



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:46 PM UTC

PDB ID : 5LNH / pdb_00005lnh
Title : Structure of full length Unliganded CodY from Bacillus subtilis
Authors : Wilkinson, A.J.; Levдикov, V.M.; Blagova, E.V.
Deposited on : 2016-08-04
Resolution : 3.00 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:

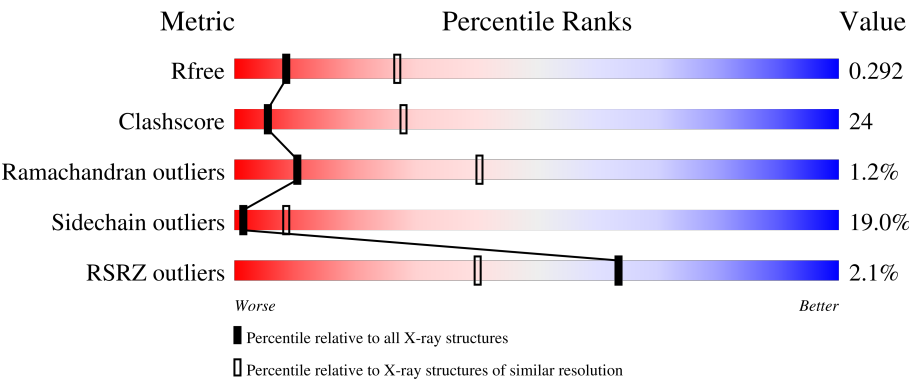
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	263	2% 51%35%10%..
1	B	263	2% 43%42%10%..
1	C	263	% 51%37%8%..
1	D	263	3% 50%35%11%..
1	E	263	3% 51%35%10%..

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Mol	Chain	Length	Quality of chain
1	F	263	2% 56% 30% 10% 2% 2%
1	G	263	2% 49% 37% 11% 2% 2%
1	H	263	2% 43% 42% 12% 2% 2%
1	I	263	2% 45% 44% 7% 2% 2%
1	K	263	0% 54% 35% 8% 2% 2%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 20090 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 GTP-sensing transcriptional pleiotropic repressor CodY.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	255	Total 2002	C 1259	N 341	O 395	Se 7	0	0	0
1	B	255	Total 2002	C 1259	N 341	O 395	Se 7	0	0	0
1	C	255	Total 2002	C 1259	N 341	O 395	Se 7	0	0	0
1	D	255	Total 2002	C 1259	N 341	O 395	Se 7	0	0	0
1	E	255	Total 2002	C 1259	N 341	O 395	Se 7	0	0	0
1	F	255	Total 2002	C 1259	N 341	O 395	Se 7	0	0	0
1	G	255	Total 2002	C 1259	N 341	O 395	Se 7	0	0	0
1	H	255	Total 2002	C 1259	N 341	O 395	Se 7	0	0	0
1	I	255	Total 2002	C 1259	N 341	O 395	Se 7	0	0	0
1	K	255	Total 2002	C 1259	N 341	O 395	Se 7	0	0	0

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	260	HIS	-	expression tag	UNP P39779
A	261	HIS	-	expression tag	UNP P39779
A	262	HIS	-	expression tag	UNP P39779
A	263	HIS	-	expression tag	UNP P39779
A	264	HIS	-	expression tag	UNP P39779
B	260	HIS	-	expression tag	UNP P39779
B	261	HIS	-	expression tag	UNP P39779
B	262	HIS	-	expression tag	UNP P39779
B	263	HIS	-	expression tag	UNP P39779

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Chain	Residue	Modelled	Actual	Comment	Reference
B	264	HIS	-	expression tag	UNP P39779
C	260	HIS	-	expression tag	UNP P39779
C	261	HIS	-	expression tag	UNP P39779
C	262	HIS	-	expression tag	UNP P39779
C	263	HIS	-	expression tag	UNP P39779
C	264	HIS	-	expression tag	UNP P39779
D	260	HIS	-	expression tag	UNP P39779
D	261	HIS	-	expression tag	UNP P39779
D	262	HIS	-	expression tag	UNP P39779
D	263	HIS	-	expression tag	UNP P39779
D	264	HIS	-	expression tag	UNP P39779
E	260	HIS	-	expression tag	UNP P39779
E	261	HIS	-	expression tag	UNP P39779
E	262	HIS	-	expression tag	UNP P39779
E	263	HIS	-	expression tag	UNP P39779
E	264	HIS	-	expression tag	UNP P39779
F	260	HIS	-	expression tag	UNP P39779
F	261	HIS	-	expression tag	UNP P39779
F	262	HIS	-	expression tag	UNP P39779
F	263	HIS	-	expression tag	UNP P39779
F	264	HIS	-	expression tag	UNP P39779
G	260	HIS	-	expression tag	UNP P39779
G	261	HIS	-	expression tag	UNP P39779
G	262	HIS	-	expression tag	UNP P39779
G	263	HIS	-	expression tag	UNP P39779
G	264	HIS	-	expression tag	UNP P39779
H	260	HIS	-	expression tag	UNP P39779
H	261	HIS	-	expression tag	UNP P39779
H	262	HIS	-	expression tag	UNP P39779
H	263	HIS	-	expression tag	UNP P39779
H	264	HIS	-	expression tag	UNP P39779
I	260	HIS	-	expression tag	UNP P39779
I	261	HIS	-	expression tag	UNP P39779
I	262	HIS	-	expression tag	UNP P39779
I	263	HIS	-	expression tag	UNP P39779
I	264	HIS	-	expression tag	UNP P39779
K	260	HIS	-	expression tag	UNP P39779
K	261	HIS	-	expression tag	UNP P39779
K	262	HIS	-	expression tag	UNP P39779
K	263	HIS	-	expression tag	UNP P39779
K	264	HIS	-	expression tag	UNP P39779

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	K	1	Total	O	S	0	0
			5	4	1		

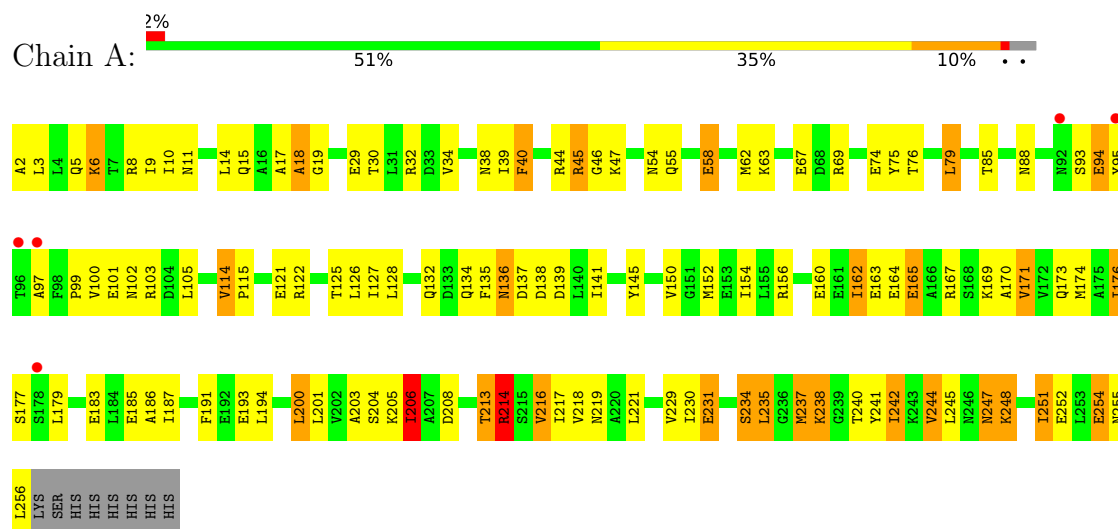
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total 4	O 4	0	0
3	B	2	Total 2	O 2	0	0
3	C	1	Total 1	O 1	0	0
3	H	1	Total 1	O 1	0	0
3	I	1	Total 1	O 1	0	0
3	K	1	Total 1	O 1	0	0

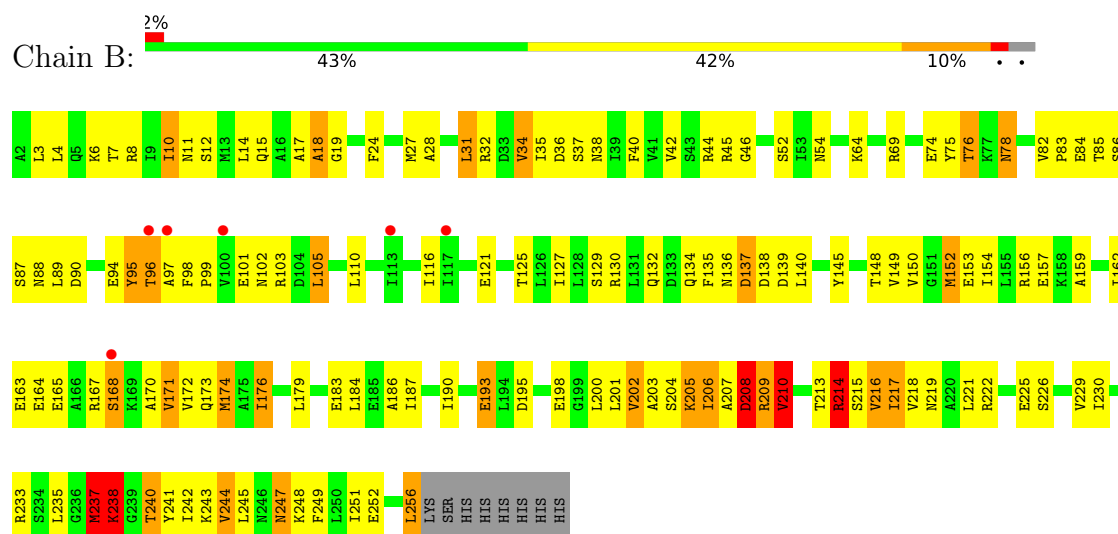
3 Residue-property plots

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: GTP-sensing transcriptional pleiotropic repressor CodY

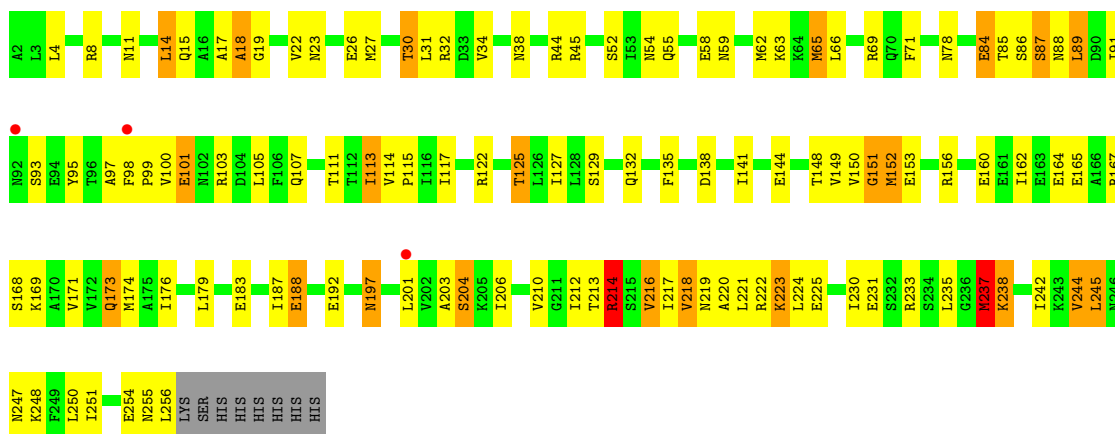


- Molecule 1: GTP-sensing transcriptional pleiotropic repressor CodY

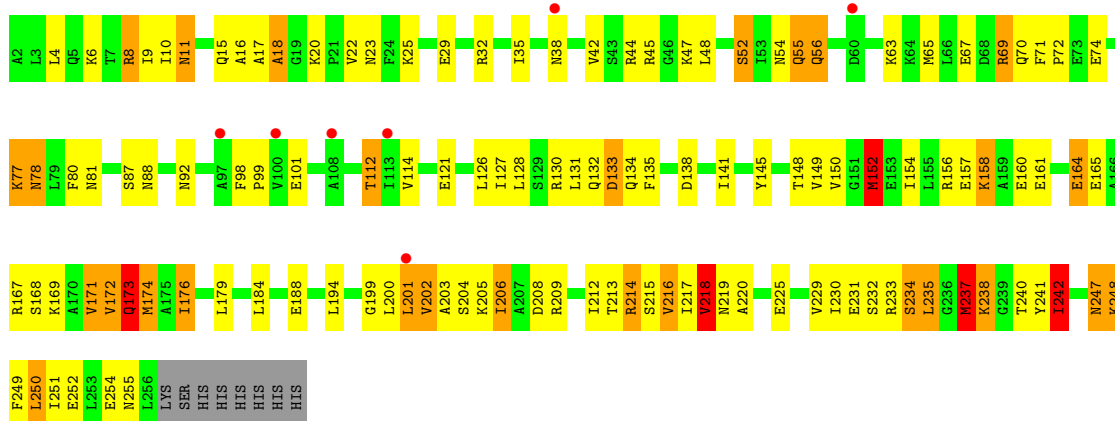


- Molecule 1: GTP-sensing transcriptional pleiotropic repressor CodY

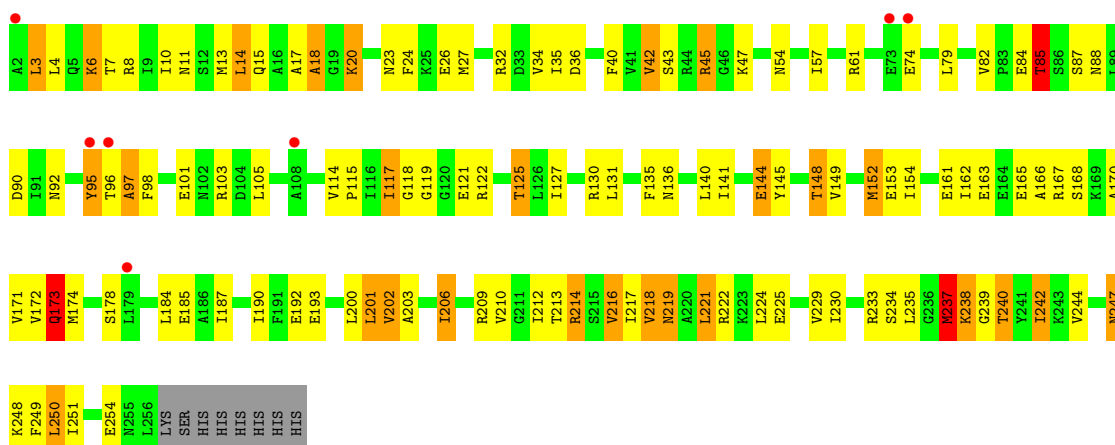




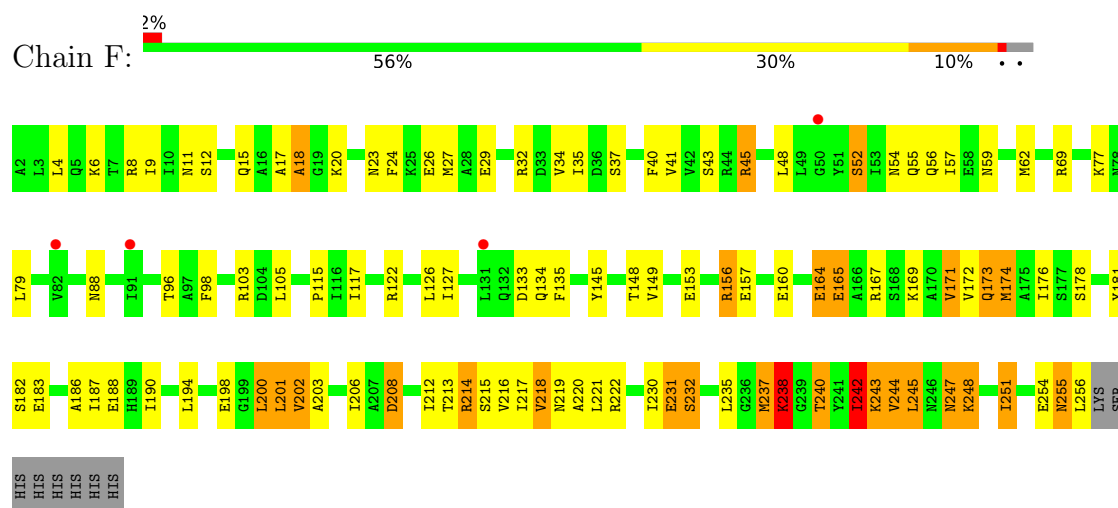
• Molecule 1: GTP-sensing transcriptional pleiotropic repressor CodY

