



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:42 AM UTC

PDB ID : 1JR3 / pdb_00001jr3
Title : Crystal Structure of the Processivity Clamp Loader Gamma Complex of E. coli DNA Polymerase III
Authors : Jeruzalmi, D.; O'Donnell, M.; Kuriyan, J.
Deposited on : 2001-08-10
Resolution : 2.70 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

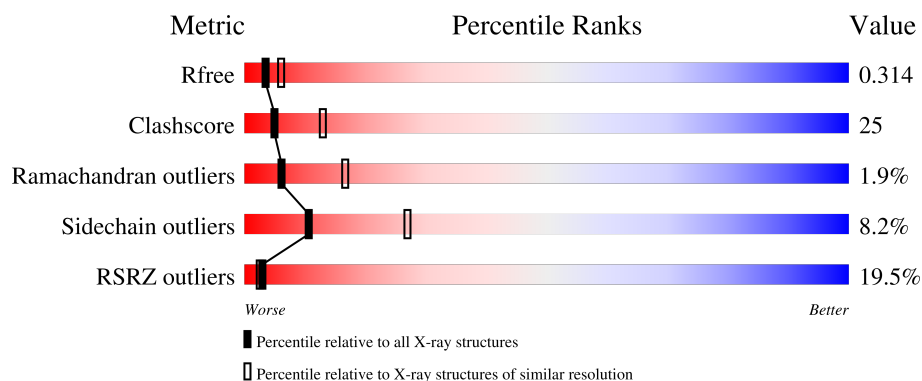
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	373	20% 53% 39% 6% .
1	B	373	22% 53% 38% 6% ..
1	C	373	14% 55% 34% 9% ..
2	D	343	17% 52% 36% 10% ..
3	E	334	23% 60% 35% 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	SO4	A	1500	-	-	X	-
5	SO4	B	2500	-	-	X	-
5	SO4	C	5500	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13845 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 DNA polymerase III subunit gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	366	Total	C	N	O	S	0	0	0
			2850	1793	514	527	16			
1	B	365	Total	C	N	O	S	0	0	0
			2838	1784	513	525	16			
1	C	366	Total	C	N	O	S	0	0	0
			2850	1793	514	527	16			

- Molecule 2 is a protein called DNA polymerase III, delta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	338	Total	C	N	O	S	0	0	0
			2687	1702	488	487	10			

- Molecule 3 is a protein called DNA polymerase III, delta' subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	334	Total	C	N	O	S	0	0	0
			2601	1655	468	465	13			

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Zn	0	0
			1	1		
4	B	1	Total	Zn	0	0
			1	1		
4	C	1	Total	Zn	0	0
			1	1		
4	E	1	Total	Zn	0	0
			1	1		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).

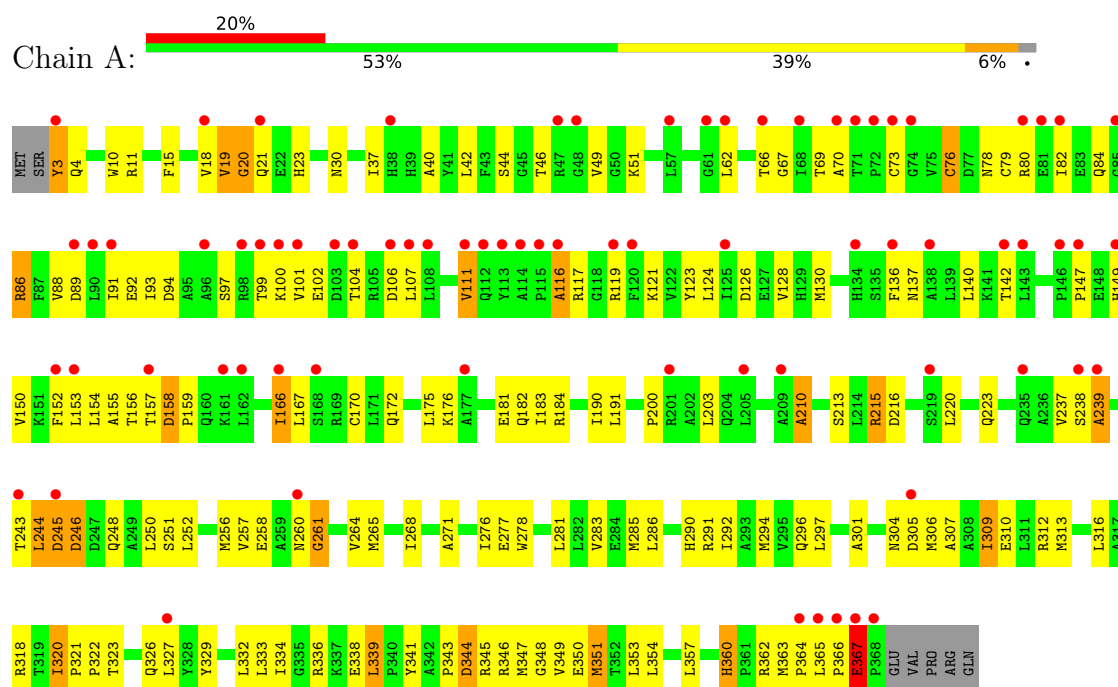


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		

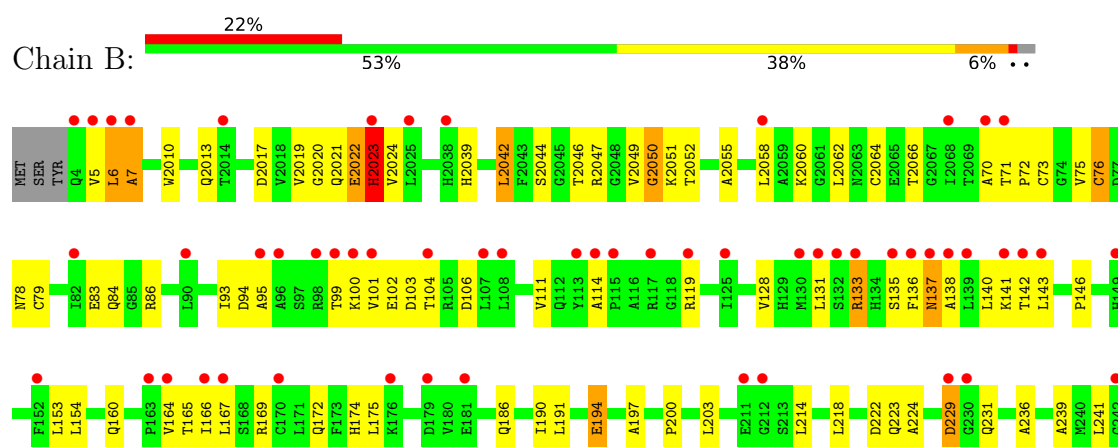
3 Residue-property plots

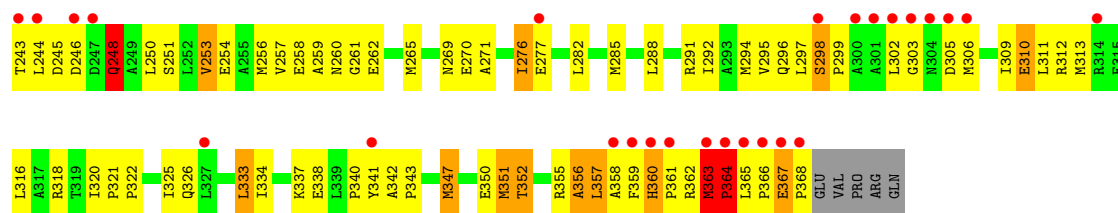
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

