,11,13	2.70	3 (42%)
1	OCS	H	50	1	6,8,9	2.75	4 (66%)	7,11,13	1.57	2 (28%)
1	OCS	F	50	1	6,8,9	2.10	4 (66%)	7,11,13	2.97	4 (57%)
1	OCS	I	50	1	6,8,9	3.84	4 (66%)	7,11,13	3.25	3 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OCS	C	50	1	6,8,9	3.78	3 (50%)	7,11,13	1.88	3 (42%)
1	OCS	E	50	1	6,8,9	4.34	3 (50%)	7,11,13	3.14	4 (57%)
1	OCS	G	50	1	6,8,9	1.53	1 (16%)	7,11,13	2.11	3 (42%)
1	OCS	A	50	1	6,8,9	2.17	2 (33%)	7,11,13	1.58	1 (14%)
1	OCS	B	50	1	6,8,9	2.83	2 (33%)	7,11,13	2.34	3 (42%)
1	OCS	J	50	1	6,8,9	3.08	4 (66%)	7,11,13	1.60	1 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OCS	D	50	1	-	0/4/7/9	-
1	OCS	H	50	1	-	0/4/7/9	-
1	OCS	F	50	1	-	0/4/7/9	-
1	OCS	I	50	1	-	0/4/7/9	-
1	OCS	C	50	1	-	0/4/7/9	-
1	OCS	E	50	1	-	0/4/7/9	-
1	OCS	G	50	1	-	0/4/7/9	-
1	OCS	A	50	1	-	0/4/7/9	-
1	OCS	B	50	1	-	0/4/7/9	-
1	OCS	J	50	1	-	0/4/7/9	-

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	50	OCS	CB-CA	-9.15	1.47	1.53
1	I	50	OCS	OD1-SG	6.42	1.63	1.45
1	C	50	OCS	OD1-SG	6.16	1.62	1.45
1	B	50	OCS	CB-CA	-5.88	1.49	1.53
1	I	50	OCS	CB-CA	-5.38	1.49	1.53
1	J	50	OCS	OD1-SG	4.93	1.59	1.45
1	C	50	OCS	OD3-SG	4.90	1.58	1.45
1	H	50	OCS	OD1-SG	4.89	1.58	1.45
1	J	50	OCS	CB-CA	-4.59	1.50	1.53
1	C	50	OCS	OD2-SG	4.51	1.64	1.47
1	E	50	OCS	OD1-SG	4.51	1.57	1.45
1	A	50	OCS	OD1-SG	4.19	1.56	1.45
1	D	50	OCS	CB-CA	-4.09	1.50	1.53
1	D	50	OCS	OD1-SG	3.32	1.54	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	50	OCS	OD3-SG	3.25	1.54	1.45
1	B	50	OCS	OD1-SG	3.12	1.53	1.45
1	A	50	OCS	CB-CA	-3.09	1.51	1.53
1	H	50	OCS	CB-CA	-2.87	1.51	1.53
1	F	50	OCS	OD1-SG	2.84	1.53	1.45
1	F	50	OCS	CB-CA	-2.67	1.51	1.53
1	F	50	OCS	OD3-SG	2.60	1.52	1.45
1	G	50	OCS	OD1-SG	2.60	1.52	1.45
1	H	50	OCS	OD3-SG	2.37	1.51	1.45
1	H	50	OCS	OD2-SG	2.32	1.55	1.47
1	I	50	OCS	OD2-SG	2.30	1.55	1.47
1	J	50	OCS	OD3-SG	2.23	1.51	1.45
1	J	50	OCS	OD2-SG	2.16	1.55	1.47
1	E	50	OCS	OD2-SG	2.09	1.55	1.47
1	F	50	OCS	O-C	2.03	1.27	1.20