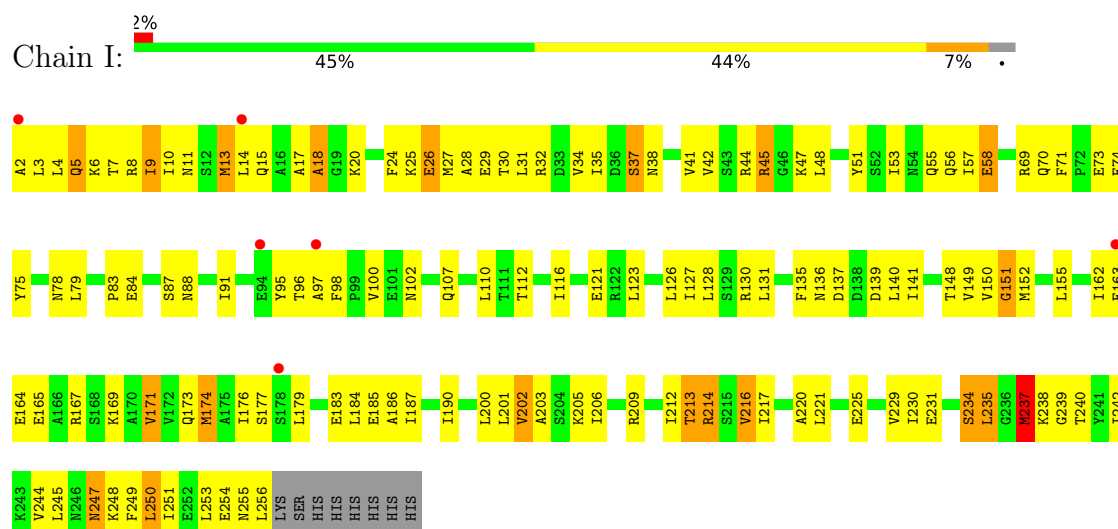


• Molecule 1: GTP-sensing transcriptional pleiotropic repressor CodY

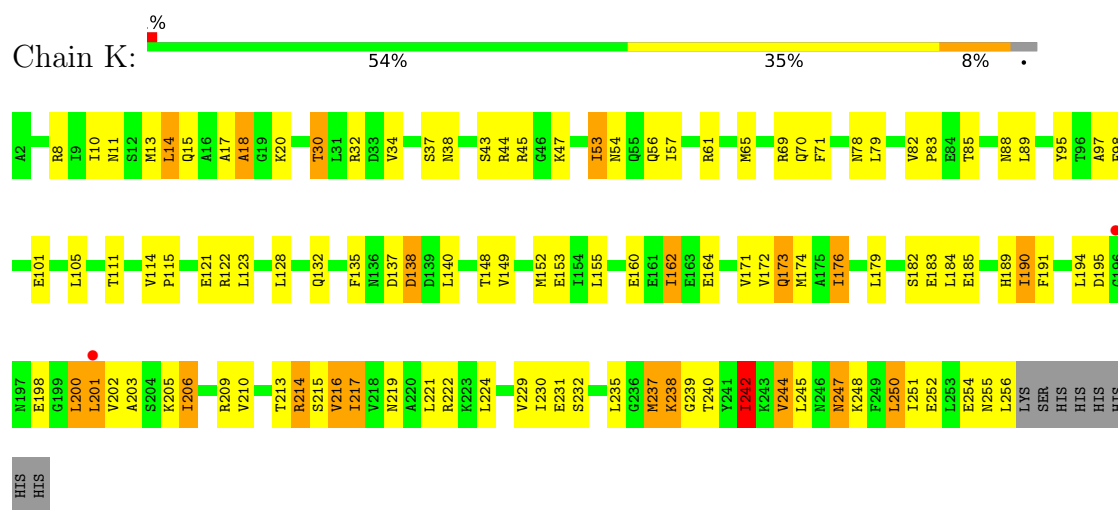


• Molecule 1: GTP-sensing transcriptional pleiotropic repressor CodY





- Molecule 1: GTP-sensing transcriptional pleiotropic repressor CodY



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	138.87Å 110.55Å 257.41Å 90.00° 91.30° 90.00°	Depositor
Resolution (Å)	46.68 – 3.00 46.68 – 3.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.68-3.00) 72.7 (46.68-3.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.26 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.230 , 0.279 (Not available) , 0.292	Depositor DCC
R_{free} test set	2880 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	94.6	Xtriage
Anisotropy	0.491	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.018 for -h,-k,l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	20090	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.93	0/2015	1.13	3/2702 (0.1%)
1	B	1.49	19/2015 (0.9%)	1.21	12/2702 (0.4%)
1	C	0.82	3/2015 (0.1%)	1.04	3/2702 (0.1%)
1	D	1.05	12/2015 (0.6%)	1.07	7/2702 (0.3%)
1	E	1.08	6/2015 (0.3%)	1.10	5/2702 (0.2%)
1	F	0.93	10/2015 (0.5%)	1.02	5/2702 (0.2%)
1	G	0.94	4/2015 (0.2%)	1.10	4/2702 (0.1%)
1	H	0.77	1/2015 (0.0%)	0.99	2/2702 (0.1%)
1	I	0.84	1/2015 (0.0%)	1.09	3/2702 (0.1%)
1	K	0.76	1/2015 (0.0%)	1.02	3/2702 (0.1%)
All	All	0.98	57/20150 (0.3%)	1.08	47/27020 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2
1	C	0	1
1	D	0	1
1	E	0	1
1	G	0	1
1	H	0	1
1	I	0	1
All	All	0	8

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	208	ASP	CG-OD1	23.72	1.70	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	173	GLN	CD-NE2	21.05	1.77	1.33
1	B	205	LYS	CD-CE	21.01	2.15	1.52
1	D	56	GLN	CD-NE2	14.57	1.63	1.33
1	B	209	ARG	CZ-NH1	14.17	1.52	1.32
1	B	208	ASP	CG-OD2	13.98	1.51	1.25
1	D	173	GLN	CD-OE1	13.93	1.50	1.23
1	D	234	SER	CB-OG	11.27	1.64	1.42
1	B	214	ARG	CZ-NH1	10.78	1.47	1.32
1	B	206	ILE	CA-CB	10.61	1.66	1.54
1	D	55	GLN	CD-NE2	9.97	1.54	1.33
1	E	144	GLU	CD-OE2	9.74	1.43	1.25
1	B	195	ASP	CG-OD2	9.65	1.43	1.25
1	F	134	GLN	CD-OE1	9.65	1.41	1.23
1	G	101	GLU	CD-OE2	9.53	1.43	1.25
1	B	209	ARG	CD-NE	8.56	1.58	1.46
1	D	55	GLN	CD-OE1	8.56	1.39	1.23
1	E	20	LYS	CB-CG	8.49	1.77	1.52
1	B	238	LYS	CE-NZ	8.31	1.74	1.49
1	B	233	ARG	CZ-NH2	8.29	1.44	1.33
1	B	209	ARG	CZ-NH2	8.24	1.44	1.33
1	F	134	GLN	CD-NE2	8.23	1.50	1.33
1	E	144	GLU	CD-OE1	8.09	1.40	1.25
1	B	214	ARG	NE-CZ	7.98	1.41	1.33
1	H	243	LYS	CE-NZ	7.94	1.73	1.49
1	D	158	LYS	CD-CE	7.91	1.76	1.52
1	D	56	GLN	CD-OE1	7.73	1.38	1.23
1	D	233	ARG	CZ-NH2	7.69	1.43	1.33
1	F	182	SER	CB-OG	7.65	1.57	1.42
1	K	198	GLU	CG-CD	7.57	1.71	1.52
1	B	209	ARG	NE-CZ	7.39	1.41	1.33
1	F	243	LYS	CD-CE	7.35	1.74	1.52
1	B	195	ASP	CG-OD1	7.32	1.39	1.25
1	B	202	VAL	CA-CB	7.17	1.61	1.53
1	C	214	ARG	NE-CZ	7.05	1.40	1.33
1	C	223	LYS	CE-NZ	6.80	1.69	1.49
1	F	243	LYS	CE-NZ	6.58	1.69	1.49
1	D	92	ASN	CG-OD1	6.57	1.36	1.23
1	G	149	VAL	CA-CB	-6.47	1.46	1.54
1	E	178	SER	CB-OG	6.30	1.54	1.42
1	B	214	ARG	CZ-NH2	6.16	1.41	1.33
1	F	231	GLU	CD-OE1	6.14	1.37	1.25
1	F	181	TYR	CE1-CZ	6.04	1.52	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	233	ARG	NE-CZ	6.01	1.39	1.33
1	F	133	ASP	CG-OD2	5.70	1.36	1.25
1	C	173	GLN	CG-CD	5.70	1.66	1.52
1	B	193	GLU	CG-CD	5.70	1.66	1.52
1	B	152	MSE	CA-C	-5.69	1.45	1.52
1	D	92	ASN	CG-ND2	5.69	1.45	1.33
1	F	133	ASP	CG-OD1	5.67	1.36	1.25
1	E	20	LYS	CG-CD	5.61	1.69	1.52
1	B	217	ILE	CA-CB	-5.56	1.48	1.54
1	I	116	ILE	CA-CB	-5.37	1.47	1.53
1	G	101	GLU	CD-OE1	5.36	1.35	1.25
1	F	181	TYR	CG-CD2	5.26	1.50	1.39
1	D	134	GLN	CD-NE2	5.09	1.44	1.33
1	G	241	TYR	CE2-CZ	5.05	1.50	1.38

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	209	ARG	NE-CZ-NH2	-9.84	110.35	119.20
1	B	214	ARG	NE-CZ-NH2	-9.77	110.41	119.20
1	D	173	GLN	OE1-CD-NE2	8.55	131.15	122.60
1	C	173	GLN	OE1-CD-NE2	-7.97	114.63	122.60
1	C	152	MSE	CB-CG-SE	-7.97	88.80	112.70
1	E	173	GLN	CG-CD-NE2	-7.37	105.34	116.40
1	F	134	GLN	OE1-CD-NE2	7.25	129.85	122.60
1	K	238	LYS	N-CA-C	-7.12	103.12	112.24
1	K	198	GLU	CB-CG-CD	-6.89	100.89	112.60
1	D	233	ARG	NE-CZ-NH1	-6.79	114.71	121.50
1	B	152	MSE	CB-CA-C	-6.43	97.62	110.42
1	I	9	ILE	CB-CA-C	-6.38	103.83	111.81
1	G	242	ILE	N-CA-C	6.37	116.76	108.35
1	D	55	GLN	OE1-CD-NE2	6.34	128.94	122.60
1	B	233	ARG	NE-CZ-NH1	-6.26	115.24	121.50
1	F	242	ILE	N-CA-C	6.20	117.63	108.45
1	B	152	MSE	CB-CG-SE	-6.11	94.36	112.70
1	C	173	GLN	CG-CD-NE2	6.07	125.50	116.40
1	E	242	ILE	N-CA-C	6.06	117.41	108.45
1	F	251	ILE	CB-CA-C	-6.05	104.23	111.97
1	B	209	ARG	CD-NE-CZ	-6.01	115.99	124.40
1	B	44	ARG	N-CA-C	-5.91	103.81	111.02
1	E	97	ALA	N-CA-C	5.90	118.47	111.33
1	B	10	ILE	CB-CA-C	-5.89	104.34	111.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	198	GLU	CB-CG-CD	-5.83	102.69	112.60
1	I	26	GLU	CB-CA-C	-5.78	101.73	110.92
1	B	233	ARG	NE-CZ-NH2	5.72	124.35	119.20
1	D	242	ILE	N-CA-C	5.66	116.51	108.42
1	B	206	ILE	CB-CG1-CD1	5.65	125.67	113.80
1	G	213	THR	N-CA-CB	5.63	118.65	109.69
1	G	97	ALA	N-CA-C	5.62	118.14	111.33
1	F	238	LYS	N-CA-C	-5.62	105.05	112.24
1	A	206	ILE	CB-CA-C	-5.54	104.79	111.88
1	D	176	ILE	CB-CA-C	-5.49	104.85	111.88
1	D	56	GLN	OE1-CD-NE2	5.48	128.08	122.60
1	B	210	VAL	CB-CA-C	-5.44	106.27	111.06
1	H	171	VAL	CB-CA-C	-5.42	104.94	111.88
1	I	44	ARG	NE-CZ-NH2	5.42	124.08	119.20
1	A	214	ARG	CB-CA-C	-5.40	101.78	110.74
1	H	242	ILE	N-CA-C	5.38	116.41	108.45
1	A	176	ILE	CB-CA-C	-5.21	105.21	111.88
1	E	172	VAL	CG1-CB-CG2	-5.14	99.50	110.80
1	E	85	THR	CB-CA-C	-5.10	102.62	109.71
1	K	242	ILE	N-CA-C	5.07	117.03	108.81
1	B	206	ILE	CB-CA-C	-5.02	105.45	111.88
1	G	150	VAL	CB-CA-C	-5.02	103.06	111.29
1	D	152	MSE	CB-CG-SE	-5.00	97.70	112.70

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	208	ASP	Sidechain
1	B	237	MSE	Peptide
1	C	237	MSE	Peptide
1	D	237	MSE	Peptide
1	E	237	MSE	Peptide
1	G	237	MSE	Peptide
1	H	237	MSE	Peptide
1	I	237	MSE	Peptide

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	2002	0	2041	108	0
1	B	2002	0	2041	128	0
1	C	2002	0	2041	85	0
1	D	2002	0	2041	107	0
1	E	2002	0	2041	97	0
1	F	2002	0	2041	85	0
1	G	2002	0	2041	96	0
1	H	2002	0	2041	123	0
1	I	2002	0	2041	104	0
1	K	2002	0	2041	81	0
2	A	10	0	0	0	0
2	B	10	0	0	1	0
2	C	5	0	0	0	0
2	E	10	0	0	1	0
2	F	5	0	0	0	0
2	G	5	0	0	0	0
2	H	5	0	0	0	0
2	I	5	0	0	0	0
2	K	5	0	0	0	0
3	A	4	0	0	0	0
3	B	2	0	0	0	0
3	C	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	K	1	0	0	0	0
All	All	20090	0	20410	959	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 24.