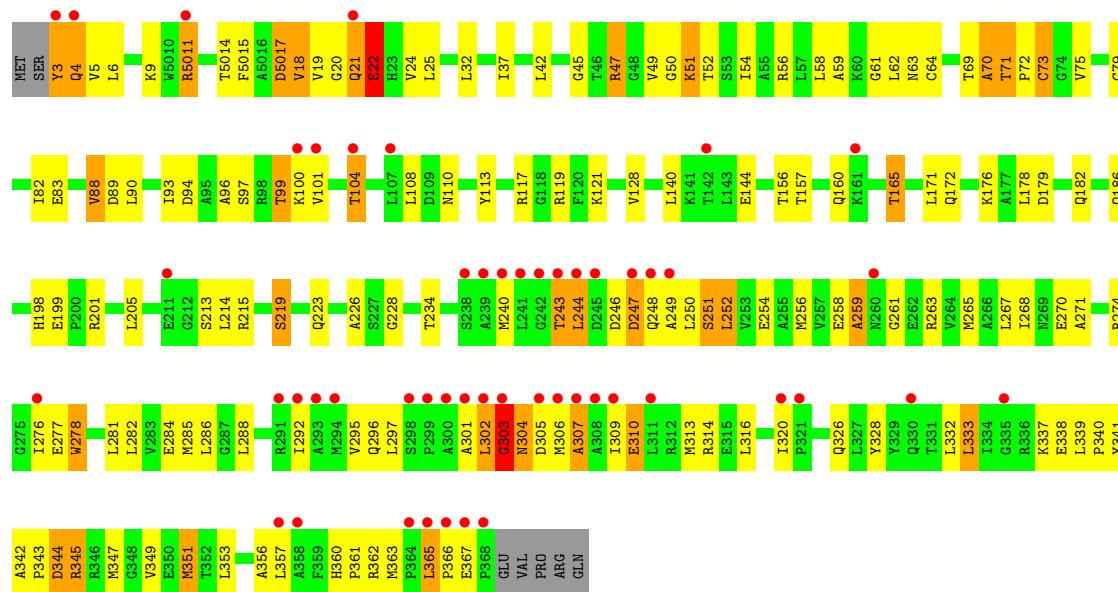


• Molecule 1: DNA polymerase III subunit gamma

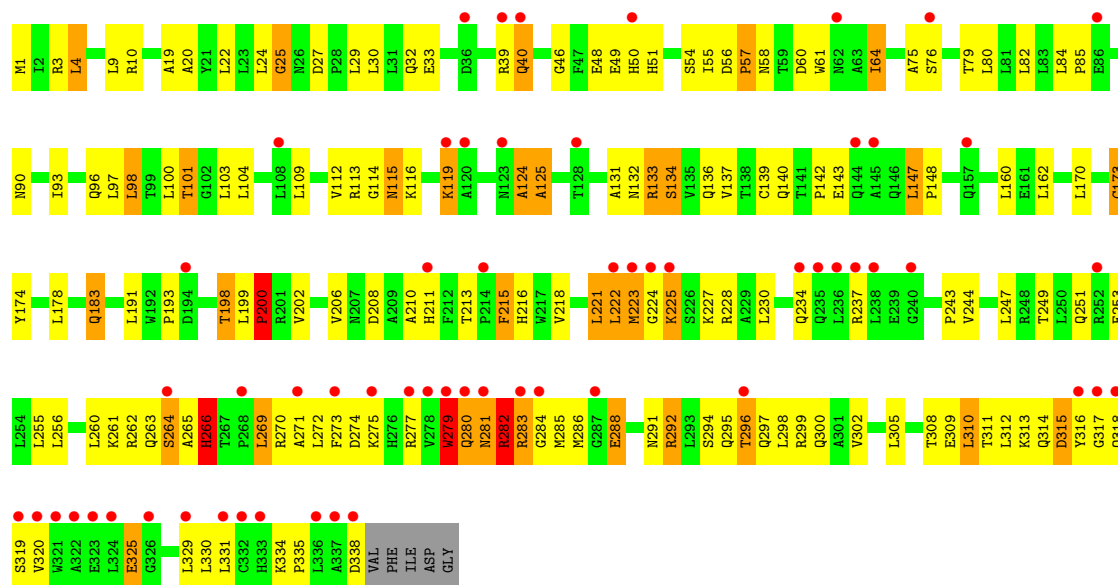




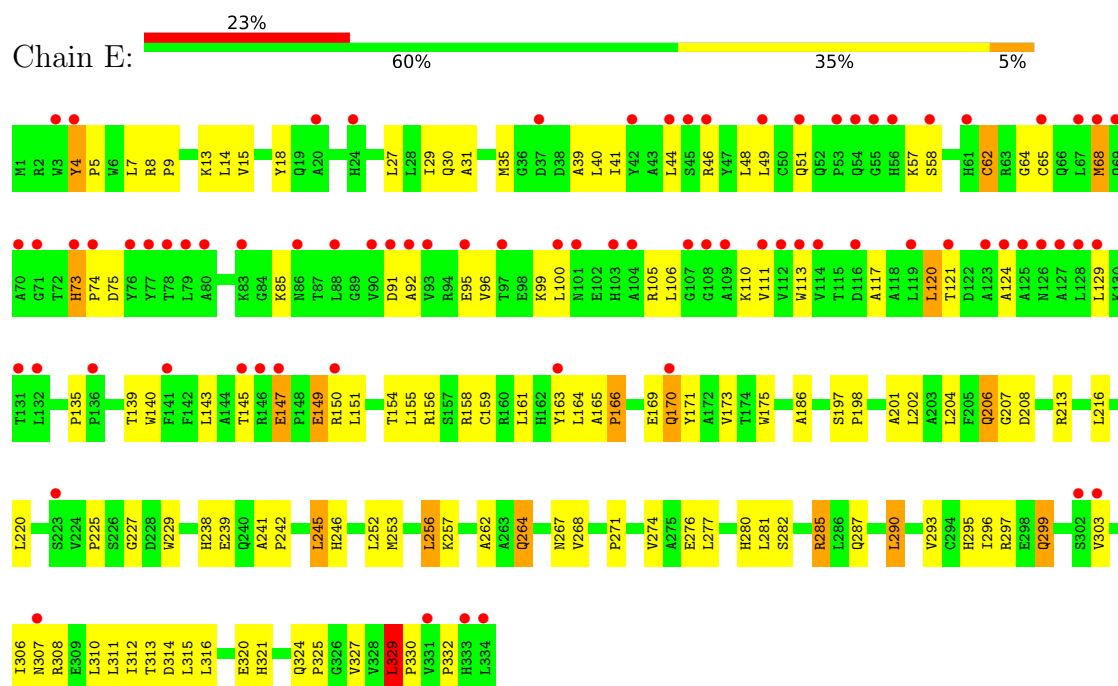
• Molecule 1: DNA polymerase III subunit gamma



• Molecule 2: DNA polymerase III, delta subunit



● Molecule 3: DNA polymerase III, delta' subunit



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	95.70Å 95.86Å 285.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	500.00 – 2.70 142.71 – 2.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (500.00-2.70) 76.8 (142.71-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	13.60	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 2.69Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.268 , 0.304 0.286 , 0.314	Depositor DCC
R_{free} test set	3031 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	65.2	Xtriage
Anisotropy	0.402	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 67.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.018 for k,h,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	13845	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.42% 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: ZN, 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	0.65	2/2898 (0.1%)	1.19	30/3930 (0.8%)
1	B	0.93	10/2885 (0.3%)	1.33	41/3912 (1.0%)
1	C	0.76	4/2898 (0.1%)	1.27	41/3930 (1.0%)
2	D	0.91	5/2735 (0.2%)	1.38	36/3716 (1.0%)
3	E	0.68	0/2666	1.13	17/3639 (0.5%)
All	All	0.80	21/14082 (0.1%)	1.26	165/19127 (0.9%)

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	1
2	D	0	4
All	All	0	5

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	315	ASP	CB-CG	24.32	2.12	1.52
1	B	363	MET	SD-CE	19.26	2.27	1.79
1	B	360	HIS	ND1-CE1	11.30	1.43	1.32
1	B	133	ARG	CZ-NH2	-11.25	1.18	1.33
2	D	310	LEU	CG-CD2	-10.36	1.18	1.52
1	B	360	HIS	CD2-NE2	9.60	1.48	1.37
1	B	360	HIS	CA-CB	9.51	1.66	1.53
1	B	363	MET	CG-SD	9.51	2.04	1.80
1	B	356	ALA	C-O	-8.92	1.12	1.24
1	B	360	HIS	CA-C	-7.99	1.42	1.52
1	B	360	HIS	CG-CD2	7.92	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	304	ASN	C-O	6.57	1.32	1.24
1	A	239	ALA	CA-CB	-6.50	1.43	1.53
2	D	283	ARG	CB-CG	5.98	1.70	1.52
2	D	315	ASP	CG-OD2	5.74	1.36	1.25
2	D	200	PRO	N-CD	-5.50	1.40	1.47
1	C	5	VAL	CA-CB	-5.45	1.47	1.54
1	B	2023	HIS	CA-C	-5.37	1.46	1.52
1	C	304	ASN	CG-ND2	-5.25	1.22	1.33
1	C	304	ASN	CA-CB	-5.25	1.44	1.53
1	A	351	MET	SD-CE	-5.24	1.66	1.79