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	50	OCS	OD2-SG-CB	-6.00	94.38	105.97
1	D	50	OCS	CA-CB-SG	-5.66	105.20	113.61
1	B	50	OCS	OD2-SG-CB	-4.96	96.40	105.97
1	E	50	OCS	OD2-SG-CB	-4.83	96.65	105.97
1	I	50	OCS	CA-CB-SG	-4.46	106.98	113.61
1	F	50	OCS	OD2-SG-CB	-4.25	97.77	105.97
1	E	50	OCS	CA-CB-SG	-4.20	107.36	113.61
1	F	50	OCS	CA-CB-SG	-4.19	107.38	113.61
1	E	50	OCS	OD3-SG-CB	4.15	112.95	106.76
1	F	50	OCS	OD3-SG-CB	4.11	112.89	106.76
1	G	50	OCS	CA-CB-SG	-3.51	108.39	113.61
1	I	50	OCS	OD2-SG-OD1	3.34	119.75	111.40
1	C	50	OCS	OD2-SG-OD3	3.10	119.14	111.40
1	J	50	OCS	CA-CB-SG	-3.09	109.01	113.61
1	A	50	OCS	OD2-SG-CB	-2.76	100.64	105.97
1	H	50	OCS	OD2-SG-OD3	2.73	118.22	111.40
1	H	50	OCS	OD1-SG-CB	-2.63	102.83	106.76
1	D	50	OCS	OD3-SG-CB	2.62	110.66	106.76
1	B	50	OCS	CA-CB-SG	-2.50	109.89	113.61
1	B	50	OCS	OD2-SG-OD1	2.49	117.62	111.40
1	G	50	OCS	OD3-SG-CB	2.49	110.47	106.76
1	F	50	OCS	OD2-SG-OD3	2.35	117.28	111.40
1	E	50	OCS	OD2-SG-OD1	2.32	117.21	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	50	OCS	OD2-SG-CB	-2.30	101.53	105.97
1	C	50	OCS	CA-CB-SG	-2.19	110.35	113.61
1	C	50	OCS	OD3-SG-CB	-2.19	103.49	106.76
1	G	50	OCS	OD2-SG-OD1	2.14	116.76	111.40

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	50	OCS	3	0
1	H	50	OCS	6	0
1	F	50	OCS	3	0
1	I	50	OCS	2	0
1	C	50	OCS	1	0
1	E	50	OCS	2	0
1	G	50	OCS	4	0
1	A	50	OCS	2	0
1	B	50	OCS	1	0
1	J	50	OCS	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	$\# Z > 2$
3	IPA	H	2004	-	3,3,3	0.51	0	3,3,3	1.86	1 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MES	F	1002	-	12,12,12	1.16	0	15,16,16	0.90	1 (6%)
3	IPA	D	2003	-	3,3,3	0.34	0	3,3,3	1.84	1 (33%)
3	IPA	G	2008	-	3,3,3	0.35	0	3,3,3	1.83	1 (33%)
2	MES	A	1001	-	12,12,12	0.94	0	15,16,16	0.69	0
3	IPA	H	2009	-	3,3,3	0.63	0	3,3,3	1.73	1 (33%)
3	IPA	J	2002	-	3,3,3	0.39	0	3,3,3	1.49	1 (33%)
3	IPA	E	2006	-	3,3,3	0.62	0	3,3,3	1.75	1 (33%)
3	IPA	J	2001	-	3,3,3	0.47	0	3,3,3	1.69	1 (33%)
3	IPA	B	2005	-	3,3,3	0.60	0	3,3,3	1.54	1 (33%)
3	IPA	F	2007	-	3,3,3	0.77	0	3,3,3	1.48	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	F	1002	-	-	1/6/14/14	0/1/1/1
2	MES	A	1001	-	-	1/6/14/14	0/1/1/1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	2008	IPA	C3-C2-C1	-3.13	89.98	113.38
3	D	2003	IPA	C3-C2-C1	-3.04	90.62	113.38
3	H	2004	IPA	C3-C2-C1	-3.01	90.83	113.38
3	E	2006	IPA	C3-C2-C1	-2.96	91.27	113.38
3	H	2009	IPA	C3-C2-C1	-2.94	91.41	113.38
3	J	2001	IPA	C3-C2-C1	-2.88	91.82	113.38
3	B	2005	IPA	C3-C2-C1	-2.62	93.80	113.38
3	J	2002	IPA	C3-C2-C1	-2.55	94.33	113.38
3	F	2007	IPA	C3-C2-C1	-2.52	94.54	113.38
2	F	1002	MES	O1S-S-C8	-2.30	103.25	106.73

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	MES	C8-C7-N4-C5
2	F	1002	MES	C8-C7-N4-C5

There are no ring outliers.