All (959) 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:F:243:LYS:CE	1:F:243:LYS:CD	1.74	1.63
1:E:20:LYS:CG	1:E:20:LYS:CB	1.77	1.58
1:D:158:LYS:CE	1:D:158:LYS:CD	1.76	1.58
1:F:243:LYS:CE	1:F:243:LYS:NZ	1.69	1.55
1:C:223:LYS:CE	1:C:223:LYS:NZ	1.69	1.54
1:H:243:LYS:CE	1:H:243:LYS:NZ	1.73	1.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:238:LYS:CE	1:B:238:LYS:NZ	1.74	1.49
1:D:234:SER:OG	1:D:234:SER:CB	1.64	1.45
1:E:173:GLN:NE2	1:E:173:GLN:CD	1.77	1.42
1:B:208:ASP:CG	1:B:208:ASP:OD1	1.70	1.35
1:E:174:MSE:HE3	1:F:174:MSE:SE	1.82	1.29
1:B:205:LYS:CD	1:B:205:LYS:CE	2.15	1.23
1:D:250:LEU:H	1:D:250:LEU:HD23	1.09	1.08
1:B:214:ARG:H	1:B:214:ARG:HD3	1.19	1.08
1:E:174:MSE:CE	1:F:174:MSE:SE	2.53	1.07
1:B:247:ASN:N	1:B:247:ASN:HD22	1.48	1.05
1:D:201:LEU:HG	1:D:206:ILE:HD11	1.38	1.02
1:B:46:GLY:HA3	1:B:76:THR:CG2	1.90	1.02
1:B:247:ASN:H	1:B:247:ASN:ND2	1.53	1.01
1:G:174:MSE:HE1	1:H:170:ALA:HB3	1.44	0.99
1:D:247:ASN:H	1:D:247:ASN:ND2	1.48	0.97
1:F:214:ARG:HD3	1:F:214:ARG:H	1.28	0.96
1:E:214:ARG:H	1:E:214:ARG:HD3	1.29	0.95
1:D:247:ASN:HD22	1:D:247:ASN:N	1.65	0.94
1:D:29:GLU:HG2	1:D:52:SER:OG	1.67	0.94
1:I:3:LEU:HA	1:I:6:LYS:HD2	1.47	0.94
1:G:12:SER:HA	1:G:15:GLN:HG3	1.48	0.94
1:A:88:ASN:HD21	1:A:135:PHE:H	0.95	0.93
1:B:88:ASN:HD21	1:B:135:PHE:H	1.17	0.92
1:K:213:THR:HG23	1:K:214:ARG:NH1	1.83	0.92
1:C:88:ASN:HD21	1:C:135:PHE:H	1.17	0.92
1:B:214:ARG:H	1:B:214:ARG:CD	1.83	0.92
1:I:58:GLU:HA	1:I:58:GLU:OE2	1.68	0.91
1:G:201:LEU:HD23	1:G:206:ILE:HD11	1.53	0.91
1:B:24:PHE:HD1	1:B:27:MSE:HE2	1.35	0.90
1:C:173:GLN:HE21	1:E:166:ALA:HA	1.35	0.90
1:E:174:MSE:HB2	1:F:174:MSE:HE1	1.52	0.89
1:E:136:ASN:O	1:E:140:LEU:HD12	1.72	0.88
1:E:247:ASN:H	1:E:247:ASN:ND2	1.66	0.87
1:A:95:TYR:HE2	1:A:97:ALA:HB3	1.37	0.87
1:E:90:ASP:OD2	1:E:92:ASN:HB2	1.75	0.87
1:K:250:LEU:H	1:K:250:LEU:HD23	1.40	0.87
1:B:95:TYR:CE2	1:B:97:ALA:HB3	2.09	0.86
1:A:88:ASN:ND2	1:A:135:PHE:H	1.71	0.85
1:A:247:ASN:H	1:A:247:ASN:HD22	1.20	0.85
1:D:174:MSE:HG3	1:E:174:MSE:HE1	1.56	0.85
1:K:213:THR:HG23	1:K:214:ARG:HH12	1.36	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:247:ASN:H	1:H:247:ASN:HD22	1.24	0.84
1:H:88:ASN:HD21	1:H:135:PHE:H	1.24	0.84
1:F:88:ASN:HD21	1:F:135:PHE:H	1.23	0.84
1:C:188:GLU:O	1:C:192:GLU:HG3	1.78	0.84
1:C:23:ASN:ND2	1:C:26:GLU:HG2	1.93	0.83
1:I:91:ILE:HD12	1:I:107:GLN:HA	1.60	0.83
1:G:201:LEU:HG	1:G:202:VAL:H	1.42	0.82
1:B:213:THR:HB	1:B:216:VAL:HG13	1.61	0.82
1:A:167:ARG:O	1:A:171:VAL:HG12	1.80	0.82
1:C:173:GLN:NE2	1:E:166:ALA:HA	1.94	0.82
1:G:14:LEU:HD13	1:G:149:VAL:HG13	1.62	0.82
1:H:145:TYR:O	1:H:149:VAL:HG23	1.79	0.82
1:F:247:ASN:H	1:F:247:ASN:HD22	1.26	0.82
1:D:250:LEU:HD23	1:D:250:LEU:N	1.94	0.81
1:H:88:ASN:HD22	1:H:110:LEU:HD13	1.45	0.81
1:I:78:ASN:HB3	1:I:98:PHE:CZ	2.15	0.81
1:G:85:THR:HG23	1:G:114:VAL:HG22	1.61	0.81
1:A:95:TYR:CE2	1:A:97:ALA:HB3	2.16	0.81
1:A:115:PRO:HB3	1:A:122:ARG:NH1	1.95	0.81
1:D:250:LEU:H	1:D:250:LEU:CD2	1.88	0.81
1:D:145:TYR:O	1:D:149:VAL:HG23	1.80	0.81
1:B:95:TYR:HH	1:B:98:PHE:HD1	1.25	0.80
1:H:24:PHE:HA	1:H:27:MSE:HE3	1.62	0.80
1:B:198:GLU:HG2	1:B:243:LYS:HG3	1.64	0.80
1:E:250:LEU:HD23	1:E:250:LEU:H	1.44	0.80
1:C:213:THR:HB	1:C:216:VAL:HG13	1.63	0.80
1:F:214:ARG:H	1:F:214:ARG:CD	1.93	0.80
1:A:46:GLY:HA3	1:A:76:THR:HG23	1.62	0.80
1:D:158:LYS:CE	1:D:158:LYS:CG	2.60	0.79
1:E:32:ARG:HD2	1:E:54:ASN:HB3	1.63	0.79
1:B:247:ASN:HD22	1:B:247:ASN:H	0.81	0.79
1:D:70:GLN:HE21	1:D:71:PHE:H	1.31	0.79
1:D:247:ASN:H	1:D:247:ASN:HD22	0.82	0.79
1:G:251:ILE:O	1:G:254:GLU:HB2	1.82	0.79
1:D:88:ASN:HD21	1:D:135:PHE:H	1.31	0.78
1:K:213:THR:HB	1:K:216:VAL:HG12	1.65	0.78
1:F:243:LYS:CE	1:F:243:LYS:CG	2.61	0.78
1:I:237:MSE:HE1	1:I:240:THR:HG22	1.64	0.78
1:K:201:LEU:HD13	1:K:202:VAL:H	1.47	0.78
1:E:201:LEU:HD13	1:E:202:VAL:H	1.48	0.78
1:G:174:MSE:HE2	1:H:174:MSE:HE1	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:171:VAL:HA	1:I:174:MSE:HE2	1.65	0.78
1:K:247:ASN:N	1:K:247:ASN:HD22	1.80	0.78
1:D:218:VAL:HG12	1:D:219:ASN:N	1.99	0.77
1:K:78:ASN:HB3	1:K:98:PHE:CE2	2.19	0.77
1:A:88:ASN:HD21	1:A:135:PHE:N	1.77	0.77
1:H:172:VAL:HG12	1:H:176:ILE:HD11	1.66	0.77
1:I:95:TYR:HE2	1:I:97:ALA:HB3	1.49	0.77
1:H:11:ASN:O	1:H:15:GLN:HG2	1.83	0.77
1:I:51:TYR:HE1	1:I:53:ILE:HD11	1.49	0.76
1:A:99:PRO:HB2	1:A:101:GLU:OE2	1.84	0.76
1:G:174:MSE:HE1	1:H:170:ALA:CB	2.15	0.76
1:D:203:ALA:HB3	1:D:237:MSE:HE1	1.66	0.76
1:K:205:LYS:HE2	1:K:209:ARG:NH2	2.00	0.76
1:H:85:THR:HG23	1:H:114:VAL:HG22	1.68	0.75
1:B:46:GLY:HA3	1:B:76:THR:HG23	1.68	0.75
1:G:214:ARG:CD	1:G:214:ARG:H	1.99	0.75
1:B:201:LEU:HD12	1:B:202:VAL:H	1.50	0.75
1:D:167:ARG:O	1:D:171:VAL:HG13	1.87	0.74
1:I:95:TYR:CE2	1:I:97:ALA:HB3	2.22	0.74
1:B:121:GLU:HG3	1:H:212:ILE:HG12	1.68	0.74
1:I:247:ASN:HD22	1:I:247:ASN:H	1.36	0.74
1:B:179:LEU:HD22	1:B:183:GLU:HB3	1.69	0.74
1:D:138:ASP:HA	1:D:141:ILE:HD12	1.70	0.74
1:A:150:VAL:HG12	1:A:154:ILE:HD11	1.70	0.74
1:I:212:ILE:HG12	1:K:121:GLU:HG3	1.69	0.74
1:A:214:ARG:H	1:A:214:ARG:HH11	1.35	0.73
1:H:149:VAL:HG13	1:H:152:MSE:HE3	1.69	0.73
1:I:78:ASN:HB3	1:I:98:PHE:CE2	2.24	0.73
1:E:213:THR:HB	1:E:216:VAL:HG13	1.71	0.73
1:B:24:PHE:CD1	1:B:27:MSE:HE2	2.21	0.73
1:C:156:ARG:O	1:C:160:GLU:HG2	1.89	0.73
1:D:169:LYS:HB3	1:F:173:GLN:HE21	1.52	0.73
1:E:203:ALA:HB3	1:E:237:MSE:SE	2.38	0.73
1:G:250:LEU:HD23	1:G:250:LEU:H	1.54	0.73
1:H:138:ASP:HA	1:H:141:ILE:HD12	1.69	0.73
1:B:95:TYR:OH	1:B:98:PHE:HD1	1.70	0.73
1:B:32:ARG:HD2	1:B:54:ASN:HB3	1.69	0.73
1:D:121:GLU:HG3	1:F:212:ILE:HG12	1.68	0.73
1:D:247:ASN:ND2	1:D:247:ASN:N	2.28	0.72
1:I:149:VAL:HA	1:I:152:MSE:HE3	1.71	0.72
1:E:20:LYS:CB	1:E:20:LYS:CD	2.67	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:214:ARG:NH2	1:H:215:SER:OG	2.23	0.72
1:K:219:ASN:HA	1:K:222:ARG:HG3	1.70	0.72
1:A:2:ALA:HA	1:A:5:GLN:NE2	2.05	0.72
1:G:11:ASN:O	1:G:15:GLN:HG2	1.90	0.71
1:F:23:ASN:HB3	1:F:26:GLU:HG3	1.72	0.71
1:F:156:ARG:HD3	1:F:160:GLU:OE2	1.89	0.71
1:G:45:ARG:H	1:G:45:ARG:HD3	1.54	0.71
1:E:95:TYR:C	1:E:95:TYR:CD1	2.68	0.71
1:E:20:LYS:CG	1:E:20:LYS:CA	2.68	0.70
1:A:54:ASN:OD1	1:A:55:GLN:HG2	1.91	0.70
1:H:193:GLU:OE2	1:H:209:ARG:NH1	2.25	0.70
1:K:247:ASN:HD22	1:K:247:ASN:H	1.39	0.70
1:D:4:LEU:HD11	1:D:8:ARG:HH11	1.55	0.70
1:F:6:LYS:HA	1:F:9:ILE:HD12	1.74	0.70
1:G:174:MSE:HE2	1:H:174:MSE:CE	2.22	0.70
1:I:231:GLU:HB2	1:I:245:LEU:HD11	1.71	0.70
1:C:88:ASN:ND2	1:C:135:PHE:H	1.90	0.70
1:B:8:ARG:O	1:B:11:ASN:HB2	1.93	0.69
1:G:146:GLY:O	1:G:150:VAL:HG23	1.92	0.69
1:A:255:ASN:C	1:A:256:LEU:HD12	2.18	0.69
1:K:252:GLU:HA	1:K:255:ASN:HD22	1.55	0.69
1:I:205:LYS:HG2	1:I:209:ARG:HH12	1.58	0.69
1:B:95:TYR:HE2	1:B:97:ALA:HB3	1.54	0.69
1:C:99:PRO:HB2	1:C:101:GLU:OE2	1.93	0.69
1:H:78:ASN:HB3	1:H:98:PHE:CE2	2.29	0.69
1:I:8:ARG:HA	1:I:11:ASN:HD22	1.56	0.69
1:K:88:ASN:HD21	1:K:135:PHE:H	1.41	0.69
1:D:22:VAL:HG21	1:D:157:GLU:HB2	1.76	0.68
1:A:30:THR:O	1:A:34:VAL:HG23	1.93	0.68
1:E:95:TYR:CE2	1:E:97:ALA:HB3	2.28	0.68
1:I:203:ALA:H	1:I:237:MSE:HE1	1.59	0.68
1:K:38:ASN:HD22	1:K:53:ILE:HG12	1.59	0.68
1:D:29:GLU:HG2	1:D:52:SER:HG	1.59	0.68
1:I:250:LEU:H	1:I:250:LEU:HD23	1.57	0.68
1:C:32:ARG:HD2	1:C:54:ASN:HB3	1.75	0.68
1:B:15:GLN:OE1	1:G:117:ILE:HG22	1.93	0.67
1:F:203:ALA:HB3	1:F:237:MSE:HE1	1.75	0.67
1:G:214:ARG:H	1:G:214:ARG:HD3	1.59	0.67
1:H:213:THR:HG22	1:H:215:SER:H	1.59	0.67
1:A:213:THR:O	1:A:217:ILE:HG13	1.92	0.67
1:C:95:TYR:OH	1:C:98:PHE:HB2	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:174:MSE:HE2	1:F:174:MSE:SE	2.45	0.67
1:E:214:ARG:H	1:E:214:ARG:CD	1.99	0.67
1:G:201:LEU:HD23	1:G:206:ILE:CD1	2.25	0.67
1:H:6:LYS:HA	1:H:9:ILE:HD12	1.77	0.67
1:I:202:VAL:HA	1:I:237:MSE:HE2	1.77	0.66
1:G:22:VAL:HG13	1:G:27:MSE:HE2	1.77	0.66
1:C:78:ASN:HB3	1:C:98:PHE:CE2	2.29	0.66
1:G:88:ASN:HD21	1:G:135:PHE:H	1.43	0.66
1:G:137:ASP:HA	1:G:140:LEU:HD12	1.78	0.66
1:A:170:ALA:CB	1:B:174:MSE:HE1	2.26	0.66
1:C:138:ASP:HA	1:C:141:ILE:HD12	1.78	0.66
1:C:223:LYS:NZ	1:C:223:LYS:CD	2.57	0.66
1:G:148:THR:HG22	1:G:152:MSE:HE3	1.78	0.66
1:H:243:LYS:NZ	1:H:243:LYS:CD	2.57	0.66
1:G:63:LYS:HA	1:G:66:LEU:HD12	1.77	0.66
1:G:229:VAL:HG11	1:G:249:PHE:CD1	2.30	0.66
1:D:70:GLN:HE21	1:D:71:PHE:N	1.93	0.66
1:H:137:ASP:HA	1:H:140:LEU:HD12	1.78	0.66
1:H:231:GLU:HB2	1:H:245:LEU:HD21	1.77	0.66
1:K:176:ILE:HA	1:K:179:LEU:CD1	2.25	0.66
1:H:32:ARG:HD2	1:H:54:ASN:HB3	1.78	0.66
1:I:214:ARG:HA	1:I:217:ILE:HD12	1.78	0.66
1:E:229:VAL:HG11	1:E:249:PHE:CD1	2.30	0.66
1:B:95:TYR:OH	1:B:98:PHE:CD1	2.49	0.65
1:D:48:LEU:HD23	1:D:69:ARG:HG3	1.76	0.65
1:K:61:ARG:HG3	1:K:105:LEU:HD13	1.78	0.65
1:I:45:ARG:NH2	1:I:47:LYS:HE2	2.12	0.65
1:A:8:ARG:HA	1:A:11:ASN:HD22	1.62	0.65
1:D:152:MSE:HE2	1:E:152:MSE:SE	2.46	0.65
1:A:14:LEU:HD23	1:A:15:GLN:HE21	1.62	0.65
1:A:145:TYR:HD2	1:A:145:TYR:O	1.79	0.65
1:K:30:THR:O	1:K:34:VAL:HG23	1.97	0.65
1:K:251:ILE:O	1:K:254:GLU:HB2	1.97	0.65
1:H:95:TYR:OH	1:H:98:PHE:HB2	1.97	0.64
1:E:115:PRO:HB2	1:E:117:ILE:CD1	2.27	0.64
1:H:8:ARG:HA	1:H:11:ASN:HD22	1.62	0.64
1:F:40:PHE:HB2	1:F:127:ILE:HB	1.78	0.64
1:G:214:ARG:HA	1:G:217:ILE:HD12	1.79	0.64
1:D:78:ASN:HB3	1:D:98:PHE:CE2	2.32	0.64
1:D:150:VAL:HG12	1:D:154:ILE:HD11	1.78	0.64
1:G:22:VAL:HG13	1:G:27:MSE:CE	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:ILE:HG22	1:A:244:VAL:HA	1.80	0.64
1:B:206:ILE:O	1:B:210:VAL:HG23	1.98	0.64
1:I:201:LEU:HG	1:I:202:VAL:H	1.63	0.64
1:G:174:MSE:SE	1:G:174:MSE:C	2.91	0.64
1:C:122:ARG:HH21	1:C:125:THR:HG23	1.63	0.63
1:I:244:VAL:HG21	1:I:250:LEU:HD22	1.80	0.63
1:I:137:ASP:HA	1:I:140:LEU:HD12	1.79	0.63
1:B:14:LEU:HD12	1:B:149:VAL:HG13	1.81	0.63
1:F:29:GLU:HG3	1:F:52:SER:OG	1.98	0.63
1:A:11:ASN:OD1	1:A:145:TYR:OH	2.12	0.63
1:H:213:THR:CG2	1:H:214:ARG:HH21	2.11	0.63
1:I:45:ARG:HH21	1:I:47:LYS:HE2	1.63	0.63
1:K:153:GLU:OE2	1:K:153:GLU:HA	1.97	0.63
1:G:11:ASN:O	1:G:15:GLN:CG	2.46	0.63
1:A:247:ASN:H	1:A:247:ASN:ND2	1.96	0.63
1:B:95:TYR:OH	1:B:98:PHE:HB2	1.99	0.63
1:C:251:ILE:O	1:C:254:GLU:HB2	1.98	0.63
1:A:63:LYS:O	1:A:67:GLU:HG3	1.99	0.62
1:A:3:LEU:HD13	1:A:138:ASP:HB3	1.80	0.62
1:H:180:SER:N	1:H:183:GLU:OE1	2.22	0.62
1:E:238:LYS:O	1:E:238:LYS:HG3	1.99	0.62
1:E:247:ASN:ND2	1:E:247:ASN:N	2.43	0.62
1:G:231:GLU:HB2	1:G:245:LEU:HD21	1.80	0.62
1:I:121:GLU:OE1	1:K:182:SER:HA	1.99	0.62
1:I:127:ILE:C	1:I:128:LEU:HD12	2.24	0.62
1:E:6:LYS:HB3	1:E:34:VAL:CG1	2.28	0.62
1:E:214:ARG:HD3	1:E:214:ARG:N	2.10	0.62
1:G:205:LYS:HD3	1:G:209:ARG:HH22	1.63	0.62
1:B:205:LYS:HD3	1:B:209:ARG:NH2	2.15	0.62
1:I:95:TYR:OH	1:I:98:PHE:HB2	1.99	0.62
1:D:194:LEU:HD11	1:D:199:GLY:HA3	1.82	0.62
1:G:168:SER:O	1:G:172:VAL:HG23	2.00	0.62
1:F:35:ILE:HG22	1:F:37:SER:HB3	1.81	0.62
1:H:210:VAL:CG1	1:H:212:ILE:HG13	2.30	0.61
1:A:39:ILE:HD13	1:A:128:LEU:HG	1.82	0.61
1:A:167:ARG:HG3	1:B:174:MSE:CG	2.29	0.61
1:B:218:VAL:CG1	1:B:222:ARG:HH12	2.13	0.61
1:I:176:ILE:HA	1:I:179:LEU:HD12	1.83	0.61
1:C:8:ARG:HA	1:C:11:ASN:ND2	2.16	0.61
1:D:77:LYS:HE2	1:D:81:ASN:HD21	1.66	0.61
1:C:213:THR:HG23	1:C:214:ARG:HH22	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:248:LYS:HD2	1:F:248:LYS:N	2.16	0.61
1:A:234:SER:C	1:A:235:LEU:HD13	2.25	0.61
1:E:233:ARG:CZ	1:H:233:ARG:HH11	2.13	0.61
1:F:167:ARG:O	1:F:171:VAL:HG13	2.01	0.61
1:H:30:THR:O	1:H:34:VAL:HG23	2.01	0.61
1:D:205:LYS:HG2	1:D:209:ARG:HH12	1.65	0.61
1:G:174:MSE:CE	1:H:170:ALA:CB	2.79	0.61
1:B:88:ASN:ND2	1:B:135:PHE:H	1.93	0.60
1:K:201:LEU:CD1	1:K:202:VAL:H	2.13	0.60
1:K:231:GLU:HB2	1:K:245:LEU:HD11	1.81	0.60
1:G:14:LEU:CD1	1:G:149:VAL:HG13	2.31	0.60
1:H:179:LEU:HD13	1:H:183:GLU:HB3	1.83	0.60
1:A:85:THR:HG23	1:A:114:VAL:HG13	1.83	0.60
1:B:86:SER:OG	1:B:89:LEU:HD11	2.00	0.60
1:B:213:THR:HG22	1:B:215:SER:H	1.66	0.60
1:C:30:THR:O	1:C:34:VAL:HG23	2.02	0.60
1:D:194:LEU:HD22	1:D:242:ILE:CD1	2.31	0.60
1:H:169:LYS:HG3	1:H:248:LYS:HG2	1.82	0.60
1:I:45:ARG:NH2	1:I:47:LYS:CE	2.65	0.60
1:H:24:PHE:HA	1:H:27:MSE:CE	2.31	0.60
1:A:248:LYS:HD2	1:A:248:LYS:N	2.16	0.59
1:C:169:LYS:HD2	1:E:173:GLN:NE2	2.17	0.59
1:D:32:ARG:HD2	1:D:54:ASN:HB3	1.84	0.59
1:E:130:ARG:HD2	1:E:135:PHE:CZ	2.37	0.59
1:A:234:SER:O	1:A:235:LEU:HD13	2.03	0.59
1:F:40:PHE:O	1:F:126:LEU:HD12	2.01	0.59
1:F:115:PRO:HB2	1:F:117:ILE:HD11	1.83	0.59
1:B:203:ALA:HB3	1:B:237:MSE:HE1	1.83	0.59
1:B:247:ASN:N	1:B:247:ASN:ND2	2.24	0.59
1:K:200:LEU:C	1:K:200:LEU:HD23	2.27	0.59
1:F:23:ASN:CB	1:F:26:GLU:HG3	2.33	0.59
1:I:88:ASN:HD21	1:I:135:PHE:H	1.51	0.59
1:G:2:ALA:HA	1:G:5:GLN:OE1	2.03	0.59
1:A:167:ARG:HG3	1:B:174:MSE:HG3	1.85	0.59
1:A:170:ALA:HB3	1:B:174:MSE:CE	2.33	0.58
1:A:219:ASN:HB2	1:B:19:GLY:O	2.02	0.58
1:C:167:ARG:O	1:C:171:VAL:HG13	2.03	0.58
1:E:115:PRO:HB2	1:E:117:ILE:HD12	1.84	0.58
1:H:247:ASN:H	1:H:247:ASN:ND2	1.95	0.58
1:I:51:TYR:CE1	1:I:53:ILE:HD11	2.36	0.58
1:D:174:MSE:HG3	1:E:174:MSE:CE	2.31	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:153:GLU:HA	1:E:153:GLU:OE2	2.01	0.58
1:K:213:THR:HG22	1:K:215:SER:H	1.68	0.58
1:B:159:ALA:O	1:B:163:GLU:HG2	2.04	0.58
1:K:171:VAL:O	1:K:174:MSE:HB3	2.03	0.58
1:K:247:ASN:H	1:K:247:ASN:ND2	2.02	0.58
1:G:199:GLY:O	1:G:241:TYR:CD1	2.57	0.58
1:G:247:ASN:HD22	1:G:247:ASN:H	1.51	0.58
1:K:206:ILE:HG22	1:K:210:VAL:HG21	1.86	0.58
1:A:170:ALA:HB3	1:B:174:MSE:HE1	1.86	0.58
1:A:214:ARG:H	1:A:214:ARG:NH1	2.01	0.58
1:B:88:ASN:HD21	1:B:135:PHE:N	1.96	0.58
1:B:167:ARG:O	1:B:171:VAL:HG13	2.04	0.57
1:B:205:LYS:HD3	1:B:209:ARG:HH22	1.69	0.57
1:K:232:SER:HB3	1:K:242:ILE:HG22	1.86	0.57
1:H:39:ILE:HD13	1:H:128:LEU:HD12	1.86	0.57
1:K:213:THR:HG22	1:K:215:SER:N	2.19	0.57
1:F:201:LEU:O	1:F:240:THR:HG23	2.04	0.57
1:F:12:SER:HA	1:F:15:GLN:HG2	1.85	0.57
1:H:13:MSE:HE2	1:H:30:THR:HB	1.85	0.57
1:K:230:ILE:HG22	1:K:244:VAL:HA	1.86	0.57
1:D:88:ASN:OD1	1:D:135:PHE:HB2	2.04	0.57
1:F:11:ASN:O	1:F:15:GLN:HG2	2.05	0.57
1:H:43:SER:HB2	1:H:45:ARG:NH1	2.20	0.57