All (165) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	315	ASP	CA-CB-CG	-22.76	89.84	112.60
2	D	280	GLN	CA-C-N	15.04	150.36	121.63
2	D	280	GLN	C-N-CA	15.04	150.36	121.63
2	D	283	ARG	CA-C-N	13.72	148.31	121.41
2	D	283	ARG	C-N-CA	13.72	148.31	121.41
1	B	363	MET	CG-SD-CE	12.09	127.49	100.90
1	B	360	HIS	N-CA-CB	11.20	129.10	110.05
1	C	75	VAL	N-CA-C	11.05	121.32	111.81
1	A	367	GLU	N-CA-C	10.89	118.02	108.22
1	B	360	HIS	CB-CA-C	-10.59	98.41	110.17
1	B	360	HIS	CA-CB-CG	10.01	123.81	113.80
1	B	360	HIS	CA-C-O	-9.93	110.46	119.59
1	B	360	HIS	CB-CG-ND1	9.61	137.11	122.70
1	C	243	THR	N-CA-C	9.44	125.06	110.42
1	C	24	VAL	N-CA-C	-9.26	102.84	111.45
1	A	301	ALA	N-CA-C	9.17	122.43	111.33
1	B	2020	GLY	N-CA-C	9.03	127.30	115.47
2	D	283	ARG	CA-C-O	8.83	130.37	120.84
1	B	133	ARG	NH1-CZ-NH2	-8.79	107.88	119.30
1	C	259	ALA	N-CA-C	8.65	125.59	113.56
2	D	75	ALA	N-CA-C	8.63	123.07	112.54
3	E	4	TYR	CA-C-N	8.26	127.94	119.19
3	E	4	TYR	C-N-CA	8.26	127.94	119.19
1	B	229	ASP	N-CA-C	-8.19	99.96	110.53
1	B	133	ARG	N-CA-C	8.12	124.77	111.37
1	B	276	ILE	CB-CA-C	-8.03	102.76	111.59
1	B	360	HIS	CE1-NE2-CD2	-7.96	101.04	109.00
2	D	280	GLN	O-C-N	-7.96	113.04	122.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	244	LEU	N-CA-C	7.84	123.14	113.50
1	A	70	ALA	N-CA-C	-7.82	103.76	113.38
1	C	19	VAL	N-CA-C	7.73	119.97	108.54
1	A	182	GLN	N-CA-C	-7.71	104.11	113.97
1	B	360	HIS	CB-CG-CD2	-7.69	121.20	131.20
1	B	7	ALA	N-CA-C	-7.69	94.43	110.80
1	C	59	ALA	N-CA-C	-7.68	102.99	111.36
3	E	206	GLN	N-CA-C	7.68	122.32	112.34
3	E	208	ASP	N-CA-C	-7.66	103.00	112.88
3	E	207	GLY	N-CA-C	-7.43	101.85	112.55
1	C	302	LEU	CA-C-N	7.41	135.92	121.41
1	C	302	LEU	C-N-CA	7.41	135.92	121.41
1	B	133	ARG	NE-CZ-NH2	7.27	125.75	119.20
1	B	141	LYS	N-CA-C	-7.21	103.51	111.36
3	E	329	LEU	CA-C-N	7.16	127.11	120.03
3	E	329	LEU	C-N-CA	7.16	127.11	120.03
1	C	20	GLY	N-CA-C	7.08	129.97	113.18
2	D	57	PRO	N-CA-C	-7.05	104.75	114.27
1	C	356	ALA	N-CA-C	-7.03	103.70	111.36
2	D	283	ARG	O-C-N	6.93	131.40	122.87
1	A	116	ALA	N-CA-C	6.86	119.59	111.71
1	A	86	ARG	N-CA-C	6.82	119.99	107.99
1	B	360	HIS	ND1-CE1-NE2	6.81	115.21	108.40
1	B	243	THR	N-CA-C	-6.80	99.14	109.95
1	B	2064	CYS	N-CA-C	6.79	119.86	110.35
3	E	186	ALA	N-CA-C	-6.78	103.51	111.03
2	D	264	SER	N-CA-C	-6.77	97.37	108.41
2	D	249	THR	N-CA-C	-6.76	104.67	113.12
1	B	298	SER	CA-C-N	6.72	128.24	119.84
1	B	298	SER	C-N-CA	6.72	128.24	119.84
1	B	363	MET	CB-CG-SD	6.70	132.81	112.70
1	C	303	GLY	N-CA-C	6.68	129.01	113.18
1	A	20	GLY	N-CA-C	6.64	128.92	113.18
2	D	134	SER	N-CA-C	6.61	120.61	110.36
1	C	244	LEU	CB-CG-CD2	-6.61	90.88	110.70
1	A	304	ASN	N-CA-C	6.59	118.25	111.14
2	D	237	ARG	N-CA-C	-6.55	105.32	113.38
2	D	277	ARG	N-CA-C	6.55	120.55	111.90
3	E	166	PRO	CA-C-N	6.54	124.37	119.66
3	E	166	PRO	C-N-CA	6.54	124.37	119.66
1	C	88	VAL	CB-CA-C	-6.50	103.57	111.88
1	C	304	ASN	N-CA-C	6.48	120.45	112.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	39	ALA	N-CA-C	6.48	119.17	111.71
2	D	124	ALA	N-CA-C	6.44	120.17	110.64
2	D	224	GLY	N-CA-C	-6.44	103.36	112.37
1	A	261	GLY	N-CA-C	6.39	119.91	112.50
1	B	359	PHE	CA-C-N	6.36	133.38	122.06
1	B	359	PHE	C-N-CA	6.36	133.38	122.06
1	C	213	SER	N-CA-C	6.32	119.70	109.40
1	C	89	ASP	N-CA-C	6.31	120.82	113.18
2	D	9	LEU	N-CA-C	6.29	117.80	111.07
1	C	5017	ASP	N-CA-C	6.28	120.56	112.26
1	C	70	ALA	N-CA-C	-6.26	105.64	113.28
1	A	215	ARG	CB-CA-C	-6.26	100.97	110.92
1	C	119	ARG	N-CA-C	6.25	118.89	111.33
1	A	244	LEU	N-CA-C	6.22	119.25	110.23
1	C	198	HIS	N-CA-C	6.20	118.59	108.55
2	D	4	LEU	N-CA-C	6.19	118.47	109.07
1	B	364	PRO	CA-N-CD	-6.18	103.34	112.00
2	D	76	SER	N-CA-C	6.10	118.48	109.69
1	C	339	LEU	N-CA-C	6.08	123.24	109.81
1	B	143	LEU	N-CA-C	6.08	118.68	111.33
2	D	288	GLU	N-CA-C	-6.04	104.77	111.36
3	E	264	GLN	N-CA-C	6.01	118.98	109.96
3	E	135	PRO	N-CA-C	6.00	118.02	110.70
2	D	210	ALA	N-CA-C	6.00	119.66	111.39
1	A	158	ASP	CA-C-N	5.98	125.66	119.56
1	A	158	ASP	C-N-CA	5.98	125.66	119.56
1	A	258	GLU	N-CA-C	-5.95	105.98	113.18
1	B	2019	VAL	N-CA-C	5.90	116.38	108.11
1	B	367	GLU	N-CA-C	5.87	113.29	108.07
1	B	75	VAL	N-CA-C	5.86	118.82	112.96
1	C	365	LEU	CA-C-N	5.84	127.03	120.66
1	C	365	LEU	C-N-CA	5.84	127.03	120.66
2	D	282	ARG	CB-CG-CD	-5.84	97.88	111.30
1	A	360	HIS	CA-C-N	5.82	125.20	118.85
1	A	360	HIS	C-N-CA	5.82	125.20	118.85
1	A	365	LEU	CA-C-N	5.79	127.10	120.85
1	A	365	LEU	C-N-CA	5.79	127.10	120.85
2	D	147	LEU	N-CA-C	-5.74	104.95	112.75
1	A	215	ARG	N-CA-C	-5.73	104.03	111.02
1	B	224	ALA	N-CA-C	-5.71	105.41	112.90
1	C	247	ASP	N-CA-C	5.70	117.50	108.67
1	C	96	ALA	N-CA-C	5.70	117.49	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	121	LYS	N-CA-C	-5.70	98.46	108.20
1	C	99	THR	N-CA-C	5.68	119.52	112.59
1	B	360	HIS	CG-CD2-NE2	5.67	112.87	107.20
2	D	61	TRP	N-CA-C	-5.64	105.28	111.82
1	A	339	LEU	N-CA-C	5.60	122.19	109.81
1	B	248	GLN	N-CA-C	5.57	117.80	111.11
1	C	21	GLN	CA-C-N	5.57	132.18	121.54
1	C	21	GLN	C-N-CA	5.57	132.18	121.54
1	A	19	VAL	N-CA-C	5.54	116.97	108.71
1	B	352	THR	N-CA-C	5.54	117.18	111.03
2	D	173	CYS	N-CA-C	-5.50	101.32	110.17
1	A	23	HIS	N-CA-C	5.47	119.06	112.38
1	B	303	GLY	N-CA-C	5.42	126.04	113.18
1	A	320	ILE	N-CA-C	5.42	113.84	107.77
3	E	293	VAL	N-CA-C	-5.41	105.10	110.62
1	A	245	ASP	N-CA-C	-5.40	102.29	110.28
2	D	291	ASN	N-CA-C	5.40	119.12	112.54
1	A	320	ILE	CA-C-N	5.39	125.93	120.38
1	A	320	ILE	C-N-CA	5.39	125.93	120.38
1	C	5015	PHE	N-CA-C	-5.39	105.41	111.28
1	C	307	ALA	N-CA-C	5.36	120.21	111.37
1	A	366	PRO	N-CA-C	5.35	120.56	111.03
1	B	270	GLU	N-CA-C	-5.32	105.49	111.28
1	A	183	ILE	N-CA-C	-5.30	105.97	111.58
2	D	283	ARG	N-CA-C	5.28	117.56	107.75
2	D	222	LEU	CB-CA-C	-5.26	104.69	111.22
2	D	225	LYS	N-CA-C	5.26	117.97	110.24
1	B	114	ALA	N-CA-C	5.25	117.13	109.84
1	C	365	LEU	N-CA-C	5.25	115.63	109.60
1	C	73	CYS	N-CA-C	-5.24	101.92	110.20
1	C	178	LEU	N-CA-C	5.24	118.23	110.48
1	C	5011	ARG	N-CA-C	-5.22	103.15	109.57
1	B	245	ASP	N-CA-C	-5.21	106.88	113.23
1	C	6	LEU	N-CA-C	5.20	117.35	111.11
1	A	210	ALA	N-CA-C	-5.20	101.98	110.20
2	D	282	ARG	CA-CB-CG	-5.19	103.73	114.10
3	E	73	HIS	CA-C-N	5.14	126.16	120.45
3	E	73	HIS	C-N-CA	5.14	126.16	120.45
2	D	104	LEU	N-CA-C	5.11	117.12	110.53
2	D	132	ASN	N-CA-C	-5.10	108.08	114.56
2	D	25	GLY	N-CA-C	5.09	117.47	110.69
1	B	347	MET	N-CA-C	-5.08	106.19	112.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	223	GLN	N-CA-C	-5.07	105.67	111.14
1	B	342	ALA	CA-C-N	5.06	125.34	119.47
1	B	342	ALA	C-N-CA	5.06	125.34	119.47
2	D	266	HIS	N-CA-C	-5.05	105.43	112.45
1	C	345	ARG	N-CA-C	5.03	117.41	111.33
1	B	241	LEU	N-CA-C	5.02	116.56	111.14
3	E	330	PRO	N-CA-C	5.02	118.94	111.41
1	C	228	GLY	N-CA-C	-5.01	106.97	115.34
1	C	199	GLU	CA-C-N	5.01	125.03	119.32
1	C	199	GLU	C-N-CA	5.01	125.03	119.32
2	D	325	GLU	N-CA-C	-5.00	105.73	111.14

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	2023	HIS	Sidechain
2	D	280	GLN	Peptide
2	D	281	ASN	Mainchain
2	D	282	ARG	Mainchain
2	D	319	SER	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	2850	0	2896	175	0
1	B	2838	0	2887	202	0
1	C	2850	0	2895	147	1
2	D	2687	0	2743	149	1
3	E	2601	0	2603	100	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
5	A	5	0	0	7	0
5	B	5	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	5	0	0	3	0
All	All	13845	0	14024	699	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 25.