10 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	2004	IPA	1	0
3	D	2003	IPA	7	0
3	G	2008	IPA	1	0
2	A	1001	MES	1	0
3	H	2009	IPA	4	0
3	J	2002	IPA	3	0
3	E	2006	IPA	3	0
3	J	2001	IPA	4	0
3	B	2005	IPA	6	0
3	F	2007	IPA	1	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 ⓘ

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, 95th 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%)	-0.36	10 (4%)	40	42	15, 27, 63, 101	0
1	B	236/250 (94%)	-0.29	16 (6%)	23	25	14, 27, 65, 98	0
1	C	236/250 (94%)	-0.22	14 (5%)	28	30	17, 28, 68, 110	0
1	D	237/250 (94%)	-0.13	10 (4%)	40	42	18, 31, 70, 102	0
1	E	235/250 (94%)	-0.14	13 (5%)	30	32	18, 33, 69, 107	0
1	F	235/250 (94%)	-0.20	14 (5%)	27	29	17, 29, 74, 100	0
1	G	237/250 (94%)	-0.15	14 (5%)	28	30	18, 31, 76, 106	0
1	H	235/250 (94%)	-0.25	14 (5%)	27	29	18, 29, 76, 102	0
1	I	236/250 (94%)	-0.17	11 (4%)	36	38	17, 32, 70, 112	0
1	J	235/250 (94%)	-0.13	14 (5%)	27	29	17, 33, 70, 109	0
All	All	2358/2500 (94%)	-0.20	130 (5%)	30	32	14, 30, 70, 112	0

All (130) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	242	TYR	5.7
1	D	5	ILE	5.4
1	G	121	ALA	5.1
1	G	4	SER	5.1
1	E	205	TYR	4.8
1	G	5	ILE	4.6
1	J	121	ALA	4.5
1	F	241	LEU	4.4
1	C	122	THR	4.1
1	H	5	ILE	4.0
1	J	106	GLN	3.9
1	F	122	THR	3.9
1	I	202	SER	3.8