1:A:3:LEU:CD1	1:A:138:ASP:HB3	2.35	0.57
1:I:169:LYS:NZ	1:K:173:GLN:NE2	2.52	0.57
1:K:32:ARG:HD2	1:K:54:ASN:HB3	1.87	0.57
1:C:183:GLU:HG2	1:C:220:ALA:HB2	1.85	0.57
1:G:168:SER:O	1:G:171:VAL:HG22	2.05	0.57
1:H:203:ALA:HB3	1:H:237:MSE:HE1	1.86	0.57
1:H:40:PHE:HB2	1:H:127:ILE:HB	1.86	0.56
1:B:99:PRO:HB2	1:B:101:GLU:OE1	2.04	0.56
1:D:201:LEU:HD12	1:D:202:VAL:H	1.70	0.56
1:C:23:ASN:ND2	1:C:26:GLU:CG	2.66	0.56
1:E:213:THR:HG23	1:E:214:ARG:CZ	2.35	0.56
1:F:237:MSE:O	1:F:238:LYS:HB2	2.05	0.56
1:H:205:LYS:HE2	1:H:209:ARG:NH2	2.20	0.56
1:I:130:ARG:HH22	1:I:139:ASP:CG	2.14	0.56
1:B:206:ILE:HG22	1:B:210:VAL:CG2	2.36	0.56
1:B:218:VAL:HG12	1:B:222:ARG:HH12	1.71	0.56
1:C:153:GLU:HA	1:C:153:GLU:OE1	2.06	0.56
1:D:165:GLU:HG3	1:D:248:LYS:NZ	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:VAL:HG12	1:A:230:ILE:HG23	1.88	0.56
1:B:46:GLY:HA3	1:B:76:THR:HG22	1.85	0.56
1:I:169:LYS:HZ3	1:K:173:GLN:NE2	2.04	0.56
1:B:214:ARG:CD	1:B:214:ARG:N	2.61	0.56
1:I:237:MSE:HE3	1:I:239:GLY:C	2.30	0.56
1:A:45:ARG:NH2	1:A:47:LYS:HD2	2.21	0.56
1:E:173:GLN:NE2	1:E:173:GLN:CG	2.66	0.56
1:H:172:VAL:O	1:H:176:ILE:HG13	2.06	0.56
1:A:251:ILE:O	1:A:254:GLU:HB2	2.06	0.56
1:B:99:PRO:HB2	1:B:101:GLU:CD	2.31	0.56
1:F:79:LEU:HD12	1:F:98:PHE:HZ	1.71	0.56
1:I:51:TYR:HE1	1:I:53:ILE:CD1	2.16	0.56
1:K:138:ASP:OD1	1:K:138:ASP:N	2.38	0.56
1:I:13:MSE:CE	1:I:27:MSE:HG2	2.36	0.55
1:C:89:LEU:CD1	1:C:113:ILE:HD11	2.36	0.55
1:I:137:ASP:O	1:I:141:ILE:HG13	2.07	0.55
1:I:167:ARG:O	1:I:171:VAL:HG13	2.05	0.55
1:K:14:LEU:HD13	1:K:149:VAL:HG22	1.88	0.55
1:A:2:ALA:HA	1:A:5:GLN:HE22	1.71	0.55
1:F:23:ASN:CG	1:F:26:GLU:HG3	2.32	0.55
1:C:148:THR:O	1:C:152:MSE:HE3	2.06	0.55
1:D:16:ALA:O	1:D:20:LYS:NZ	2.39	0.55
1:I:24:PHE:HA	1:I:27:MSE:HE3	1.87	0.55
1:K:8:ARG:HA	1:K:11:ASN:HD22	1.72	0.55
1:I:212:ILE:HG22	1:I:216:VAL:HG23	1.89	0.55
1:C:179:LEU:O	1:E:162:ILE:HD11	2.07	0.55
1:I:25:LYS:O	1:I:28:ALA:HB3	2.07	0.55
1:K:38:ASN:HD22	1:K:53:ILE:CG1	2.19	0.55
1:D:4:LEU:HD11	1:D:8:ARG:NH1	2.20	0.55
1:K:85:THR:HG23	1:K:114:VAL:HG22	1.89	0.55
1:H:173:GLN:HA	1:H:176:ILE:HD12	1.89	0.55
1:A:156:ARG:HD3	1:A:160:GLU:OE2	2.06	0.55
1:B:4:LEU:O	1:B:7:THR:OG1	2.23	0.55
1:D:71:PHE:HD1	1:D:72:PRO:HD2	1.71	0.55
1:H:213:THR:HB	1:H:216:VAL:HG12	1.88	0.55
1:D:172:VAL:HG21	1:D:249:PHE:HA	1.88	0.54
1:G:218:VAL:HG12	1:G:219:ASN:N	2.22	0.54
1:K:205:LYS:HE2	1:K:209:ARG:HH22	1.71	0.54
1:D:99:PRO:HB2	1:D:101:GLU:OE2	2.08	0.54
1:G:167:ARG:O	1:G:171:VAL:HG13	2.08	0.54
1:C:113:ILE:HG23	1:C:127:ILE:HG13	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:99:PRO:HG2	1:H:102:ASN:ND2	2.22	0.54
1:I:121:GLU:HG2	1:I:123:LEU:HD23	1.89	0.54
1:B:206:ILE:HG22	1:B:210:VAL:HG21	1.90	0.54
1:A:160:GLU:O	1:A:164:GLU:HG2	2.08	0.54
1:B:172:VAL:O	1:B:176:ILE:HG13	2.08	0.54
1:D:158:LYS:CD	1:D:158:LYS:NZ	2.67	0.54
1:H:88:ASN:ND2	1:H:110:LEU:HD13	2.19	0.54
1:A:247:ASN:HD22	1:A:247:ASN:N	1.98	0.54
1:D:88:ASN:ND2	1:D:135:PHE:H	2.03	0.54
1:I:30:THR:O	1:I:34:VAL:HG23	2.08	0.54
1:I:78:ASN:OD1	1:I:102:ASN:ND2	2.41	0.54
1:D:11:ASN:O	1:D:15:GLN:HG2	2.07	0.54
1:D:234:SER:CB	1:D:234:SER:HG	2.08	0.54
1:G:48:LEU:HD13	1:G:65:MSE:SE	2.58	0.54
1:H:24:PHE:CD1	1:H:27:MSE:HE1	2.43	0.54
1:A:171:VAL:HA	1:A:174:MSE:HE3	1.89	0.54
1:A:237:MSE:HG3	1:A:238:LYS:H	1.71	0.54
1:F:6:LYS:HD2	1:F:34:VAL:HG13	1.88	0.54
1:H:218:VAL:O	1:H:222:ARG:HG3	2.07	0.54
1:I:201:LEU:HD23	1:I:206:ILE:HD11	1.89	0.54
1:E:4:LEU:O	1:E:7:THR:OG1	2.26	0.53
1:H:87:SER:HA	1:H:112:THR:OG1	2.08	0.53
1:H:130:ARG:HG3	1:H:135:PHE:CE1	2.43	0.53
1:I:247:ASN:HD22	1:I:247:ASN:N	2.04	0.53
1:F:160:GLU:O	1:F:164:GLU:HG2	2.08	0.53
1:H:167:ARG:O	1:H:171:VAL:HG23	2.08	0.53
1:B:6:LYS:O	1:B:10:ILE:HD12	2.08	0.53
1:H:63:LYS:O	1:H:67:GLU:HG3	2.07	0.53
1:K:172:VAL:HG12	1:K:176:ILE:HD12	1.89	0.53
1:B:237:MSE:SE	1:B:240:THR:HG22	2.58	0.53
1:E:216:VAL:O	1:E:217:ILE:C	2.52	0.53
1:H:150:VAL:O	1:H:154:ILE:HD12	2.08	0.53
1:C:197:ASN:ND2	1:C:244:VAL:HG22	2.24	0.53
1:D:205:LYS:HG2	1:D:209:ARG:NH1	2.23	0.53
1:G:48:LEU:HD23	1:G:69:ARG:HE	1.74	0.53
1:H:116:ILE:HG22	1:H:123:LEU:HB2	1.90	0.53
1:I:190:ILE:HD11	1:I:217:ILE:HG23	1.91	0.53
1:B:34:VAL:HG12	1:B:35:ILE:HG13	1.89	0.53
1:H:16:ALA:O	1:H:20:LYS:NZ	2.41	0.53
1:H:203:ALA:HB3	1:H:237:MSE:CE	2.39	0.53
1:F:201:LEU:HG	1:F:202:VAL:H	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:169:LYS:HE2	1:C:248:LYS:HE2	1.90	0.53
1:C:218:VAL:HG12	1:C:219:ASN:N	2.23	0.53
1:A:40:PHE:CE2	1:A:62:MSE:HE1	2.44	0.52
1:G:206:ILE:N	1:G:206:ILE:HD13	2.24	0.52
1:H:201:LEU:HG	1:H:206:ILE:HD11	1.90	0.52
1:C:4:LEU:O	1:C:8:ARG:HG3	2.08	0.52
1:F:88:ASN:HD21	1:F:135:PHE:N	2.00	0.52
1:I:230:ILE:HG22	1:I:244:VAL:HA	1.91	0.52
1:D:6:LYS:HA	1:D:9:ILE:HD12	1.92	0.52
1:F:200:LEU:O	1:F:200:LEU:HD23	2.10	0.52
1:G:190:ILE:O	1:G:193:GLU:HB3	2.10	0.52
1:I:251:ILE:O	1:I:254:GLU:HB2	2.09	0.52
1:D:88:ASN:HD21	1:D:135:PHE:N	2.02	0.52
1:D:234:SER:O	1:D:235:LEU:HD13	2.09	0.52
1:E:24:PHE:CD1	1:E:27:MSE:CE	2.93	0.52
1:A:174:MSE:O	1:A:177:SER:HB3	2.10	0.52
1:C:95:TYR:CE2	1:C:97:ALA:HB3	2.45	0.52
1:E:214:ARG:CD	1:E:214:ARG:N	2.71	0.52
1:G:32:ARG:HD3	1:G:52:SER:OG	2.09	0.52
1:G:231:GLU:CB	1:G:245:LEU:HD21	2.39	0.52
1:C:212:ILE:HG12	1:E:121:GLU:HG3	1.92	0.52
1:G:95:TYR:CD1	1:G:95:TYR:C	2.87	0.52
1:H:214:ARG:HA	1:H:217:ILE:HD12	1.92	0.52
1:I:128:LEU:HD12	1:I:128:LEU:N	2.25	0.52
1:B:116:ILE:HD12	1:B:125:THR:N	2.24	0.52
1:H:132:GLN:HE21	1:H:132:GLN:N	2.08	0.52
1:B:136:ASN:O	1:B:139:ASP:HB2	2.10	0.51
1:D:194:LEU:HD22	1:D:242:ILE:HD11	1.91	0.51
1:D:225:GLU:OE2	1:D:232:SER:HB3	2.09	0.51
1:I:165:GLU:HG3	1:I:248:LYS:NZ	2.25	0.51
1:I:216:VAL:O	1:I:217:ILE:C	2.53	0.51
1:A:145:TYR:O	1:A:145:TYR:CD2	2.61	0.51
1:B:11:ASN:O	1:B:15:GLN:HG2	2.10	0.51
1:E:3:LEU:O	1:E:3:LEU:HD12	2.09	0.51
1:E:40:PHE:HB2	1:E:127:ILE:HB	1.92	0.51
1:E:168:SER:O	1:E:171:VAL:HG12	2.10	0.51
1:F:45:ARG:H	1:F:45:ARG:HD3	1.76	0.51
1:I:176:ILE:HA	1:I:179:LEU:CD1	2.40	0.51
1:K:255:ASN:C	1:K:256:LEU:HD12	2.36	0.51
1:G:13:MSE:O	1:G:13:MSE:HE2	2.10	0.51
1:D:44:ARG:HG3	1:D:80:PHE:HE2	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:237:MSE:HE2	1:E:240:THR:HB	1.93	0.51
1:B:87:SER:HB3	1:B:140:LEU:HD21	1.92	0.51
1:B:230:ILE:HG22	1:B:244:VAL:HA	1.92	0.51
1:E:247:ASN:H	1:E:247:ASN:HD22	1.53	0.51
1:H:61:ARG:NH1	1:H:72:PRO:HG2	2.25	0.51
1:C:11:ASN:O	1:C:14:LEU:HB3	2.10	0.51
1:C:174:MSE:CG	1:D:167:ARG:HG3	2.40	0.51
1:H:249:PHE:C	1:H:249:PHE:CD2	2.88	0.51
1:B:167:ARG:O	1:B:170:ALA:HB3	2.11	0.51
1:G:247:ASN:H	1:G:247:ASN:ND2	2.08	0.51
1:F:247:ASN:HD22	1:F:247:ASN:N	2.04	0.51
1:A:231:GLU:HG3	1:A:245:LEU:HD11	1.92	0.51
1:H:12:SER:HA	1:H:15:GLN:HG3	1.93	0.51
1:A:203:ALA:HB3	1:A:237:MSE:HE1	1.92	0.50
1:B:3:LEU:HD13	1:B:138:ASP:HB3	1.93	0.50
1:G:24:PHE:CD1	1:G:27:MSE:HE3	2.46	0.50
1:I:29:GLU:O	1:I:32:ARG:HB3	2.11	0.50
1:I:57:ILE:HG12	1:I:131:LEU:HD13	1.93	0.50
1:I:187:ILE:HD11	1:I:220:ALA:HB1	1.93	0.50
1:A:14:LEU:HD23	1:A:15:GLN:NE2	2.24	0.50
1:C:188:GLU:O	1:C:192:GLU:CG	2.57	0.50
1:E:170:ALA:HB1	1:F:174:MSE:HE3	1.92	0.50
1:K:229:VAL:HG12	1:K:230:ILE:HG23	1.93	0.50
1:A:137:ASP:O	1:A:141:ILE:HG13	2.11	0.50
1:D:165:GLU:CG	1:D:248:LYS:HZ1	2.25	0.50
1:G:32:ARG:HD2	1:G:53:ILE:C	2.36	0.50
1:H:130:ARG:HD2	1:H:133:ASP:HB2	1.94	0.50
1:I:45:ARG:HH21	1:I:47:LYS:CE	2.21	0.50
1:K:206:ILE:O	1:K:210:VAL:HG23	2.12	0.50
1:B:164:GLU:O	1:B:168:SER:OG	2.29	0.50
1:C:101:GLU:H	1:C:101:GLU:CD	2.18	0.50
1:H:203:ALA:HB3	1:H:237:MSE:SE	2.62	0.50
1:I:244:VAL:HG21	1:I:250:LEU:CD2	2.41	0.50
1:B:205:LYS:CE	1:B:205:LYS:CG	2.88	0.50
1:C:95:TYR:HE2	1:C:97:ALA:HB3	1.76	0.50
1:E:218:VAL:HG12	1:E:219:ASN:N	2.27	0.50
1:H:216:VAL:O	1:H:217:ILE:C	2.54	0.50
1:F:156:ARG:CD	1:F:160:GLU:OE2	2.60	0.50
1:H:45:ARG:HD3	1:H:45:ARG:H	1.76	0.50
1:I:8:ARG:O	1:I:11:ASN:HB2	2.12	0.50
1:A:79:LEU:HD11	1:A:125:THR:HG21	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:ILE:O	1:A:221:LEU:HD22	2.12	0.50
1:E:201:LEU:O	1:E:240:THR:HG23	2.12	0.50
1:H:149:VAL:HA	1:H:152:MSE:CE	2.42	0.50
1:F:251:ILE:O	1:F:254:GLU:HB2	2.11	0.50
1:A:204:SER:HA	1:A:214:ARG:HG3	1.93	0.50
1:C:168:SER:O	1:C:171:VAL:HG22	2.12	0.50
1:G:88:ASN:OD1	1:G:135:PHE:HB2	2.12	0.50
1:K:179:LEU:HD23	1:K:183:GLU:HB3	1.94	0.50
1:E:23:ASN:OD1	1:E:23:ASN:C	2.55	0.49
1:G:163:GLU:O	1:G:167:ARG:HB2	2.12	0.49
1:A:186:ALA:O	1:A:187:ILE:C	2.56	0.49
1:B:204:SER:O	1:B:207:ALA:HB3	2.12	0.49
1:C:65:MSE:HG3	1:C:71:PHE:CE1	2.47	0.49
1:D:173:GLN:NE2	1:D:176:ILE:HD12	2.28	0.49
1:E:217:ILE:O	1:E:221:LEU:HD22	2.12	0.49
1:B:95:TYR:CD1	1:B:95:TYR:C	2.90	0.49
1:C:59:ASN:ND2	1:C:62:MSE:HG2	2.27	0.49
1:C:213:THR:HA	1:C:214:ARG:HH12	1.77	0.49
1:D:168:SER:O	1:D:171:VAL:HG22	2.12	0.49
1:E:11:ASN:O	1:E:15:GLN:HG2	2.11	0.49
1:E:171:VAL:O	1:E:174:MSE:HB3	2.13	0.49
1:F:214:ARG:CD	1:F:214:ARG:N	2.71	0.49
1:A:101:GLU:HG2	1:A:102:ASN:OD1	2.11	0.49
1:B:145:TYR:O	1:B:149:VAL:HG23	2.12	0.49
1:I:83:PRO:HG2	1:I:84:GLU:HG2	1.94	0.49
1:C:89:LEU:HD12	1:C:113:ILE:HD11	1.94	0.49
1:C:88:ASN:HD21	1:C:135:PHE:N	1.99	0.49
1:C:203:ALA:HB3	1:C:237:MSE:CE	2.43	0.49
1:D:165:GLU:HG3	1:D:248:LYS:HZ1	1.77	0.49
1:G:145:TYR:O	1:G:148:THR:HB	2.12	0.49
1:A:95:TYR:HD2	1:A:97:ALA:H	1.60	0.49
1:B:38:ASN:HB2	1:B:129:SER:OG	2.12	0.49
1:C:115:PRO:HB3	1:C:122:ARG:CZ	2.42	0.49
1:G:172:VAL:O	1:G:176:ILE:HG13	2.11	0.49
1:I:6:LYS:HA	1:I:9:ILE:HD12	1.94	0.49
1:K:213:THR:O	1:K:216:VAL:CG1	2.60	0.49
1:K:252:GLU:HA	1:K:255:ASN:ND2	2.25	0.49
1:D:156:ARG:O	1:D:160:GLU:HG3	2.12	0.49
1:G:130:ARG:NH1	1:G:134:GLN:O	2.45	0.49
1:G:171:VAL:O	1:G:174:MSE:HG3	2.12	0.49
1:H:205:LYS:HE2	1:H:209:ARG:HH21	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:165:GLU:CG	1:D:248:LYS:NZ	2.76	0.49
1:H:23:ASN:OD1	1:H:23:ASN:C	2.55	0.49
1:H:95:TYR:HE1	1:H:103:ARG:NH1	2.11	0.49
1:A:241:TYR:C	1:A:241:TYR:CD2	2.91	0.49
1:E:115:PRO:HB3	1:E:122:ARG:CZ	2.43	0.49
1:F:88:ASN:ND2	1:F:135:PHE:H	2.02	0.49
1:I:229:VAL:HG12	1:I:230:ILE:HG23	1.95	0.49
1:K:213:THR:O	1:K:216:VAL:HG13	2.13	0.49
1:C:62:MSE:SE	1:C:65:MSE:HE2	2.63	0.48
1:C:78:ASN:HD21	1:C:99:PRO:HD3	1.78	0.48
1:D:237:MSE:HG3	1:D:238:LYS:N	2.28	0.48
1:I:4:LEU:HB3	1:I:5:GLN:OE1	2.13	0.48
1:K:216:VAL:O	1:K:217:ILE:C	2.56	0.48
1:C:214:ARG:H	1:C:214:ARG:NH1	2.12	0.48
1:I:231:GLU:HB2	1:I:245:LEU:CD1	2.43	0.48
1:C:231:GLU:HB2	1:C:245:LEU:HD21	1.94	0.48
1:C:255:ASN:C	1:C:256:LEU:HD12	2.38	0.48
1:E:88:ASN:HD21	1:E:135:PHE:H	1.60	0.48
1:F:169:LYS:HG3	1:F:248:LYS:HG2	1.93	0.48
1:F:255:ASN:N	1:F:255:ASN:HD22	2.12	0.48
1:A:170:ALA:HB1	1:B:174:MSE:HE1	1.95	0.48
1:A:214:ARG:HA	1:A:217:ILE:HD12	1.95	0.48
1:I:45:ARG:H	1:I:45:ARG:HD3	1.78	0.48
1:A:162:ILE:HD12	1:G:184:LEU:HD12	1.95	0.48
1:D:23:ASN:C	1:D:23:ASN:OD1	2.56	0.48
1:F:17:ALA:O	1:F:18:ALA:C	2.57	0.48
1:H:13:MSE:SE	1:H:27:MSE:HG2	2.63	0.48
1:H:252:GLU:OE1	1:H:252:GLU:HA	2.12	0.48
1:I:37:SER:HA	1:I:55:GLN:NE2	2.28	0.48
1:A:201:LEU:HD23	1:A:206:ILE:CD1	2.44	0.48
1:B:85:THR:HB	1:G:8:ARG:NH2	2.28	0.48
1:C:15:GLN:OE1	1:C:15:GLN:HA	2.14	0.48
1:D:252:GLU:O	1:D:255:ASN:HB2	2.13	0.48
1:E:57:ILE:HG12	1:E:131:LEU:HD12	1.95	0.48
1:E:82:VAL:HG22	1:E:97:ALA:HB1	1.96	0.48
1:E:238:LYS:O	1:E:238:LYS:CG	2.61	0.48
1:I:17:ALA:O	1:I:18:ALA:C	2.56	0.48
1:A:40:PHE:CZ	1:A:62:MSE:HE1	2.48	0.48
1:D:65:MSE:SE	1:D:65:MSE:C	3.07	0.48
1:D:173:GLN:HG2	1:F:169:LYS:HB2	1.96	0.48
1:F:216:VAL:O	1:F:217:ILE:C	2.56	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:112:THR:HG1	1:H:135:PHE:HD2	1.60	0.48
1:A:194:LEU:HD22	1:A:242:ILE:CD1	2.43	0.48
1:D:164:GLU:HG2	1:D:167:ARG:HH22	1.79	0.48
1:B:31:LEU:HB3	1:B:35:ILE:HD12	1.95	0.48
1:C:216:VAL:O	1:C:217:ILE:C	2.57	0.48
1:F:145:TYR:O	1:F:149:VAL:HG23	2.14	0.48
1:I:2:ALA:HA	1:I:5:GLN:NE2	2.29	0.47
1:F:243:LYS:CD	1:F:243:LYS:NZ	2.73	0.47
1:B:153:GLU:OE2	1:B:153:GLU:HA	2.13	0.47
1:F:115:PRO:HB3	1:F:122:ARG:CZ	2.44	0.47
1:G:115:PRO:HB3	1:G:122:ARG:CZ	2.44	0.47
1:I:58:GLU:OE2	1:I:58:GLU:CA	2.50	0.47
1:A:103:ARG:C	1:A:105:LEU:H	2.21	0.47
1:B:40:PHE:HB2	1:B:127:ILE:HB	1.95	0.47
1:A:187:ILE:O	1:A:191:PHE:HD1	1.98	0.47
1:E:213:THR:CG2	1:E:214:ARG:CZ	2.92	0.47
1:A:17:ALA:O	1:A:18:ALA:C	2.57	0.47
1:E:20:LYS:CG	1:E:20:LYS:N	2.78	0.47
1:E:167:ARG:HD3	1:F:178:SER:OG	2.14	0.47
1:E:190:ILE:CD1	1:E:221:LEU:HD11	2.44	0.47
1:F:6:LYS:HB3	1:F:34:VAL:CG1	2.44	0.47
1:G:95:TYR:CE2	1:G:97:ALA:HB3	2.50	0.47
1:I:213:THR:HB	1:I:216:VAL:HG22	1.96	0.47
1:A:88:ASN:ND2	1:A:134:GLN:OE1	2.48	0.47
1:D:101:GLU:CD	1:D:101:GLU:H	2.23	0.47
1:H:99:PRO:HG2	1:H:102:ASN:HD22	1.79	0.47
1:C:213:THR:HA	1:C:214:ARG:NH1	2.30	0.47
1:D:234:SER:C	1:D:235:LEU:HD13	2.39	0.47
1:B:28:ALA:HB1	1:B:52:SER:HB2	1.97	0.47
1:B:203:ALA:HB3	1:B:237:MSE:CE	2.44	0.47
1:D:201:LEU:HD12	1:D:202:VAL:HG23	1.97	0.47
1:E:35:ILE:O	1:E:36:ASP:HB3	2.15	0.47
1:F:6:LYS:HB3	1:F:34:VAL:HG13	1.95	0.47
1:G:174:MSE:CE	1:H:170:ALA:HB1	2.45	0.47
1:H:122:ARG:NH2	1:H:125:THR:HG23	2.30	0.47
1:A:58:GLU:OE2	1:A:58:GLU:HA	2.15	0.47
1:A:214:ARG:NH1	1:A:214:ARG:N	2.63	0.47
1:C:174:MSE:HG2	1:D:167:ARG:HG3	1.97	0.47
1:F:243:LYS:HD3	1:F:245:LEU:CD2	2.45	0.47
1:K:56:GLN:HA	1:K:56:GLN:NE2	2.30	0.47
1:C:91:ILE:HD12	1:C:107:GLN:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:158:LYS:O	1:D:161:GLU:HB3	2.15	0.46
1:I:183:GLU:O	1:I:186:ALA:HB3	2.15	0.46
1:K:176:ILE:O	1:K:179:LEU:HD12	2.15	0.46
1:A:216:VAL:O	1:A:217:ILE:C	2.57	0.46
1:B:229:VAL:HG11	1:B:249:PHE:CD1	2.50	0.46
1:C:204:SER:HA	1:C:214:ARG:HG3	1.97	0.46
1:E:230:ILE:HG22	1:E:244:VAL:HA	1.97	0.46
1:E:251:ILE:O	1:E:254:GLU:HB2	2.15	0.46
1:G:174:MSE:HG2	1:H:174:MSE:SE	2.65	0.46
1:I:79:LEU:HD23	1:I:79:LEU:HA	1.74	0.46
1:B:179:LEU:CD2	1:B:183:GLU:HB3	2.44	0.46
1:E:11:ASN:ND2	2:E:301:SO4:O4	2.48	0.46
1:H:230:ILE:HG22	1:H:244:VAL:HA	1.97	0.46
1:I:75:TYR:O	1:I:78:ASN:HB2	2.15	0.46
1:A:121:GLU:HG2	1:A:122:ARG:N	2.30	0.46