All (699) 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:B:363:MET:CG	1:B:363:MET:SD	2.04	1.45
1:C:304:ASN:ND2	2:D:234:GLN:OE1	1.61	1.30
1:B:363:MET:SD	1:B:363:MET:CE	2.27	1.21
2:D:315:ASP:CG	2:D:315:ASP:CB	2.12	1.21
1:C:94:ASP:H	1:C:100:LYS:NZ	1.40	1.17
1:C:304:ASN:ND2	2:D:234:GLN:CD	2.02	1.17
1:B:360:HIS:HB3	1:B:363:MET:CB	1.77	1.13
1:B:360:HIS:HB3	1:B:363:MET:HB2	1.11	1.09
1:C:246:ASP:HB3	1:C:274:ARG:HD3	1.38	1.06
1:C:69:THR:HG22	1:C:71:THR:H	1.15	1.05
2:D:223:MET:SD	2:D:292:ARG:HB3	1.99	1.03
1:B:360:HIS:ND1	1:B:363:MET:HE2	1.74	1.02
1:B:363:MET:HB3	1:B:364:PRO:HD2	1.42	1.01
2:D:25:GLY:HA3	2:D:139:CYS:O	1.59	1.01
1:B:355:ARG:HH21	3:E:332:PRO:HD3	1.23	0.99
2:D:119:LYS:H	2:D:119:LYS:HD3	1.26	0.99
1:C:304:ASN:ND2	2:D:234:GLN:NE2	2.10	0.98
2:D:315:ASP:HB2	2:D:318:GLN:CG	1.94	0.98
1:A:239:ALA:HB1	1:B:2023:HIS:CE1	2.00	0.97
2:D:310:LEU:HD22	2:D:314:GLN:HE21	1.27	0.97
1:B:357:LEU:HA	1:B:363:MET:SD	2.05	0.97
1:A:351:MET:HA	1:A:351:MET:HE3	1.46	0.94
1:C:18:VAL:HG22	1:C:25:LEU:HD11	1.47	0.94
1:A:100:LYS:CD	1:B:133:ARG:HH21	1.82	0.93
1:A:100:LYS:HD3	1:B:133:ARG:NH2	1.82	0.93
1:A:239:ALA:HB1	1:B:2023:HIS:NE2	1.83	0.92
1:C:94:ASP:H	1:C:100:LYS:HZ3	0.96	0.91
2:D:213:THR:H	2:D:216:HIS:HD2	1.13	0.90
1:C:94:ASP:N	1:C:100:LYS:NZ	2.21	0.89
1:C:362:ARG:HE	1:C:363:MET:HE2	1.39	0.88
1:C:94:ASP:C	1:C:100:LYS:HZ1	1.81	0.88
1:B:357:LEU:O	1:B:363:MET:SD	2.31	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:363:MET:CB	1:B:364:PRO:HD2	2.04	0.87
1:A:271:ALA:HB1	1:A:276:ILE:HD11	1.57	0.86
1:B:309:ILE:CG2	1:B:313:MET:HG2	2.05	0.86
1:B:200:PRO:HB2	1:B:305:ASP:HB2	1.57	0.86
1:A:351:MET:CE	1:B:326:GLN:HE22	1.90	0.85
1:C:179:ASP:HB3	1:C:182:GLN:HB2	1.58	0.83
3:E:8:ARG:HG3	3:E:9:PRO:HD3	1.60	0.83
1:B:356:ALA:O	1:B:363:MET:HE3	1.77	0.83
2:D:55:ILE:HD13	2:D:97:LEU:HD11	1.59	0.83
2:D:312:LEU:HB2	2:D:320:VAL:HG21	1.60	0.83
1:A:351:MET:HE2	1:B:326:GLN:HE22	1.42	0.82
1:C:3:TYR:O	1:C:4:GLN:HG3	1.79	0.82
1:A:99:THR:HG22	1:A:99:THR:O	1.78	0.81
1:B:357:LEU:HA	1:B:363:MET:CE	2.09	0.81
1:B:360:HIS:HB3	1:B:363:MET:CG	2.10	0.81
2:D:315:ASP:HB2	2:D:318:GLN:HG3	1.63	0.81
1:B:253:VAL:O	1:B:257:VAL:HG23	1.80	0.81
1:A:94:ASP:O	1:A:100:LYS:HE3	1.81	0.80
1:B:99:THR:O	1:B:99:THR:HG22	1.81	0.80
3:E:58:SER:HB3	3:E:65:CYS:SG	2.21	0.80
1:C:304:ASN:ND2	2:D:234:GLN:HE22	1.77	0.80
1:A:309:ILE:HG13	1:A:313:MET:HG2	1.62	0.80
1:B:360:HIS:ND1	1:B:363:MET:CE	2.44	0.80
1:C:94:ASP:N	1:C:100:LYS:HZ3	1.77	0.79
1:A:67:GLY:HA2	1:A:119:ARG:HH12	1.47	0.79
1:A:97:SER:OG	1:A:100:LYS:HE3	1.83	0.79
1:B:360:HIS:CB	1:B:363:MET:CG	2.61	0.78
1:B:259:ALA:HB2	1:B:363:MET:CG	2.12	0.78
1:A:80:ARG:O	1:A:84:GLN:HG3	1.82	0.78
2:D:310:LEU:HD22	2:D:314:GLN:NE2	1.98	0.78
2:D:244:VAL:HG22	2:D:312:LEU:HD21	1.64	0.78
1:A:93:ILE:CG2	1:A:100:LYS:NZ	2.47	0.78
1:A:271:ALA:CB	1:A:276:ILE:HD11	2.13	0.78
1:C:45:GLY:O	1:C:51:LYS:HE2	1.84	0.77
1:B:363:MET:HB3	1:B:364:PRO:CD	2.14	0.77
1:A:128:VAL:HG11	1:A:154:LEU:HD22	1.67	0.77
1:B:244:LEU:HD21	1:B:276:ILE:HG12	1.66	0.77
1:C:4:GLN:OE1	1:C:9:LYS:HD2	1.84	0.77
2:D:300:GLN:OE1	2:D:335:PRO:CG	2.32	0.76
1:A:281:LEU:HD23	1:A:285:MET:HE2	1.68	0.76
1:B:360:HIS:HB2	1:B:363:MET:SD	2.26	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:99:THR:HG22	1:C:99:THR:O	1.83	0.76
1:A:111:VAL:HG11	1:A:142:THR:HG21	1.66	0.76
1:B:2042:LEU:HB3	1:B:172:GLN:HB3	1.67	0.76
1:C:248:GLN:HG3	1:C:267:LEU:HB3	1.65	0.76
2:D:222:LEU:O	2:D:223:MET:HB2	1.83	0.76
1:B:257:VAL:O	1:B:360:HIS:HE1	1.69	0.75
1:A:276:ILE:HD13	1:A:281:LEU:HD12	1.69	0.75
1:C:271:ALA:HB1	1:C:276:ILE:HD12	1.68	0.75
1:B:2013:GLN:HE22	1:B:83:GLU:HG2	1.49	0.75
1:B:259:ALA:CB	1:B:363:MET:HG2	2.17	0.74
3:E:5:PRO:O	3:E:8:ARG:HG2	1.87	0.74
1:A:94:ASP:O	1:A:100:LYS:CE	2.35	0.74
2:D:310:LEU:HD13	2:D:314:GLN:NE2	2.01	0.74
1:B:357:LEU:CA	1:B:363:MET:SD	2.75	0.74
2:D:147:LEU:HB3	2:D:148:PRO:HD3	1.69	0.74
2:D:315:ASP:CG	2:D:315:ASP:CA	2.61	0.74
1:A:156:THR:HG22	1:A:158:ASP:H	1.54	0.73
2:D:273:PHE:HB3	2:D:279:TRP:CB	2.18	0.73
1:B:355:ARG:NH2	3:E:332:PRO:HD3	2.01	0.73
1:A:93:ILE:HG22	1:A:100:LYS:NZ	2.03	0.73
1:A:100:LYS:CE	1:B:133:ARG:HH21	2.00	0.73
1:B:360:HIS:CG	1:B:363:MET:HG3	2.23	0.73
1:B:358:ALA:HA	1:B:364:PRO:HG2	1.71	0.72
2:D:82:LEU:HD21	2:D:100:LEU:HD12	1.70	0.72
1:B:271:ALA:HB1	1:B:276:ILE:CD1	2.19	0.72
3:E:49:LEU:HD23	3:E:68:MET:SD	2.29	0.72
3:E:117:ALA:O	3:E:120:LEU:HD22	1.89	0.72
1:B:259:ALA:HB1	1:B:363:MET:HG2	1.72	0.72
1:B:73:CYS:O	1:B:79:CYS:SG	2.48	0.71
1:C:94:ASP:H	1:C:100:LYS:HZ1	1.35	0.71
2:D:223:MET:SD	2:D:292:ARG:CB	2.78	0.71
2:D:300:GLN:OE1	2:D:335:PRO:HG3	1.91	0.70
1:A:326:GLN:NE2	1:C:351:MET:SD	2.65	0.70
1:A:360:HIS:HB3	1:A:363:MET:O	1.91	0.70
2:D:313:LYS:O	2:D:316:TYR:CZ	2.44	0.70
1:A:276:ILE:HG22	1:A:277:GLU:H	1.56	0.70
2:D:222:LEU:HD11	2:D:285:MET:HE3	1.74	0.70
2:D:222:LEU:HD12	2:D:285:MET:HG2	1.74	0.69
1:A:94:ASP:O	1:A:100:LYS:NZ	2.25	0.69