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Mol	Chain	Res	Type	RSRZ
1	I	242	TYR	3.7
1	F	202	SER	3.7
1	D	242	TYR	3.7
1	D	4	SER	3.7
1	H	205	TYR	3.6
1	F	106	GLN	3.6
1	G	122	THR	3.6
1	D	121	ALA	3.6
1	C	201	GLU	3.5
1	G	124	THR	3.5
1	E	203	GLY	3.4
1	H	122	THR	3.4
1	B	204	GLN	3.4
1	C	204	GLN	3.4
1	G	204	GLN	3.4
1	I	204	GLN	3.3
1	C	124	THR	3.3
1	I	205	TYR	3.3
1	A	121	ALA	3.2
1	C	121	ALA	3.2
1	D	243	GLU	3.2
1	A	122	THR	3.2
1	H	124	THR	3.2
1	A	204	GLN	3.2
1	B	121	ALA	3.1
1	F	238	ALA	3.1
1	J	116	LEU	3.1
1	J	5	ILE	3.0
1	G	203	GLY	3.0
1	E	241	LEU	3.0
1	H	123	HIS	3.0
1	H	201	GLU	2.9
1	F	121	ALA	2.9
1	E	201	GLU	2.9
1	B	202	SER	2.9
1	B	242	TYR	2.9
1	B	238	ALA	2.9
1	H	204	GLN	2.8
1	E	238	ALA	2.8
1	H	121	ALA	2.8
1	I	201	GLU	2.8
1	J	201	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	239	LYS	2.8
1	E	121	ALA	2.8
1	I	122	THR	2.7
1	B	106	GLN	2.7
1	E	204	GLN	2.7
1	D	122	THR	2.7
1	J	4	SER	2.7
1	C	2	PRO	2.7
1	C	120	SER	2.7
1	B	124	THR	2.7
1	E	122	THR	2.7
1	F	203	GLY	2.7
1	C	202	SER	2.7
1	F	118	ALA	2.6
1	I	121	ALA	2.6
1	F	124	THR	2.6
1	B	2	PRO	2.6
1	E	202	SER	2.6
1	G	202	SER	2.6
1	J	204	GLN	2.6
1	B	119	GLU	2.6
1	D	203	GLY	2.6
1	C	242	TYR	2.6
1	H	4	SER	2.6
1	I	124	THR	2.5
1	J	241	LEU	2.5
1	H	118	ALA	2.5
1	C	203	GLY	2.5
1	D	124	THR	2.5
1	E	118	ALA	2.5
1	J	2	PRO	2.4
1	B	203	GLY	2.4
1	G	120	SER	2.4
1	A	116	LEU	2.4
1	J	3	GLY	2.3
1	D	205	TYR	2.3
1	F	205	TYR	2.3
1	A	120	SER	2.3
1	G	118	ALA	2.3
1	F	42	HIS	2.3
1	F	240	LEU	2.3
1	J	122	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	J	124	THR	2.3
1	A	42	HIS	2.3
1	J	203	GLY	2.2
1	C	4	SER	2.2
1	G	106	GLN	2.2
1	J	239	LYS	2.2
1	I	116	LEU	2.2
1	D	239	LYS	2.2
1	B	122	THR	2.2
1	C	5	ILE	2.2
1	C	116	LEU	2.2
1	F	107	GLY	2.2
1	G	123	HIS	2.2
1	A	124	THR	2.2
1	B	120	SER	2.2
1	I	239	LYS	2.2
1	B	42	HIS	2.2
1	A	205	TYR	2.1
1	A	2	PRO	2.1
1	H	42	HIS	2.1
1	E	124	THR	2.1
1	G	119	GLU	2.1
1	F	123	HIS	2.1
1	H	202	SER	2.1
1	E	123	HIS	2.1
1	H	2	PRO	2.1
1	B	116	LEU	2.0
1	C	205	TYR	2.0
1	G	205	TYR	2.0
1	H	239	LYS	2.0
1	B	201	GLU	2.0
1	I	106	GLN	2.0
1	B	241	LEU	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	OCS	A	50	9/10	0.97	0.08	20,24,36,41	0
1	OCS	G	50	9/10	0.97	0.10	23,27,37,47	0
1	OCS	I	50	9/10	0.97	0.07	27,29,37,37	0
1	OCS	J	50	9/10	0.97	0.07	23,28,36,38	0
1	OCS	E	50	9/10	0.98	0.08	22,27,37,42	0
1	OCS	F	50	9/10	0.98	0.07	20,23,35,36	0
1	OCS	B	50	9/10	0.98	0.07	23,25,33,34	0
1	OCS	H	50	9/10	0.98	0.07	24,27,30,40	0
1	OCS	C	50	9/10	0.98	0.06	24,25,34,36	0
1	OCS	D	50	9/10	0.98	0.07	16,26,38,43	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	IPA	F	2007	4/4	0.78	0.17	39,40,43,45	0
3	IPA	E	2006	4/4	0.80	0.19	52,57,61,62	0
2	MES	F	1002	12/12	0.80	0.18	70,75,82,84	0
3	IPA	H	2004	4/4	0.81	0.22	55,61,61,63	0
3	IPA	B	2005	4/4	0.86	0.15	40,42,46,47	0
3	IPA	H	2009	4/4	0.86	0.16	38,46,47,53	0
3	IPA	J	2002	4/4	0.87	0.13	38,39,39,41	0
3	IPA	J	2001	4/4	0.90	0.14	32,38,40,42	0
2	MES	A	1001	12/12	0.91	0.10	41,51,65,66	0
3	IPA	G	2008	4/4	0.91	0.14	31,34,42,46	0
3	IPA	D	2003	4/4	0.93	0.10	33,38,40,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.