1:B:27:MSE:HE3	1:B:150:VAL:HG22	1.97	0.46
1:B:27:MSE:HE1	1:B:150:VAL:HA	1.97	0.46
1:I:87:SER:HA	1:I:112:THR:HG23	1.97	0.46
1:D:202:VAL:O	1:D:206:ILE:HG12	2.15	0.46
1:F:103:ARG:C	1:F:105:LEU:H	2.23	0.46
1:A:103:ARG:C	1:A:105:LEU:N	2.74	0.46
1:B:103:ARG:C	1:B:105:LEU:H	2.23	0.46
1:C:85:THR:HG23	1:C:114:VAL:HG22	1.98	0.46
1:G:251:ILE:HD13	1:G:251:ILE:HA	1.78	0.46
1:H:172:VAL:HG12	1:H:176:ILE:CD1	2.43	0.46
1:A:29:GLU:O	1:A:32:ARG:HB3	2.16	0.46
1:A:169:LYS:HG3	1:A:248:LYS:HG2	1.96	0.46
1:A:200:LEU:O	1:A:200:LEU:HD23	2.16	0.46
1:C:165:GLU:O	1:C:169:LYS:HG3	2.16	0.46
1:D:205:LYS:HD3	1:D:209:ARG:HH22	1.81	0.46
1:D:237:MSE:HG3	1:D:238:LYS:H	1.80	0.46
1:G:6:LYS:HA	1:G:9:ILE:HD12	1.96	0.46
1:G:249:PHE:CD2	1:G:249:PHE:C	2.94	0.46
1:H:27:MSE:O	1:H:31:LEU:HD23	2.16	0.46
1:G:4:LEU:CD1	1:G:8:ARG:HD2	2.46	0.46
1:I:148:THR:HG22	1:I:152:MSE:HE2	1.97	0.46
1:A:6:LYS:HD2	1:A:34:VAL:HG13	1.97	0.45
1:B:153:GLU:CD	1:B:156:ARG:HH21	2.23	0.45
1:E:190:ILE:O	1:E:193:GLU:HB3	2.16	0.45
1:A:2:ALA:O	1:A:6:LYS:HG2	2.16	0.45
1:B:198:GLU:CG	1:B:243:LYS:HG3	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:213:THR:O	1:G:216:VAL:HG13	2.16	0.45
1:H:187:ILE:HD12	1:H:224:LEU:HD12	1.98	0.45
1:A:114:VAL:HA	1:A:115:PRO:HD2	1.83	0.45
1:B:90:ASP:HB3	1:B:110:LEU:HD23	1.98	0.45
1:C:149:VAL:HA	1:C:152:MSE:HE3	1.97	0.45
1:D:38:ASN:ND2	1:D:55:GLN:O	2.47	0.45
1:E:6:LYS:HB3	1:E:34:VAL:HG13	1.97	0.45
1:B:34:VAL:HG12	1:B:35:ILE:N	2.31	0.45
1:B:37:SER:HB2	1:B:130:ARG:HD2	1.99	0.45
1:B:145:TYR:O	1:B:145:TYR:HD2	1.99	0.45
1:E:4:LEU:HG	1:E:8:ARG:HD2	1.98	0.45
1:E:95:TYR:OH	1:E:98:PHE:HB2	2.15	0.45
1:E:233:ARG:NE	1:H:233:ARG:HH11	2.15	0.45
1:A:40:PHE:CD2	1:A:40:PHE:N	2.85	0.45
1:B:137:ASP:HA	1:B:140:LEU:HD12	1.99	0.45
1:F:48:LEU:HD23	1:F:69:ARG:HG3	1.99	0.45
1:F:115:PRO:HB2	1:F:117:ILE:CD1	2.46	0.45
1:F:172:VAL:HG12	1:F:176:ILE:HD12	1.98	0.45
1:F:183:GLU:O	1:F:186:ALA:HB3	2.17	0.45
1:G:6:LYS:HB3	1:G:34:VAL:CG1	2.46	0.45
1:G:62:MSE:O	1:G:65:MSE:HB3	2.16	0.45
1:G:250:LEU:H	1:G:250:LEU:CD2	2.27	0.45
1:H:31:LEU:HD12	1:H:35:ILE:HD11	1.97	0.45
1:H:177:SER:OG	1:H:178:SER:N	2.49	0.45
1:K:232:SER:CB	1:K:242:ILE:HG22	2.45	0.45
1:A:38:ASN:O	1:A:128:LEU:HA	2.17	0.45
1:I:249:PHE:CE1	1:I:253:LEU:HD13	2.52	0.45
1:A:150:VAL:HG12	1:A:154:ILE:CD1	2.44	0.45
1:B:24:PHE:HD1	1:B:27:MSE:CE	2.16	0.45
1:H:202:VAL:O	1:H:206:ILE:HG12	2.17	0.45
1:B:252:GLU:O	1:B:256:LEU:HD13	2.17	0.45
1:C:213:THR:HG23	1:C:214:ARG:NH2	2.31	0.45
1:D:25:LYS:O	1:D:29:GLU:HG3	2.17	0.45
1:D:203:ALA:HB3	1:D:237:MSE:CE	2.43	0.45
1:E:206:ILE:HD13	1:E:209:ARG:HH11	1.82	0.45
1:I:5:GLN:OE1	1:I:5:GLN:N	2.49	0.45
1:I:203:ALA:HB3	1:I:237:MSE:SE	2.67	0.45
1:A:167:ARG:HG3	1:B:174:MSE:HG2	1.97	0.45
1:B:225:GLU:HG3	1:B:230:ILE:O	2.17	0.45
1:D:17:ALA:O	1:D:18:ALA:C	2.60	0.45
1:D:206:ILE:HD13	1:D:206:ILE:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:88:ASN:HD21	1:G:134:GLN:HA	1.82	0.45
1:B:95:TYR:CG	1:B:96:THR:N	2.85	0.44
1:H:88:ASN:ND2	1:H:135:PHE:H	2.04	0.44
1:I:183:GLU:O	1:I:187:ILE:HG12	2.17	0.44
1:D:204:SER:HA	1:D:214:ARG:HG3	2.00	0.44
1:G:91:ILE:HD13	1:G:107:GLN:HA	1.99	0.44
1:H:182:SER:HA	1:H:185:GLU:HB2	2.00	0.44
1:H:218:VAL:HG13	1:H:219:ASN:N	2.31	0.44
1:K:137:ASP:HA	1:K:140:LEU:HD12	2.00	0.44
1:A:121:GLU:HG3	1:G:212:ILE:HG12	1.98	0.44
1:D:179:LEU:HD13	1:D:184:LEU:HA	2.00	0.44
1:D:241:TYR:CG	1:D:242:ILE:N	2.85	0.44
1:G:184:LEU:O	1:G:185:GLU:C	2.59	0.44
1:H:39:ILE:CD1	1:H:128:LEU:HD12	2.46	0.44
1:K:214:ARG:H	1:K:214:ARG:HD3	1.82	0.44
1:E:162:ILE:HG13	1:E:163:GLU:N	2.31	0.44
1:F:251:ILE:O	1:F:255:ASN:ND2	2.51	0.44
1:B:103:ARG:C	1:B:105:LEU:N	2.76	0.44
1:H:86:SER:HB3	1:H:89:LEU:HD11	1.99	0.44
1:B:95:TYR:OH	1:B:98:PHE:CB	2.66	0.44
1:C:8:ARG:HA	1:C:11:ASN:CG	2.43	0.44
1:D:8:ARG:NH1	1:E:144:GLU:OE2	2.50	0.44
1:D:214:ARG:CD	1:D:214:ARG:H	2.30	0.44
1:I:70:GLN:HG3	1:I:71:PHE:N	2.32	0.44
1:K:8:ARG:O	1:K:11:ASN:HB2	2.18	0.44
1:E:250:LEU:HG	1:E:251:ILE:H	1.83	0.44
1:F:237:MSE:HG3	1:F:238:LYS:H	1.83	0.44
1:G:174:MSE:HE2	1:H:170:ALA:HB1	1.99	0.44
1:H:51:TYR:HE2	1:H:69:ARG:HH21	1.66	0.44
1:K:121:GLU:HG2	1:K:122:ARG:N	2.32	0.44
1:A:145:TYR:CD2	1:A:145:TYR:C	2.95	0.44
1:A:216:VAL:HA	1:B:19:GLY:HA3	1.99	0.44
1:C:78:ASN:HD21	1:C:99:PRO:CD	2.31	0.44
1:D:217:ILE:O	1:D:220:ALA:HB3	2.18	0.44
1:A:164:GLU:O	1:A:165:GLU:C	2.61	0.43
1:B:99:PRO:HB2	1:B:101:GLU:OE2	2.17	0.43
1:D:169:LYS:HD2	1:F:173:GLN:NE2	2.33	0.43
1:D:213:THR:HG22	1:D:215:SER:H	1.83	0.43
1:D:214:ARG:HA	1:D:217:ILE:HD12	1.99	0.43
1:E:148:THR:O	1:E:152:MSE:HE3	2.18	0.43
1:A:6:LYS:HA	1:A:9:ILE:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:VAL:HG23	1:A:126:LEU:HB3	2.00	0.43
1:A:179:LEU:HD22	1:A:183:GLU:HB3	1.99	0.43
1:B:241:TYR:CD2	1:B:241:TYR:C	2.96	0.43
1:C:17:ALA:O	1:C:18:ALA:C	2.61	0.43
1:E:17:ALA:O	1:E:18:ALA:C	2.61	0.43
1:H:23:ASN:CG	1:H:26:GLU:HG2	2.42	0.43
1:K:250:LEU:H	1:K:250:LEU:CD2	2.13	0.43
1:C:38:ASN:OD1	1:C:55:GLN:HG2	2.19	0.43
1:E:95:TYR:CG	1:E:96:THR:N	2.84	0.43
1:H:12:SER:HA	1:H:15:GLN:CG	2.47	0.43
1:H:218:VAL:CG1	1:H:219:ASN:N	2.81	0.43
1:I:234:SER:O	1:I:235:LEU:HD13	2.19	0.43
1:K:14:LEU:HD23	1:K:15:GLN:NE2	2.34	0.43
1:H:61:ARG:HH12	1:H:72:PRO:HG2	1.83	0.43
1:K:61:ARG:O	1:K:61:ARG:HD3	2.18	0.43
1:C:187:ILE:HD11	1:C:220:ALA:HB1	2.00	0.43
1:G:186:ALA:O	1:G:187:ILE:C	2.60	0.43
1:K:65:MSE:HG3	1:K:71:PHE:CZ	2.53	0.43
1:A:238:LYS:HD3	1:A:238:LYS:HA	1.68	0.43
1:B:216:VAL:O	1:B:217:ILE:C	2.61	0.43
1:B:241:TYR:C	1:B:242:ILE:HG13	2.44	0.43
1:G:54:ASN:CG	1:G:55:GLN:HE21	2.25	0.43
1:H:210:VAL:HG13	1:H:212:ILE:HG13	2.00	0.43
1:C:87:SER:O	1:C:89:LEU:HD23	2.19	0.43
1:D:130:ARG:HD2	1:D:133:ASP:O	2.19	0.43
1:F:213:THR:HG22	1:F:215:SER:N	2.34	0.43
1:G:100:VAL:HA	1:G:103:ARG:HE	1.84	0.43
1:G:252:GLU:OE1	1:G:252:GLU:HA	2.19	0.43
1:K:78:ASN:CB	1:K:98:PHE:CE2	2.97	0.43
1:A:136:ASN:OD1	1:A:139:ASP:OD1	2.36	0.43
1:B:64:LYS:HE2	2:B:302:SO4:O2	2.19	0.43
1:B:84:GLU:O	1:B:85:THR:C	2.62	0.43
1:B:150:VAL:O	1:B:154:ILE:HG13	2.19	0.43
1:C:238:LYS:HD3	1:C:238:LYS:HA	1.87	0.43
1:E:237:MSE:HA	1:E:239:GLY:O	2.17	0.43
1:H:187:ILE:HD12	1:H:224:LEU:CD1	2.49	0.43
1:H:247:ASN:ND2	1:H:247:ASN:N	2.63	0.43
1:I:37:SER:HA	1:I:55:GLN:HE21	1.83	0.43
1:I:150:VAL:O	1:I:151:GLY:C	2.61	0.43
1:A:252:GLU:O	1:A:256:LEU:HD13	2.19	0.43
1:B:82:VAL:HA	1:B:83:PRO:HD3	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:153:GLU:OE2	1:F:153:GLU:HA	2.18	0.43
1:G:230:ILE:HG22	1:G:244:VAL:HA	2.01	0.43
1:H:80:PHE:CD1	1:H:80:PHE:C	2.97	0.43
1:C:150:VAL:O	1:C:151:GLY:C	2.62	0.43
1:D:35:ILE:HD13	1:D:128:LEU:HD21	2.00	0.43
1:E:118:GLY:O	1:E:119:GLY:C	2.62	0.43
1:F:232:SER:HB2	1:F:242:ILE:CG2	2.49	0.43
1:G:255:ASN:HD22	1:G:255:ASN:N	2.17	0.43
1:H:201:LEU:HG	1:H:206:ILE:CD1	2.49	0.43
1:A:256:LEU:HD12	1:A:256:LEU:N	2.34	0.42
1:K:123:LEU:HD23	1:K:123:LEU:HA	1.81	0.42
1:F:186:ALA:O	1:F:187:ILE:C	2.62	0.42
1:I:203:ALA:H	1:I:237:MSE:CE	2.28	0.42
1:A:15:GLN:OE1	1:H:117:ILE:HG22	2.19	0.42
1:A:156:ARG:O	1:A:160:GLU:HG3	2.19	0.42
1:E:11:ASN:OD1	1:E:145:TYR:OH	2.31	0.42
1:E:212:ILE:CG2	1:E:216:VAL:HG22	2.49	0.42
1:F:4:LEU:O	1:F:8:ARG:HG3	2.19	0.42
1:G:201:LEU:HG	1:G:202:VAL:N	2.17	0.42
1:H:11:ASN:OD1	1:H:145:TYR:OH	2.09	0.42
1:H:150:VAL:HG12	1:H:154:ILE:HD11	2.02	0.42
1:I:148:THR:O	1:I:152:MSE:HE3	2.19	0.42
1:A:19:GLY:O	1:B:219:ASN:HB2	2.20	0.42
1:A:94:GLU:O	1:A:94:GLU:HG3	2.19	0.42
1:B:78:ASN:HD22	1:B:78:ASN:HA	1.63	0.42
1:D:229:VAL:HG11	1:D:249:PHE:CD1	2.54	0.42
1:E:206:ILE:HD13	1:E:209:ARG:HD3	2.01	0.42
1:G:58:GLU:OE2	1:G:58:GLU:HA	2.19	0.42
1:G:156:ARG:HD2	1:G:160:GLU:OE1	2.18	0.42
1:K:38:ASN:O	1:K:128:LEU:HA	2.19	0.42
1:A:11:ASN:O	1:A:15:GLN:HG2	2.19	0.42
1:B:27:MSE:CE	1:B:150:VAL:HG22	2.50	0.42
1:C:22:VAL:HG13	1:C:27:MSE:CE	2.49	0.42
1:C:27:MSE:HE1	1:C:153:GLU:OE2	2.20	0.42
1:D:42:VAL:HG21	1:D:127:ILE:HD12	2.02	0.42
1:D:148:THR:HG22	1:D:152:MSE:HE3	2.01	0.42
1:I:131:LEU:HD12	1:I:131:LEU:HA	1.72	0.42
1:K:95:TYR:OH	1:K:98:PHE:HB2	2.19	0.42
1:K:115:PRO:HB3	1:K:122:ARG:CZ	2.49	0.42
1:B:145:TYR:O	1:B:145:TYR:CD2	2.73	0.42
1:B:173:GLN:O	1:B:174:MSE:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:47:LYS:HG2	1:D:48:LEU:N	2.33	0.42
1:D:87:SER:HA	1:D:112:THR:OG1	2.18	0.42
1:F:32:ARG:HD2	1:F:54:ASN:HB3	2.01	0.42
1:F:103:ARG:C	1:F:105:LEU:N	2.75	0.42
1:F:230:ILE:HG22	1:F:244:VAL:HA	2.00	0.42
1:G:103:ARG:C	1:G:105:LEU:N	2.78	0.42
1:G:197:ASN:HD22	1:G:197:ASN:H	1.67	0.42
1:H:17:ALA:O	1:H:18:ALA:C	2.63	0.42
1:K:95:TYR:N	1:K:95:TYR:CD1	2.87	0.42
1:A:127:ILE:C	1:A:128:LEU:HD12	2.45	0.42
1:B:75:TYR:O	1:B:76:THR:C	2.61	0.42
1:B:171:VAL:O	1:B:174:MSE:HB3	2.20	0.42
1:C:19:GLY:N	1:D:216:VAL:HG12	2.35	0.42
1:D:216:VAL:O	1:D:217:ILE:C	2.61	0.42
1:E:229:VAL:CG1	1:E:249:PHE:CD1	2.99	0.42
1:I:31:LEU:HB3	1:I:35:ILE:HD12	2.01	0.42
1:A:75:TYR:O	1:A:76:THR:C	2.63	0.42
1:A:217:ILE:O	1:A:221:LEU:CD2	2.68	0.42
1:B:95:TYR:OH	1:B:98:PHE:N	2.52	0.42
1:B:237:MSE:HG3	1:B:238:LYS:H	1.85	0.42
1:C:84:GLU:HA	1:C:115:PRO:HG2	2.01	0.42
1:C:85:THR:OG1	1:C:114:VAL:HG13	2.20	0.42
1:F:59:ASN:HB3	1:F:62:MSE:HB2	2.01	0.42
1:I:4:LEU:HD21	1:I:8:ARG:NH1	2.34	0.42
1:B:149:VAL:O	1:B:150:VAL:C	2.61	0.42
1:D:38:ASN:O	1:D:128:LEU:HA	2.19	0.42
1:F:213:THR:HB	1:F:216:VAL:HG23	2.02	0.42
1:H:132:GLN:HE21	1:H:132:GLN:H	1.67	0.42
1:H:149:VAL:HA	1:H:152:MSE:HE2	2.02	0.42
1:H:215:SER:O	1:H:218:VAL:HG12	2.20	0.42
1:I:38:ASN:HD21	1:I:55:GLN:HG3	1.85	0.42
1:I:202:VAL:HA	1:I:237:MSE:CE	2.48	0.42
1:I:234:SER:C	1:I:235:LEU:HD13	2.45	0.42
1:K:185:GLU:O	1:K:189:HIS:HD2	2.03	0.42
1:A:8:ARG:O	1:A:11:ASN:HB2	2.20	0.42
1:D:248:LYS:HD2	1:D:248:LYS:HA	1.74	0.42
1:I:8:ARG:HA	1:I:11:ASN:ND2	2.28	0.42
1:I:201:LEU:HG	1:I:202:VAL:HG23	2.02	0.42
1:K:17:ALA:O	1:K:18:ALA:C	2.63	0.42
1:B:35:ILE:O	1:B:36:ASP:HB3	2.20	0.41
1:E:103:ARG:C	1:E:105:LEU:H	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:250:LEU:H	1:E:250:LEU:CD2	2.13	0.41
1:F:43:SER:HB2	1:F:45:ARG:NH1	2.35	0.41
1:G:103:ARG:C	1:G:105:LEU:H	2.27	0.41
1:G:169:LYS:HG3	1:G:248:LYS:HG2	2.00	0.41
1:H:155:LEU:HD23	1:H:155:LEU:HA	1.74	0.41
1:I:41:VAL:HG22	1:I:126:LEU:CD1	2.50	0.41
1:A:95:TYR:CD2	1:A:97:ALA:N	2.88	0.41
1:G:204:SER:O	1:G:208:ASP:OD1	2.37	0.41
1:I:47:LYS:HG2	1:I:48:LEU:N	2.34	0.41
1:B:190:ILE:O	1:B:193:GLU:HB2	2.19	0.41
1:C:144:GLU:OE2	1:F:8:ARG:NE	2.53	0.41
1:K:206:ILE:HG22	1:K:210:VAL:CG2	2.50	0.41
1:B:14:LEU:HD23	1:B:14:LEU:C	2.45	0.41
1:B:37:SER:OG	1:B:38:ASN:N	2.53	0.41
1:B:78:ASN:HB3	1:B:98:PHE:CE2	2.55	0.41
1:C:222:ARG:HB2	1:C:222:ARG:CZ	2.50	0.41
1:E:27:MSE:SE	1:E:153:GLU:HG3	2.70	0.41
1:G:26:GLU:O	1:G:29:GLU:HB2	2.21	0.41
1:G:216:VAL:O	1:G:217:ILE:C	2.63	0.41
1:H:24:PHE:CD1	1:H:27:MSE:CE	3.03	0.41
1:K:82:VAL:HA	1:K:83:PRO:HD3	1.85	0.41
1:K:176:ILE:HA	1:K:179:LEU:HD13	2.00	0.41
1:B:17:ALA:O	1:B:18:ALA:C	2.62	0.41
1:E:45:ARG:HD3	1:E:45:ARG:H	1.86	0.41
1:F:218:VAL:O	1:F:222:ARG:HG3	2.20	0.41
1:H:214:ARG:H	1:H:214:ARG:HG3	1.60	0.41
1:K:45:ARG:H	1:K:45:ARG:HD3	1.85	0.41
1:K:172:VAL:HG12	1:K:176:ILE:CD1	2.51	0.41
1:C:63:LYS:HA	1:C:66:LEU:HD12	2.02	0.41
1:E:14:LEU:HD12	1:E:149:VAL:HG13	2.02	0.41
1:F:23:ASN:CG	1:F:26:GLU:CG	2.94	0.41
1:I:205:LYS:HG2	1:I:209:ARG:NH1	2.32	0.41
1:B:200:LEU:HB2	1:B:240:THR:O	2.21	0.41
1:F:243:LYS:HD3	1:F:245:LEU:HD23	2.01	0.41
1:G:231:GLU:OE2	1:G:243:LYS:HD3	2.21	0.41
1:H:10:ILE:HA	1:H:13:MSE:HE3	2.01	0.41
1:H:103:ARG:C	1:H:105:LEU:H	2.29	0.41
1:I:250:LEU:H	1:I:250:LEU:CD2	2.18	0.41
1:A:44:ARG:C	1:A:46:GLY:H	2.29	0.41
1:C:44:ARG:HH21	1:C:45:ARG:HG3	1.86	0.41
1:C:103:ARG:C	1:C:105:LEU:H	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:212:ILE:CG2	1:D:216:VAL:HG22	2.51	0.41
1:F:165:GLU:HG2	1:F:248:LYS:NZ	2.36	0.41
1:G:12:SER:CA	1:G:15:GLN:HG3	2.33	0.41
1:I:186:ALA:O	1:I:187:ILE:C	2.63	0.41
1:B:101:GLU:HG2	1:B:102:ASN:OD1	2.21	0.41
1:B:186:ALA:O	1:B:187:ILE:C	2.63	0.41
1:C:65:MSE:HG3	1:C:71:PHE:CZ	2.56	0.41
1:C:254:GLU:C	1:C:256:LEU:H	2.29	0.41
1:D:251:ILE:O	1:D:254:GLU:HB2	2.21	0.41
1:E:84:GLU:O	1:E:85:THR:C	2.63	0.41
1:F:24:PHE:HA	1:F:27:MSE:HE2	2.02	0.41
1:F:219:ASN:HA	1:F:222:ARG:HG3	2.03	0.41
1:G:205:LYS:HG2	1:G:209:ARG:NH1	2.36	0.41
1:I:78:ASN:CB	1:I:98:PHE:CE2	3.01	0.41
1:I:88:ASN:HD22	1:I:110:LEU:HD22	1.86	0.41
1:K:162:ILE:H	1:K:162:ILE:HG12	1.56	0.41
1:K:174:MSE:HE2	1:K:174:MSE:HB2	1.65	0.41
1:K:190:ILE:HG22	1:K:191:PHE:CD1	2.56	0.41
1:B:206:ILE:HG22	1:B:210:VAL:HG23	2.03	0.41
1:D:63:LYS:HE2	1:D:67:GLU:HG3	2.03	0.41
1:D:200:LEU:HB2	1:D:240:THR:O	2.21	0.41
1:G:206:ILE:HG22	1:G:210:VAL:CG2	2.51	0.41
1:H:103:ARG:C	1:H:105:LEU:N	2.79	0.41
1:K:32:ARG:CD	1:K:54:ASN:HB3	2.51	0.41
1:K:95:TYR:HE2	1:K:97:ALA:HB3	1.86	0.41
1:H:48:LEU:HD13	1:H:65:MSE:SE	2.71	0.40
1:H:153:GLU:O	1:H:157:GLU:HB2	2.21	0.40
1:B:3:LEU:O	1:B:4:LEU:C	2.65	0.40
1:C:38:ASN:HB2	1:C:129:SER:OG	2.22	0.40
1:D:169:LYS:CB	1:F:173:GLN:HE21	2.27	0.40
1:E:42:VAL:HG23	1:E:125:THR:O	2.21	0.40
1:E:103:ARG:C	1:E:105:LEU:N	2.79	0.40
1:E:170:ALA:HB1	1:F:174:MSE:CE	2.51	0.40
1:F:183:GLU:HG2	1:F:220:ALA:HB2	2.04	0.40
1:G:132:GLN:NE2	1:G:133:ASP:OD1	2.47	0.40
1:H:32:ARG:N	1:H:39:ILE:HG13	2.36	0.40
1:H:135:PHE:HA	1:H:139:ASP:OD1	2.20	0.40
1:I:70:GLN:HE21	1:I:71:PHE:H	1.69	0.40
1:K:79:LEU:HD23	1:K:79:LEU:HA	1.79	0.40
1:K:160:GLU:O	1:K:164:GLU:HG2	2.21	0.40
1:C:225:GLU:HB2	1:C:230:ILE:CD1	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:187:ILE:HD12	1:E:224:LEU:CD1	2.52	0.40
1:F:208:ASP:OD2	1:F:208:ASP:N	2.53	0.40
1:H:78:ASN:HB3	1:H:98:PHE:CZ	2.57	0.40
1:H:250:LEU:HD22	1:H:250:LEU:HA	1.69	0.40
1:I:38:ASN:O	1:I:128:LEU:HA	2.21	0.40
1:B:110:LEU:HD13	1:B:134:GLN:OE1	2.22	0.40
1:D:234:SER:OG	1:D:234:SER:CA	2.58	0.40
1:H:46:GLY:C	1:H:70:GLN:HE22	2.29	0.40
1:K:203:ALA:HB3	1:K:237:MSE:SE	2.71	0.40
1:K:237:MSE:HA	1:K:239:GLY:O	2.21	0.40