1:A:86:ARG:NH2	1:B:138:ALA:HA	2.08	0.69
2:D:213:THR:H	2:D:216:HIS:CD2	2.04	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:338:GLU:O	1:B:341:TYR:HB2	1.93	0.69
1:A:306:MET:HE1	1:A:313:MET:HE2	1.75	0.68
3:E:169:GLU:O	3:E:173:VAL:HG23	1.92	0.68
1:A:73:CYS:O	1:A:79:CYS:SG	2.50	0.68
2:D:55:ILE:O	2:D:85:PRO:HG3	1.93	0.68
2:D:202:VAL:O	2:D:206:VAL:HG23	1.92	0.68
1:C:93:ILE:CG2	1:C:100:LYS:NZ	2.57	0.68
1:C:93:ILE:HG23	1:C:100:LYS:NZ	2.09	0.68
1:A:93:ILE:CG2	1:A:100:LYS:HZ3	2.06	0.68
1:C:73:CYS:O	1:C:79:CYS:SG	2.51	0.68
3:E:111:VAL:HG12	3:E:140:TRP:HB2	1.75	0.68
1:A:367:GLU:HG3	1:B:322:PRO:HD2	1.74	0.68
2:D:116:LYS:HB3	2:D:140:GLN:HE21	1.59	0.68
1:A:67:GLY:HA2	1:A:119:ARG:NH1	2.07	0.68
1:A:94:ASP:C	1:A:100:LYS:HZ1	2.01	0.68
1:B:93:ILE:HG22	1:B:100:LYS:HZ3	1.58	0.68
1:C:18:VAL:CG2	1:C:25:LEU:HD11	2.24	0.68
2:D:308:THR:HG23	2:D:320:VAL:HG13	1.75	0.67
1:A:11:ARG:HH22	1:B:165:THR:HG22	1.59	0.67
1:B:254:GLU:OE2	1:B:312:ARG:HD3	1.94	0.67
1:B:259:ALA:CB	1:B:363:MET:CG	2.72	0.67
1:B:260:ASN:O	1:B:262:GLU:N	2.27	0.67
1:A:351:MET:HE2	1:B:326:GLN:NE2	2.08	0.67
1:C:73:CYS:O	1:C:73:CYS:SG	2.53	0.67
1:B:223:GLN:HE21	3:E:158:ARG:HE	1.43	0.67
1:B:358:ALA:HA	1:B:364:PRO:CG	2.25	0.67
3:E:31:ALA:HB2	3:E:164:LEU:HB3	1.76	0.67
1:C:165:THR:HG23	2:D:32:GLN:HE22	1.59	0.67
1:B:309:ILE:HG22	1:B:313:MET:HG2	1.74	0.66
1:C:110:ASN:HB3	1:C:113:TYR:HD1	1.58	0.66
1:A:256:MET:HE2	1:A:353:LEU:HD21	1.77	0.66
1:B:271:ALA:HB1	1:B:276:ILE:HD12	1.75	0.66
1:C:93:ILE:HG23	1:C:100:LYS:HZ2	1.58	0.66
3:E:64:GLY:O	3:E:68:MET:HB2	1.96	0.66
3:E:74:PRO:HB3	3:E:105:ARG:HD2	1.76	0.66
1:A:181:GLU:HG2	1:A:184:ARG:HD2	1.77	0.66
1:B:93:ILE:HG22	1:B:100:LYS:NZ	2.10	0.65
1:B:347:MET:O	1:B:351:MET:HG2	1.96	0.65
2:D:274:ASP:HA	2:D:279:TRP:CE3	2.32	0.65
2:D:281:ASN:C	2:D:283:ARG:H	2.02	0.65
1:B:2013:GLN:NE2	1:B:83:GLU:HG2	2.12	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:8:ARG:CG	3:E:9:PRO:HD3	2.25	0.64
3:E:73:HIS:HD2	3:E:75:ASP:H	1.45	0.64
1:A:111:VAL:HG11	1:A:142:THR:CG2	2.28	0.64
2:D:48:GLU:HG3	2:D:49:GLU:N	2.13	0.64
1:A:256:MET:HE1	1:A:332:LEU:HD11	1.80	0.64
1:B:356:ALA:O	1:B:363:MET:CE	2.45	0.64
1:A:261:GLY:HA3	1:B:297:LEU:HD21	1.80	0.64
1:B:309:ILE:HG21	1:B:313:MET:HG2	1.77	0.64
2:D:273:PHE:HB3	2:D:279:TRP:CG	2.33	0.64
3:E:149:GLU:C	3:E:151:LEU:H	2.05	0.64
1:C:268:ILE:HD11	1:C:353:LEU:CD1	2.28	0.64
1:A:344:ASP:HB3	1:A:347:MET:HE3	1.78	0.64
1:B:360:HIS:CG	1:B:363:MET:CG	2.80	0.64
1:C:254:GLU:O	1:C:258:GLU:HG3	1.98	0.64
1:A:73:CYS:O	1:A:73:CYS:SG	2.56	0.63
1:A:107:LEU:HD11	1:B:133:ARG:NH1	2.14	0.63
2:D:222:LEU:CD1	2:D:285:MET:HG2	2.29	0.63
3:E:329:LEU:H	3:E:329:LEU:HD23	1.63	0.63
1:B:6:LEU:O	1:B:218:LEU:HB3	1.98	0.63
1:C:281:LEU:HG	1:C:285:MET:HE2	1.81	0.63
2:D:315:ASP:HB2	2:D:318:GLN:HG2	1.80	0.62
3:E:147:GLU:O	3:E:147:GLU:HG2	1.98	0.62
1:A:256:MET:HE2	1:A:353:LEU:CD2	2.29	0.62
1:B:100:LYS:HB2	1:B:103:ASP:OD1	1.99	0.62
2:D:281:ASN:C	2:D:283:ARG:N	2.57	0.62
1:A:343:PRO:HG2	1:A:347:MET:SD	2.38	0.62
1:A:93:ILE:HG23	1:A:100:LYS:NZ	2.14	0.62
2:D:24:LEU:HA	2:D:114:GLY:O	2.00	0.62
2:D:256:LEU:O	2:D:260:LEU:HG	2.00	0.62
3:E:161:LEU:HD12	3:E:161:LEU:H	1.64	0.62
1:C:328:TYR:O	1:C:332:LEU:HD23	1.99	0.62
1:C:263:ARG:O	1:C:267:LEU:HG	2.00	0.62
1:C:271:ALA:HB1	1:C:276:ILE:CD1	2.30	0.62
1:A:239:ALA:CB	1:B:2023:HIS:CE1	2.78	0.62
1:B:337:LYS:HG3	1:B:338:GLU:N	2.12	0.62
1:B:102:GLU:HB3	1:B:106:ASP:HB2	1.80	0.61
1:C:246:ASP:HB3	1:C:274:ARG:CD	2.24	0.61
3:E:129:LEU:HD11	3:E:158:ARG:HH11	1.64	0.61
1:A:250:LEU:HD22	1:A:309:ILE:HD12	1.82	0.61
1:A:86:ARG:HH21	1:B:138:ALA:HA	1.63	0.61
1:A:100:LYS:CD	1:B:133:ARG:NH2	2.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:246:ASP:CB	1:C:274:ARG:HD3	2.24	0.61
1:B:316:LEU:HD22	1:B:320:ILE:HD11	1.81	0.61
3:E:73:HIS:CD2	3:E:75:ASP:H	2.18	0.61
1:A:100:LYS:HD3	1:B:133:ARG:HH21	1.44	0.61
1:C:304:ASN:HD22	2:D:234:GLN:CD	2.03	0.61
1:B:338:GLU:OE2	3:E:295:HIS:NE2	2.34	0.60
1:B:363:MET:CG	1:B:364:PRO:HD2	2.31	0.60
1:C:94:ASP:O	1:C:100:LYS:HE3	1.99	0.60
1:C:268:ILE:HD11	1:C:353:LEU:HD12	1.83	0.60
1:A:97:SER:HG	1:A:100:LYS:HE3	1.65	0.60
1:A:30:ASN:HD22	1:C:226:ALA:HA	1.66	0.60
1:B:70:ALA:O	1:B:72:PRO:HD3	2.01	0.60
1:C:51:LYS:HB2	5:C:5500:SO4:O3	2.02	0.60
1:C:302:LEU:HD13	1:C:310:GLU:HG2	1.84	0.60
1:A:362:ARG:O	1:A:363:MET:HG3	2.02	0.60
1:C:284:GLU:O	1:C:288:LEU:HG	2.02	0.60
3:E:303:VAL:HB	3:E:306:ILE:HD11	1.83	0.60
1:B:140:LEU:HD21	1:B:166:ILE:HG12	1.83	0.60
1:A:3:TYR:O	1:A:4:GLN:HG3	2.01	0.59
1:A:88:VAL:HG11	1:A:116:ALA:HB3	1.83	0.59
2:D:269:LEU:HG	2:D:273:PHE:CE1	2.37	0.59
1:A:152:PHE:O	1:A:153:LEU:HD23	2.02	0.59
1:A:316:LEU:HD22	1:A:320:ILE:HD11	1.84	0.59
1:A:292:ILE:O	1:A:296:GLN:HG3	2.02	0.59
3:E:117:ALA:HB2	3:E:143:LEU:HD12	1.83	0.59
1:A:21:GLN:OE1	1:A:175:LEU:HD22	2.02	0.59
1:C:343:PRO:HG2	1:C:347:MET:SD	2.42	0.59
1:B:265:MET:HE1	1:B:350:GLU:HB3	1.85	0.59
1:B:246:ASP:HB2	1:B:248:GLN:HG2	1.85	0.59