There are no symmetry-related clashes.

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	253/263 (96%)	229 (90%)	19 (8%)	5 (2%)	6	28
1	B	253/263 (96%)	229 (90%)	22 (9%)	2 (1%)	16	50
1	C	253/263 (96%)	231 (91%)	18 (7%)	4 (2%)	7	34
1	D	253/263 (96%)	229 (90%)	20 (8%)	4 (2%)	7	34
1	E	253/263 (96%)	229 (90%)	21 (8%)	3 (1%)	10	40
1	F	253/263 (96%)	228 (90%)	22 (9%)	3 (1%)	10	40
1	G	253/263 (96%)	229 (90%)	21 (8%)	3 (1%)	10	40
1	H	253/263 (96%)	235 (93%)	16 (6%)	2 (1%)	16	50
1	I	253/263 (96%)	227 (90%)	23 (9%)	3 (1%)	10	40
1	K	253/263 (96%)	228 (90%)	23 (9%)	2 (1%)	16	50
All	All	2530/2630 (96%)	2294 (91%)	205 (8%)	31 (1%)	10	40

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	18	ALA
1	A	237	MSE
1	B	18	ALA
1	B	237	MSE
1	C	18	ALA
1	C	237	MSE
1	D	18	ALA
1	D	237	MSE
1	E	18	ALA
1	E	237	MSE
1	F	18	ALA
1	F	237	MSE
1	G	18	ALA
1	G	237	MSE
1	H	18	ALA
1	H	237	MSE
1	I	18	ALA
1	I	237	MSE
1	K	18	ALA
1	K	237	MSE
1	A	74	GLU
1	E	74	GLU
1	A	58	GLU
1	D	74	GLU
1	G	74	GLU
1	D	218	VAL
1	C	58	GLU
1	A	218	VAL
1	C	151	GLY
1	I	151	GLY
1	F	218	VAL

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	221/222 (100%)	182 (82%)	39 (18%)	2	10
1	B	221/222 (100%)	181 (82%)	40 (18%)	2	9
1	C	221/222 (100%)	181 (82%)	40 (18%)	2	9
1	D	221/222 (100%)	184 (83%)	37 (17%)	2	12
1	E	221/222 (100%)	171 (77%)	50 (23%)	1	5
1	F	221/222 (100%)	182 (82%)	39 (18%)	2	10
1	G	221/222 (100%)	182 (82%)	39 (18%)	2	10
1	H	221/222 (100%)	174 (79%)	47 (21%)	1	6
1	I	221/222 (100%)	177 (80%)	44 (20%)	1	7
1	K	221/222 (100%)	177 (80%)	44 (20%)	1	7
All	All	2210/2220 (100%)	1791 (81%)	419 (19%)	1	8

All (419) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LYS
1	A	10	ILE
1	A	40	PHE
1	A	45	ARG
1	A	69	ARG
1	A	79	LEU
1	A	93	SER
1	A	94	GLU
1	A	100	VAL
1	A	114	VAL
1	A	132	GLN
1	A	136	ASN
1	A	152	MSE
1	A	162	ILE
1	A	163	GLU
1	A	165	GLU
1	A	171	VAL
1	A	173	GLN
1	A	176	ILE
1	A	185	GLU
1	A	193	GLU
1	A	200	LEU
1	A	205	LYS
1	A	206	ILE