1:A:93:ILE:HG22	1:A:100:LYS:HZ3	1.65	0.59
1:C:47:ARG:O	1:C:47:ARG:HG3	2.03	0.59
1:B:363:MET:CB	1:B:364:PRO:CD	2.78	0.58
1:C:205:LEU:CD1	1:C:234:THR:HG23	2.33	0.58
2:D:263:GLN:HG2	2:D:266:HIS:HD2	1.68	0.58
1:A:30:ASN:ND2	1:C:226:ALA:HA	2.18	0.58
1:A:341:TYR:HB2	1:B:333:LEU:HD11	1.84	0.58
1:C:93:ILE:CG2	1:C:100:LYS:HZ2	2.17	0.58
3:E:41:ILE:HG21	3:E:113:TRP:CD1	2.38	0.58
3:E:46:ARG:CZ	3:E:68:MET:HG3	2.33	0.58
1:A:257:VAL:HG11	1:A:320:ILE:CD1	2.34	0.58
1:B:367:GLU:HB3	1:B:368:PRO:HD2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:GLY:HA2	1:C:72:PRO:HG3	1.85	0.58
2:D:222:LEU:HD12	2:D:285:MET:SD	2.44	0.58
1:B:2058:LEU:HD23	1:B:153:LEU:HD22	1.86	0.58
1:C:259:ALA:HB3	1:C:363:MET:CE	2.33	0.58
3:E:8:ARG:HG3	3:E:9:PRO:CD	2.33	0.58
1:A:93:ILE:CG2	1:A:100:LYS:HZ2	2.17	0.57
1:B:94:ASP:O	1:B:100:LYS:HE2	2.03	0.57
1:B:360:HIS:CB	1:B:363:MET:SD	2.92	0.57
1:C:282:LEU:CD2	1:C:332:LEU:HD12	2.34	0.57
2:D:10:ARG:HH12	2:D:40:GLN:NE2	2.00	0.57
1:B:128:VAL:HG11	1:B:154:LEU:HD22	1.87	0.57
1:B:229:ASP:O	1:B:231:GLN:N	2.34	0.57
2:D:279:TRP:CG	2:D:279:TRP:O	2.57	0.57
1:A:291:ARG:HH11	1:A:306:MET:HG3	1.69	0.57
2:D:222:LEU:HD12	2:D:285:MET:CG	2.33	0.57
1:A:49:VAL:O	5:A:1500:SO4:S	2.63	0.57
1:C:304:ASN:OD1	1:C:305:ASP:N	2.37	0.57
1:C:306:MET:HE1	1:C:313:MET:HE2	1.86	0.57
1:A:94:ASP:C	1:A:100:LYS:NZ	2.62	0.57
2:D:10:ARG:HH22	2:D:40:GLN:HE22	1.51	0.57
1:B:186:GLN:HG2	1:B:214:LEU:HD21	1.86	0.57
2:D:221:LEU:HD13	2:D:331:LEU:HD12	1.86	0.57
3:E:308:ARG:O	3:E:312:ILE:HG13	2.04	0.57
1:B:357:LEU:C	1:B:363:MET:SD	2.88	0.56
2:D:273:PHE:CE1	2:D:283:ARG:HG3	2.39	0.56
1:B:296:GLN:NE2	1:B:325:ILE:HD12	2.20	0.56
1:C:205:LEU:HD11	1:C:234:THR:HG23	1.87	0.56
1:C:328:TYR:OH	1:C:361:PRO:HD2	2.05	0.56
2:D:170:LEU:O	2:D:173:CYS:O	2.24	0.56
1:B:194:GLU:HA	1:B:194:GLU:OE1	2.05	0.56
1:C:259:ALA:HB3	1:C:363:MET:HE3	1.87	0.56
1:B:95:ALA:HA	1:B:100:LYS:HZ1	1.71	0.56
1:C:362:ARG:HH21	1:C:363:MET:CE	2.19	0.56
3:E:280:HIS:O	3:E:281:LEU:HD23	2.05	0.56
1:C:69:THR:HG22	1:C:71:THR:N	2.01	0.56
1:B:259:ALA:HB2	1:B:363:MET:SD	2.46	0.56
1:C:295:VAL:HG22	1:C:301:ALA:HB3	1.88	0.56
1:A:99:THR:O	1:A:99:THR:CG2	2.51	0.56
1:C:309:ILE:HG22	1:C:313:MET:HG2	1.88	0.56
1:A:40:ALA:HB1	1:A:170:CYS:SG	2.46	0.55
1:A:156:THR:HG22	1:A:158:ASP:N	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:5011:ARG:HD3	1:C:83:GLU:OE2	2.07	0.55
2:D:39:ARG:NH2	2:D:50:HIS:HB3	2.21	0.55
2:D:218:VAL:HA	2:D:221:LEU:HB2	1.88	0.55
2:D:296:THR:HG22	2:D:299:ARG:NH1	2.21	0.55
1:B:360:HIS:HD2	1:B:361:PRO:O	1.90	0.55
2:D:308:THR:CG2	2:D:320:VAL:HG13	2.37	0.55
1:B:338:GLU:OE2	3:E:295:HIS:CE1	2.60	0.55
2:D:310:LEU:HD11	3:E:299:GLN:NE2	2.21	0.55
1:A:351:MET:HE1	1:B:326:GLN:HE22	1.69	0.55
1:B:355:ARG:NH1	3:E:287:GLN:HB3	2.22	0.55
2:D:313:LYS:O	2:D:316:TYR:CE2	2.60	0.55
1:B:259:ALA:HB2	1:B:363:MET:HG3	1.89	0.55
1:A:91:ILE:HD12	1:A:123:TYR:CE2	2.42	0.54
1:C:104:THR:O	1:C:108:LEU:HG	2.08	0.54
1:C:297:LEU:HD23	2:D:334:LYS:O	2.06	0.54
2:D:282:ARG:O	2:D:285:MET:HB3	2.07	0.54
1:C:3:TYR:O	1:C:3:TYR:CD2	2.60	0.54
1:A:97:SER:OG	1:A:100:LYS:CE	2.54	0.54
1:A:281:LEU:HD23	1:A:285:MET:CE	2.36	0.54
3:E:213:ARG:NH2	3:E:267:ASN:OD1	2.39	0.54
1:C:307:ALA:HA	1:C:310:GLU:HG3	1.89	0.54
1:A:346:ARG:O	1:A:350:GLU:HG3	2.07	0.54
1:B:360:HIS:CG	1:B:363:MET:CE	2.90	0.54
2:D:264:SER:O	2:D:265:ALA:HB3	2.07	0.54
3:E:4:TYR:HB3	3:E:5:PRO:HD2	1.89	0.54
3:E:201:ALA:O	3:E:204:LEU:HB2	2.06	0.54
1:C:49:VAL:O	5:C:5500:SO4:S	2.66	0.54
1:C:248:GLN:O	1:C:252:LEU:N	2.39	0.54
2:D:1:MET:HA	2:D:134:SER:O	2.08	0.54
1:C:205:LEU:CD2	1:C:243:THR:HG23	2.38	0.54
2:D:48:GLU:HG3	2:D:49:GLU:H	1.73	0.54
1:B:244:LEU:HD11	1:B:276:ILE:HD13	1.90	0.54
1:A:265:MET:HG3	1:B:294:MET:HE1	1.89	0.53
2:D:271:ALA:O	2:D:275:LYS:HG2	2.07	0.53
1:C:259:ALA:CB	1:C:363:MET:HE3	2.39	0.53
1:C:276:ILE:HG22	1:C:277:GLU:N	2.24	0.53
2:D:262:ARG:NH2	3:E:320:GLU:OE1	2.42	0.53
1:A:351:MET:HA	1:A:351:MET:CE	2.30	0.53
1:C:94:ASP:N	1:C:100:LYS:HZ1	1.93	0.53
1:B:296:GLN:HE22	1:B:325:ILE:HD12	1.73	0.53
1:B:302:LEU:HD22	1:B:306:MET:HG2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:171:LEU:HA	2:D:183:GLN:HE22	1.73	0.53
2:D:119:LYS:H	2:D:119:LYS:CD	2.05	0.53
2:D:255:LEU:HD22	3:E:313:THR:HG21	1.91	0.53
3:E:306:ILE:HG22	3:E:307:ASN:H	1.73	0.53
1:A:86:ARG:HE	1:B:137:ASN:HB2	1.73	0.53
1:A:261:GLY:CA	1:B:297:LEU:HD21	2.39	0.53
1:A:307:ALA:HA	1:A:310:GLU:HB2	1.90	0.53
1:B:244:LEU:HD21	1:B:276:ILE:CG1	2.37	0.53
2:D:93:ILE:HG23	2:D:97:LEU:HD13	1.91	0.53
1:A:107:LEU:HD11	1:B:133:ARG:HH12	1.71	0.53
1:A:276:ILE:HG22	1:A:277:GLU:N	2.24	0.53
1:A:354:LEU:CD2	1:B:297:LEU:HD22	2.39	0.53
1:B:366:PRO:HB3	3:E:282:SER:HB2	1.91	0.53
1:C:366:PRO:C	1:C:367:GLU:HG3	2.32	0.53
2:D:218:VAL:HG11	2:D:253:GLU:HG3	1.91	0.53
2:D:311:THR:HG23	2:D:318:GLN:CD	2.34	0.53
1:B:84:GLN:HB3	1:B:86:ARG:NH2	2.24	0.53
1:B:259:ALA:CB	1:B:363:MET:SD	2.97	0.53
2:D:25:GLY:O	2:D:115:ASN:HA	2.08	0.53