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Mol	Chain	Res	Type
1	A	208	ASP
1	A	213	THR
1	A	214	ARG
1	A	216	VAL
1	A	231	GLU
1	A	234	SER
1	A	235	LEU
1	A	238	LYS
1	A	240	THR
1	A	242	ILE
1	A	244	VAL
1	A	247	ASN
1	A	248	LYS
1	A	251	ILE
1	A	254	GLU
1	B	12	SER
1	B	31	LEU
1	B	34	VAL
1	B	42	VAL
1	B	45	ARG
1	B	69	ARG
1	B	74	GLU
1	B	76	THR
1	B	78	ASN
1	B	94	GLU
1	B	95	TYR
1	B	96	THR
1	B	105	LEU
1	B	132	GLN
1	B	137	ASP
1	B	148	THR
1	B	152	MSE
1	B	157	GLU
1	B	162	ILE
1	B	165	GLU
1	B	168	SER
1	B	171	VAL
1	B	174	MSE
1	B	176	ILE
1	B	184	LEU
1	B	208	ASP
1	B	210	VAL

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Mol	Chain	Res	Type
1	B	214	ARG
1	B	216	VAL
1	B	221	LEU
1	B	226	SER
1	B	235	LEU
1	B	238	LYS
1	B	240	THR
1	B	244	VAL
1	B	245	LEU
1	B	247	ASN
1	B	248	LYS
1	B	251	ILE
1	B	256	LEU
1	C	14	LEU
1	C	30	THR
1	C	31	LEU
1	C	52	SER
1	C	65	MSE
1	C	69	ARG
1	C	84	GLU
1	C	86	SER
1	C	87	SER
1	C	89	LEU
1	C	93	SER
1	C	100	VAL
1	C	101	GLU
1	C	111	THR
1	C	113	ILE
1	C	117	ILE
1	C	125	THR
1	C	132	GLN
1	C	162	ILE
1	C	164	GLU
1	C	176	ILE
1	C	188	GLU
1	C	197	ASN
1	C	201	LEU
1	C	204	SER
1	C	206	ILE
1	C	210	VAL
1	C	214	ARG
1	C	216	VAL

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Mol	Chain	Res	Type
1	C	218	VAL
1	C	221	LEU
1	C	224	LEU
1	C	233	ARG
1	C	235	LEU
1	C	238	LYS
1	C	242	ILE
1	C	244	VAL
1	C	245	LEU
1	C	247	ASN
1	C	250	LEU
1	D	8	ARG
1	D	10	ILE
1	D	11	ASN
1	D	45	ARG
1	D	52	SER
1	D	56	GLN
1	D	69	ARG
1	D	77	LYS
1	D	78	ASN
1	D	112	THR
1	D	114	VAL
1	D	126	LEU
1	D	131	LEU
1	D	132	GLN
1	D	133	ASP
1	D	152	MSE
1	D	164	GLU
1	D	171	VAL
1	D	172	VAL
1	D	173	GLN
1	D	174	MSE
1	D	188	GLU
1	D	201	LEU
1	D	202	VAL
1	D	206	ILE
1	D	208	ASP
1	D	214	ARG
1	D	216	VAL
1	D	218	VAL
1	D	230	ILE
1	D	231	GLU

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Mol	Chain	Res	Type
1	D	235	LEU
1	D	238	LYS
1	D	242	ILE
1	D	247	ASN
1	D	248	LYS
1	D	250	LEU
1	E	3	LEU
1	E	6	LYS
1	E	10	ILE
1	E	13	MSE
1	E	14	LEU
1	E	26	GLU
1	E	42	VAL
1	E	43	SER
1	E	45	ARG
1	E	47	LYS
1	E	61	ARG
1	E	79	LEU
1	E	85	THR
1	E	87	SER
1	E	95	TYR
1	E	101	GLU
1	E	114	VAL
1	E	117	ILE
1	E	125	THR
1	E	141	ILE
1	E	148	THR
1	E	152	MSE
1	E	154	ILE
1	E	161	GLU
1	E	165	GLU
1	E	173	GLN
1	E	184	LEU
1	E	185	GLU
1	E	192	GLU
1	E	200	LEU
1	E	201	LEU
1	E	202	VAL
1	E	206	ILE
1	E	210	VAL
1	E	214	ARG
1	E	216	VAL

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Mol	Chain	Res	Type
1	E	218	VAL
1	E	219	ASN
1	E	221	LEU
1	E	222	ARG
1	E	225	GLU
1	E	234	SER
1	E	235	LEU
1	E	237	MSE
1	E	238	LYS
1	E	240	THR
1	E	242	ILE
1	E	247	ASN
1	E	248	LYS
1	E	250	LEU
1	F	20	LYS
1	F	41	VAL
1	F	45	ARG
1	F	52	SER
1	F	55	GLN
1	F	56	GLN
1	F	57	ILE
1	F	77	LYS
1	F	96	THR
1	F	148	THR
1	F	156	ARG
1	F	157	GLU
1	F	164	GLU
1	F	165	GLU
1	F	171	VAL
1	F	173	GLN
1	F	174	MSE
1	F	188	GLU
1	F	190	ILE
1	F	194	LEU
1	F	200	LEU
1	F	201	LEU
1	F	202	VAL
1	F	206	ILE
1	F	208	ASP
1	F	214	ARG
1	F	221	LEU
1	F	231	GLU

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Mol	Chain	Res	Type
1	F	232	SER
1	F	235	LEU
1	F	238	LYS
1	F	240	THR
1	F	242	ILE
1	F	244	VAL
1	F	245	LEU
1	F	247	ASN
1	F	248	LYS
1	F	255	ASN
1	F	256	LEU
1	G	10	ILE
1	G	13	MSE
1	G	14	LEU
1	G	15	GLN
1	G	29	GLU
1	G	42	VAL
1	G	43	SER
1	G	47	LYS
1	G	57	ILE
1	G	69	ARG
1	G	95	TYR
1	G	100	VAL
1	G	101	GLU
1	G	111	THR
1	G	125	THR
1	G	132	GLN
1	G	133	ASP
1	G	154	ILE
1	G	155	LEU
1	G	164	GLU
1	G	165	GLU
1	G	174	MSE
1	G	176	ILE
1	G	177	SER
1	G	194	LEU
1	G	204	SER
1	G	206	ILE
1	G	214	ARG
1	G	216	VAL
1	G	218	VAL
1	G	221	LEU

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Mol	Chain	Res	Type
1	G	238	LYS
1	G	240	THR
1	G	242	ILE
1	G	245	LEU
1	G	247	ASN
1	G	250	LEU
1	G	251	ILE
1	G	256	LEU
1	H	6	LYS
1	H	7	THR
1	H	8	ARG
1	H	13	MSE
1	H	14	LEU
1	H	15	GLN
1	H	30	THR
1	H	35	ILE
1	H	41	VAL
1	H	42	VAL
1	H	56	GLN
1	H	66	LEU
1	H	69	ARG
1	H	78	ASN
1	H	86	SER
1	H	94	GLU
1	H	95	TYR
1	H	101	GLU
1	H	103	ARG
1	H	112	THR
1	H	113	ILE
1	H	125	THR
1	H	128	LEU
1	H	132	GLN
1	H	139	ASP
1	H	157	GLU
1	H	163	GLU
1	H	164	GLU
1	H	165	GLU
1	H	179	LEU
1	H	184	LEU
1	H	192	GLU
1	H	200	LEU
1	H	201	LEU

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Mol	Chain	Res	Type
1	H	204	SER
1	H	206	ILE
1	H	210	VAL
1	H	214	ARG
1	H	216	VAL
1	H	221	LEU
1	H	230	ILE
1	H	235	LEU
1	H	242	ILE
1	H	245	LEU
1	H	247	ASN
1	H	250	LEU
1	H	256	LEU
1	I	5	GLN
1	I	7	THR
1	I	10	ILE
1	I	13	MSE
1	I	14	LEU
1	I	15	GLN
1	I	20	LYS
1	I	26	GLU
1	I	37	SER
1	I	42	VAL
1	I	45	ARG
1	I	56	GLN
1	I	58	GLU
1	I	69	ARG
1	I	73	GLU
1	I	74	GLU
1	I	96	THR
1	I	100	VAL
1	I	136	ASN
1	I	155	LEU
1	I	162	ILE
1	I	163	GLU
1	I	164	GLU
1	I	171	VAL
1	I	173	GLN
1	I	174	MSE
1	I	177	SER
1	I	184	LEU
1	I	185	GLU

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Mol	Chain	Res	Type
1	I	200	LEU
1	I	202	VAL
1	I	213	THR
1	I	214	ARG
1	I	216	VAL
1	I	221	LEU
1	I	225	GLU
1	I	234	SER
1	I	235	LEU
1	I	238	LYS
1	I	242	ILE
1	I	247	ASN
1	I	250	LEU
1	I	255	ASN
1	I	256	LEU
1	K	10	ILE
1	K	13	MSE
1	K	14	LEU
1	K	20	LYS
1	K	30	THR
1	K	37	SER
1	K	43	SER
1	K	44	ARG
1	K	47	LYS
1	K	53	ILE
1	K	57	ILE
1	K	69	ARG
1	K	70	GLN
1	K	89	LEU
1	K	101	GLU
1	K	111	THR
1	K	132	GLN
1	K	138	ASP
1	K	148	THR
1	K	152	MSE
1	K	155	LEU
1	K	162	ILE
1	K	173	GLN
1	K	176	ILE
1	K	184	LEU
1	K	190	ILE
1	K	194	LEU

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Mol	Chain	Res	Type
1	K	195	ASP
1	K	200	LEU
1	K	201	LEU
1	K	206	ILE
1	K	214	ARG
1	K	216	VAL
1	K	217	ILE
1	K	221	LEU
1	K	224	LEU
1	K	235	LEU
1	K	238	LYS
1	K	240	THR
1	K	242	ILE
1	K	244	VAL
1	K	247	ASN
1	K	248	LYS
1	K	250	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	70	GLN
1	A	88	ASN
1	A	132	GLN
1	A	134	GLN
1	A	173	GLN
1	A	189	HIS
1	A	247	ASN
1	B	15	GLN
1	B	88	ASN
1	B	173	GLN
1	B	189	HIS
1	B	247	ASN
1	C	23	ASN
1	C	78	ASN
1	C	88	ASN
1	C	173	GLN
1	C	197	ASN
1	D	70	GLN
1	D	78	ASN
1	D	81	ASN

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Mol	Chain	Res	Type
1	D	88	ASN
1	D	102	ASN
1	D	173	GLN
1	D	197	ASN
1	D	247	ASN
1	E	173	GLN
1	E	219	ASN
1	E	246	ASN
1	E	247	ASN
1	F	55	GLN
1	F	56	GLN
1	F	70	GLN
1	F	88	ASN
1	F	136	ASN
1	F	173	GLN
1	F	189	HIS
1	F	247	ASN
1	F	255	ASN
1	G	59	ASN
1	G	88	ASN
1	G	102	ASN
1	G	189	HIS
1	G	197	ASN
1	G	247	ASN
1	G	255	ASN
1	H	55	GLN
1	H	70	GLN
1	H	78	ASN
1	H	88	ASN
1	H	102	ASN
1	H	132	GLN
1	H	173	GLN
1	H	189	HIS
1	I	70	GLN
1	I	88	ASN
1	I	189	HIS
1	I	247	ASN
1	K	5	GLN
1	K	15	GLN
1	K	56	GLN
1	K	78	ASN
1	K	88	ASN

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Mol	Chain	Res	Type
1	K	92	ASN
1	K	134	GLN
1	K	173	GLN
1	K	189	HIS
1	K	247	ASN
1	K	255	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	B	302	-	4,4,4	0.27	0	6,6,6	0.16	0
2	SO4	C	301	-	4,4,4	1.18	0	6,6,6	0.59	0
2	SO4	E	302	-	4,4,4	0.51	0	6,6,6	0.16	0
2	SO4	H	301	-	4,4,4	0.63	0	6,6,6	0.15	0
2	SO4	A	301	-	4,4,4	0.57	0	6,6,6	0.33	0
2	SO4	B	301	-	4,4,4	0.31	0	6,6,6	0.34	0
2	SO4	G	301	-	4,4,4	0.29	0	6,6,6	0.43	0
2	SO4	I	301	-	4,4,4	0.28	0	6,6,6	0.21	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	E	301	-	4,4,4	0.70	0	6,6,6	0.36	0
2	SO4	A	302	-	4,4,4	0.27	0	6,6,6	0.20	0
2	SO4	K	301	-	4,4,4	0.69	0	6,6,6	0.27	0
2	SO4	F	301	-	4,4,4	0.33	0	6,6,6	0.26	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	302	SO4	1	0
2	E	301	SO4	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	248/263 (94%)	0.43	5 (2%)	65	41	69, 86, 96, 106	0
1	B	248/263 (94%)	0.47	6 (2%)	59	36	69, 86, 96, 106	0
1	C	248/263 (94%)	0.12	3 (1%)	76	55	69, 86, 96, 106	0
1	D	248/263 (94%)	0.38	7 (2%)	55	32	69, 86, 96, 106	0
1	E	248/263 (94%)	0.14	7 (2%)	55	32	69, 86, 96, 106	0
1	F	248/263 (94%)	0.13	4 (1%)	70	47	69, 86, 96, 106	0
1	G	248/263 (94%)	0.25	6 (2%)	59	36	69, 86, 96, 106	0
1	H	248/263 (94%)	0.21	5 (2%)	65	41	69, 86, 96, 106	0
1	I	248/263 (94%)	0.20	6 (2%)	59	36	69, 86, 96, 106	0
1	K	248/263 (94%)	0.07	2 (0%)	82	64	69, 86, 96, 106	0
All	All	2480/2630 (94%)	0.24	51 (2%)	63	40	69, 86, 97, 106	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	100	VAL	4.0
1	H	108	ALA	4.0
1	I	97	ALA	3.5
1	G	95	TYR	3.1
1	G	176	ILE	3.0
1	D	97	ALA	2.9
1	E	73	GLU	2.9
1	H	110	LEU	2.8
1	E	179	LEU	2.8
1	F	131	LEU	2.7
1	B	97	ALA	2.7
1	I	2	ALA	2.7
1	B	96	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	201	LEU	2.6
1	A	95	TYR	2.6
1	K	201	LEU	2.6
1	D	201	LEU	2.5
1	F	82	VAL	2.5
1	F	91	ILE	2.5
1	H	105	LEU	2.5
1	A	97	ALA	2.4
1	D	113	ILE	2.4
1	C	92	ASN	2.4
1	E	95	TYR	2.4
1	E	96	THR	2.4
1	H	109	GLY	2.3
1	E	108	ALA	2.3
1	A	178	SER	2.3
1	G	131	LEU	2.3
1	I	178	SER	2.3
1	I	14	LEU	2.2
1	A	96	THR	2.2
1	D	108	ALA	2.2
1	G	201	LEU	2.2
1	A	92	ASN	2.2
1	C	98	PHE	2.2
1	G	203	ALA	2.2
1	H	201	LEU	2.2
1	K	196	GLY	2.2
1	D	60	ASP	2.2
1	D	100	VAL	2.1
1	B	117	ILE	2.1
1	E	74	GLU	2.1
1	E	2	ALA	2.1
1	I	163	GLU	2.1
1	B	113	ILE	2.1
1	F	50	GLY	2.1
1	I	94	GLU	2.1
1	B	168	SER	2.1
1	G	196	GLY	2.0
1	D	38	ASN	2.0

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

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

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(Å ²)	Q<0.9
2	SO4	F	301	5/5	0.73	0.14	180,180,180,181	0
2	SO4	K	301	5/5	0.76	0.25	184,185,185,185	0
2	SO4	E	302	5/5	0.78	0.23	198,199,199,199	0
2	SO4	B	302	5/5	0.79	0.08	162,162,163,163	0
2	SO4	A	302	5/5	0.80	0.08	160,160,160,160	0
2	SO4	H	301	5/5	0.85	0.13	173,174,174,174	0
2	SO4	C	301	5/5	0.85	0.15	148,149,149,150	0
2	SO4	E	301	5/5	0.89	0.13	160,160,160,160	0
2	SO4	G	301	5/5	0.89	0.14	140,140,141,141	0
2	SO4	B	301	5/5	0.90	0.15	143,143,144,144	0
2	SO4	I	301	5/5	0.91	0.12	148,148,148,149	0
2	SO4	A	301	5/5	0.91	0.14	157,158,158,159	0

6.5 Other polymers [i](#)

There are no such residues in this entry.