1:A:191:LEU:HD12	1:A:203:LEU:HD21	1.91	0.52
1:B:360:HIS:HB2	1:B:363:MET:CE	2.39	0.52
1:B:271:ALA:HB1	1:B:276:ILE:HD11	1.90	0.52
2:D:309:GLU:O	2:D:313:LYS:HG3	2.09	0.52
1:A:100:LYS:HB3	1:B:133:ARG:CZ	2.39	0.52
1:B:291:ARG:HD2	1:B:306:MET:SD	2.49	0.52
2:D:273:PHE:HB3	2:D:279:TRP:HB2	1.90	0.52
3:E:268:VAL:O	3:E:271:PRO:HD3	2.09	0.52
1:B:277:GLU:HB3	3:E:149:GLU:HG2	1.90	0.52
1:B:360:HIS:O	1:B:363:MET:HB2	2.09	0.52
3:E:238:HIS:ND1	3:E:239:GLU:N	2.56	0.52
1:A:360:HIS:HD2	1:A:363:MET:H	1.57	0.52
1:A:278:TRP:HB3	1:A:349:VAL:HG21	1.91	0.52
3:E:68:MET:HE3	3:E:68:MET:HA	1.92	0.52
1:A:281:LEU:CD2	1:A:285:MET:HE2	2.36	0.52
1:B:360:HIS:CG	1:B:363:MET:SD	3.02	0.52
3:E:27:LEU:O	3:E:143:LEU:N	2.39	0.52
1:B:257:VAL:HG11	1:B:320:ILE:CD1	2.40	0.52
1:B:352:THR:O	1:B:355:ARG:HB3	2.10	0.52
2:D:310:LEU:O	2:D:314:GLN:HG3	2.11	0.52
1:B:250:LEU:HD23	1:B:312:ARG:HH11	1.75	0.51
1:A:252:LEU:HD13	1:A:281:LEU:HD21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:93:ILE:HG22	1:C:100:LYS:NZ	2.25	0.51
2:D:10:ARG:HH22	2:D:40:GLN:NE2	2.08	0.51
1:A:213:SER:OG	1:A:216:ASP:HB2	2.11	0.51
1:A:334:ILE:O	1:A:338:GLU:HG3	2.09	0.51
1:C:343:PRO:CG	1:C:347:MET:SD	2.99	0.51
1:A:51:LYS:HE2	5:A:1500:SO4:O4	2.11	0.51
1:A:181:GLU:HA	1:A:184:ARG:HB3	1.93	0.51
3:E:311:LEU:O	3:E:314:ASP:HB3	2.11	0.51
1:C:243:THR:HG22	1:C:244:LEU:N	2.26	0.51
1:C:303:GLY:HA3	1:C:306:MET:HG2	1.93	0.51
3:E:100:LEU:HD13	3:E:139:THR:HG21	1.93	0.51
2:D:261:LYS:HE3	2:D:295:GLN:HE21	1.76	0.51
2:D:300:GLN:OE1	2:D:335:PRO:HG2	2.09	0.51
3:E:139:THR:HG22	3:E:140:TRP:N	2.26	0.51
1:C:201:ARG:O	1:C:205:LEU:HG	2.11	0.50
2:D:315:ASP:HB2	2:D:318:GLN:CD	2.36	0.50
1:A:341:TYR:HB2	1:B:333:LEU:CD1	2.41	0.50
1:B:2049:VAL:O	5:B:2500:SO4:S	2.69	0.50
1:B:357:LEU:HA	1:B:363:MET:HE1	1.91	0.50
2:D:294:SER:H	2:D:297:GLN:NE2	2.08	0.50
1:B:338:GLU:CD	3:E:295:HIS:HE2	2.18	0.50
3:E:151:LEU:HD21	3:E:155:LEU:HD12	1.93	0.50
1:B:2060:LYS:HE3	1:B:79:CYS:HB3	1.93	0.50
1:A:3:TYR:HB2	1:B:2039:HIS:CE1	2.46	0.50
1:C:302:LEU:HG	1:C:314:ARG:NH1	2.26	0.50
1:B:360:HIS:CB	1:B:363:MET:CB	2.68	0.50
1:C:49:VAL:HG12	1:C:50:GLY:N	2.27	0.50
3:E:46:ARG:NH1	3:E:68:MET:HG3	2.27	0.50
1:A:89:ASP:HB3	1:A:121:LYS:HA	1.92	0.50
1:A:102:GLU:HB3	1:A:106:ASP:CB	2.41	0.50
2:D:96:GLN:O	2:D:100:LEU:HG	2.12	0.50
1:A:100:LYS:HG2	1:B:133:ARG:HE	1.77	0.50
1:A:360:HIS:CD2	1:A:362:ARG:H	2.30	0.50
1:B:288:LEU:O	1:B:292:ILE:HG13	2.12	0.50
2:D:312:LEU:HB2	2:D:320:VAL:CG2	2.35	0.50
1:A:107:LEU:CD1	1:B:133:ARG:HH12	2.25	0.49
1:A:297:LEU:HD21	1:C:261:GLY:HA3	1.93	0.49
3:E:312:ILE:O	3:E:316:LEU:HG	2.12	0.49
1:A:44:SER:HB2	1:A:159:PRO:HG3	1.94	0.49
1:A:244:LEU:HB3	1:A:248:GLN:HB2	1.95	0.49
1:A:329:TYR:CG	1:C:351:MET:HE3	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2052:THR:O	1:B:2055:ALA:HB3	2.13	0.49
1:C:51:LYS:HE3	5:C:5500:SO4:O3	2.12	0.49
2:D:199:LEU:HB3	2:D:200:PRO:HD3	1.94	0.49
2:D:274:ASP:HA	2:D:279:TRP:CZ3	2.47	0.49
1:B:276:ILE:HG22	1:B:277:GLU:N	2.28	0.49
1:A:92:GLU:HG2	1:A:124:LEU:HD23	1.94	0.49
2:D:22:LEU:HD22	2:D:112:VAL:HB	1.94	0.49
1:A:100:LYS:HE2	1:B:133:ARG:HH21	1.75	0.49
1:B:236:ALA:O	1:B:239:ALA:HB3	2.12	0.49
1:C:99:THR:O	1:C:99:THR:CG2	2.53	0.49
2:D:27:ASP:HB3	2:D:30:LEU:HB2	1.93	0.49
2:D:183:GLN:HE21	2:D:183:GLN:HA	1.78	0.49
3:E:41:ILE:HG21	3:E:113:TRP:CG	2.47	0.49
3:E:57:LYS:HG3	3:E:58:SER:H	1.78	0.49
1:C:69:THR:HG22	1:C:70:ALA:N	2.28	0.49
2:D:20:ALA:O	2:D:134:SER:HB2	2.12	0.49
2:D:296:THR:HG22	2:D:299:ARG:HH12	1.77	0.49
3:E:145:THR:HG22	3:E:147:GLU:N	2.27	0.49
1:A:238:SER:HB2	1:A:243:THR:O	2.13	0.49
1:A:354:LEU:HD11	1:B:294:MET:SD	2.53	0.49
1:C:82:ILE:HG23	1:C:90:LEU:CD2	2.42	0.48
1:A:294:MET:HE1	1:C:265:MET:HE2	1.93	0.48
1:B:140:LEU:HD22	1:B:169:ARG:CZ	2.43	0.48
1:B:338:GLU:HA	1:B:341:TYR:CD1	2.48	0.48
1:C:270:GLU:HG2	1:C:274:ARG:NH1	2.28	0.48
1:B:302:LEU:HD11	1:B:313:MET:CB	2.43	0.48
1:C:244:LEU:HA	1:C:244:LEU:HD23	1.51	0.48
1:B:5:VAL:HG13	1:B:222:ASP:CG	2.38	0.48
1:C:140:LEU:O	1:C:144:GLU:HG3	2.14	0.48
2:D:310:LEU:HD21	3:E:306:ILE:HD13	1.96	0.48
3:E:85:LYS:NZ	3:E:85:LYS:HB3	2.28	0.48
1:B:229:ASP:C	1:B:231:GLN:N	2.71	0.48
1:C:22:GLU:H	1:C:22:GLU:HG3	1.09	0.48
1:A:66:THR:HG22	1:A:66:THR:O	2.14	0.48
1:B:302:LEU:HD11	1:B:313:MET:HB2	1.94	0.48
3:E:306:ILE:HG22	3:E:307:ASN:N	2.29	0.48
1:A:101:VAL:HG12	1:A:102:GLU:HG3	1.96	0.48
1:C:307:ALA:HA	1:C:310:GLU:CD	2.38	0.48
2:D:10:ARG:NH2	2:D:40:GLN:HE22	2.11	0.48
1:B:260:ASN:O	1:B:260:ASN:OD1	2.32	0.48
1:C:326:GLN:CD	2:D:338:ASP:OD2	2.56	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:57:LYS:HD2	3:E:57:LYS:HA	1.67	0.48
1:B:358:ALA:C	1:B:360:HIS:H	2.22	0.47
1:C:205:LEU:HD22	1:C:243:THR:HG23	1.95	0.47
3:E:145:THR:HG22	3:E:147:GLU:H	1.78	0.47
1:C:32:LEU:HD11	1:C:58:LEU:HD12	1.95	0.47
1:B:2013:GLN:HE22	1:B:83:GLU:CG	2.22	0.47
1:C:256:MET:CE	1:C:332:LEU:HD21	2.44	0.47
2:D:281:ASN:O	2:D:283:ARG:N	2.47	0.47
3:E:241:ALA:N	3:E:242:PRO:HD2	2.29	0.47
1:A:216:ASP:O	1:A:220:LEU:HG	2.15	0.47
1:A:291:ARG:NH1	1:A:306:MET:HG3	2.29	0.47
2:D:48:GLU:CG	2:D:49:GLU:N	2.76	0.47
2:D:98:LEU:O	2:D:101:THR:HG22	2.14	0.47
1:B:257:VAL:HG11	1:B:320:ILE:HD13	1.95	0.47
1:C:292:ILE:O	1:C:296:GLN:HG3	2.14	0.47
1:C:333:LEU:CD1	1:C:337:LYS:HE3	2.45	0.47
2:D:310:LEU:HD13	2:D:314:GLN:HE22	1.77	0.47
1:B:2024:VAL:HG11	1:B:175:LEU:HD21	1.96	0.47
1:A:271:ALA:HB1	1:A:276:ILE:CD1	2.36	0.47
1:A:316:LEU:HB3	1:A:320:ILE:HD12	1.96	0.47
1:C:286:LEU:HD11	1:C:333:LEU:HA	1.96	0.47
1:A:126:ASP:HA	1:A:155:ALA:HB3	1.96	0.47
1:A:362:ARG:C	1:A:363:MET:HG3	2.40	0.47
1:B:2044:SER:OG	1:B:174:HIS:HA	2.15	0.47
1:B:244:LEU:HD11	1:B:276:ILE:CG2	2.45	0.47
3:E:227:GLY:O	3:E:229:TRP:HD1	1.98	0.47
1:B:256:MET:HA	1:B:357:LEU:HD11	1.97	0.47
1:C:50:GLY:O	1:C:54:ILE:HG13	2.15	0.47
2:D:60:ASP:O	2:D:64:ILE:HD12	2.15	0.47
2:D:263:GLN:HB2	2:D:272:LEU:HD21	1.97	0.47
1:A:147:PRO:HG2	1:A:150:VAL:HB	1.96	0.46
1:A:200:PRO:HG2	1:A:305:ASP:CG	2.40	0.46
3:E:241:ALA:O	3:E:245:LEU:HD22	2.14	0.46
1:A:294:MET:SD	1:C:265:MET:HE2	2.55	0.46
1:A:149:HIS:CD2	1:A:149:HIS:H	2.34	0.46
1:B:246:ASP:HB2	1:B:248:GLN:CG	2.45	0.46
1:B:343:PRO:HG3	1:B:347:MET:SD	2.56	0.46
1:A:93:ILE:HG23	1:A:100:LYS:HZ3	1.76	0.46
1:B:165:THR:O	1:B:169:ARG:HG3	2.15	0.46
2:D:284:GLY:O	2:D:288:GLU:HB2	2.16	0.46
2:D:311:THR:HG23	2:D:318:GLN:OE1	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:ASP:O	1:A:250:LEU:HB2	2.16	0.46
1:B:2042:LEU:HB3	1:B:172:GLN:CB	2.42	0.46
1:B:316:LEU:HD22	1:B:320:ILE:CD1	2.45	0.46
1:B:338:GLU:HA	1:B:341:TYR:HD1	1.81	0.46
2:D:315:ASP:CB	2:D:318:GLN:HG2	2.45	0.46
1:A:257:VAL:HG11	1:A:320:ILE:HD13	1.97	0.46
1:B:2051:LYS:HB2	1:B:2051:LYS:HE3	1.76	0.46
2:D:213:THR:N	2:D:216:HIS:HD2	1.96	0.46
2:D:251:GLN:OE1	3:E:307:ASN:ND2	2.49	0.46
2:D:263:GLN:OE1	2:D:272:LEU:HD11	2.15	0.46
3:E:95:GLU:O	3:E:99:LYS:HB2	2.16	0.46
1:B:2042:LEU:HD12	1:B:172:GLN:OE1	2.16	0.46
1:A:257:VAL:O	1:A:360:HIS:HE1	1.99	0.46
1:C:94:ASP:O	1:C:100:LYS:CE	2.63	0.46
1:C:94:ASP:CA	1:C:100:LYS:HZ1	2.29	0.46
2:D:222:LEU:CD1	2:D:285:MET:SD	3.04	0.46
3:E:257:LYS:HB3	3:E:262:ALA:HB3	1.98	0.46
1:A:21:GLN:HE22	1:A:49:VAL:HG13	1.81	0.46
1:B:302:LEU:HD23	1:B:302:LEU:HA	1.54	0.46
1:C:56:ARG:NH1	1:C:82:ILE:O	2.49	0.46
1:C:186:GLN:HG2	1:C:214:LEU:HD21	1.98	0.46
2:D:174:TYR:CE2	2:D:211:HIS:CE1	3.04	0.46
1:A:51:LYS:HB2	1:A:51:LYS:HE3	1.77	0.45
1:A:260:ASN:OD1	1:A:260:ASN:O	2.35	0.45
1:B:291:ARG:O	1:B:295:VAL:HG23	2.16	0.45
2:D:222:LEU:CD1	2:D:285:MET:HE3	2.42	0.45
3:E:27:LEU:CD2	3:E:29:ILE:HD11	2.46	0.45
3:E:282:SER:OG	3:E:285:ARG:HB2	2.16	0.45
1:A:252:LEU:CD1	1:A:281:LEU:HD21	2.47	0.45
1:A:333:LEU:CD2	1:C:338:GLU:HB3	2.46	0.45
1:B:197:ALA:HB3	1:B:231:GLN:HG2	1.98	0.45
1:C:219:SER:O	1:C:223:GLN:HG3	2.17	0.45
1:C:344:ASP:O	1:C:347:MET:HB3	2.16	0.45
2:D:19:ALA:CB	2:D:133:ARG:HD3	2.45	0.45
2:D:247:LEU:HD11	2:D:308:THR:HG22	1.98	0.45
2:D:279:TRP:O	2:D:279:TRP:CD2	2.69	0.45
1:B:2051:LYS:HB2	5:B:2500:SO4:O3	2.17	0.45
1:A:215:ARG:NH2	5:A:1500:SO4:O2	2.50	0.45
2:D:312:LEU:O	2:D:312:LEU:HG	2.15	0.45
3:E:14:LEU:HD13	3:E:44:LEU:HD11	1.98	0.45
1:C:362:ARG:NE	1:C:363:MET:HE2	2.19	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:48:GLU:CG	2:D:49:GLU:H	2.30	0.45
2:D:213:THR:C	2:D:215:PHE:N	2.75	0.45
3:E:51:GLN:HB2	3:E:62:CYS:HB2	1.98	0.45
1:A:73:CYS:SG	1:A:76:CYS:HB3	2.56	0.45
1:C:270:GLU:HG2	1:C:274:ARG:CZ	2.46	0.45
2:D:315:ASP:HB2	2:D:318:GLN:NE2	2.31	0.45
1:B:361:PRO:O	1:B:362:ARG:HB2	2.15	0.45
2:D:198:THR:HB	2:D:200:PRO:HD2	1.98	0.45
3:E:27:LEU:HG	3:E:29:ILE:CD1	2.47	0.45
3:E:253:MET:O	3:E:256:LEU:N	2.49	0.45
3:E:299:GLN:HE21	3:E:311:LEU:HD21	1.82	0.45
1:B:258:GLU:O	1:B:259:ALA:HB3	2.17	0.45
2:D:27:ASP:OD2	2:D:178:LEU:HD12	2.17	0.45
2:D:221:LEU:HD23	2:D:221:LEU:HA	1.47	0.45
2:D:225:LYS:HE3	2:D:227:LYS:HD2	1.99	0.45
2:D:298:LEU:O	2:D:302:VAL:HG23	2.16	0.45
1:B:2066:THR:O	1:B:2066:THR:HG22	2.17	0.45
1:A:21:GLN:NE2	1:A:176:LYS:O	2.49	0.44
1:A:86:ARG:HH21	1:B:138:ALA:CA	2.27	0.44
1:B:2062:LEU:O	1:B:119:ARG:HD2	2.18	0.44
1:B:140:LEU:HD11	1:B:165:THR:HB	1.99	0.44
1:B:142:THR:O	1:B:146:PRO:N	2.50	0.44
1:C:248:GLN:O	1:C:252:LEU:HB2	2.17	0.44
3:E:30:GLN:HA	3:E:145:THR:O	2.17	0.44
1:C:316:LEU:HD22	1:C:320:ILE:HD11	1.98	0.44
2:D:223:MET:HE3	2:D:223:MET:HB3	1.59	0.44
1:A:37:ILE:HD12	1:A:62:LEU:HD21	1.98	0.44
1:A:102:GLU:HB3	1:A:106:ASP:HB2	1.99	0.44
1:A:147:PRO:HB2	1:A:149:HIS:CD2	2.52	0.44
1:C:42:LEU:HD23	1:C:172:GLN:HG2	1.99	0.44
1:C:307:ALA:HA	1:C:310:GLU:CG	2.47	0.44
1:C:363:MET:HE3	1:C:363:MET:HB2	1.67	0.44
2:D:25:GLY:N	2:D:114:GLY:O	2.41	0.44
2:D:315:ASP:H	2:D:318:GLN:HE21	1.65	0.44
3:E:324:GLN:HA	3:E:325:PRO:HD3	1.86	0.44
1:B:343:PRO:HB2	3:E:246:HIS:ND1	2.33	0.44
2:D:57:PRO:HB3	2:D:90:ASN:ND2	2.33	0.44
1:A:215:ARG:CZ	5:A:1500:SO4:O1	2.65	0.44
1:B:2010:TRP:CE2	1:B:190:ILE:HG23	2.53	0.44
1:B:131:LEU:HB2	1:B:136:PHE:CD1	2.52	0.44
1:C:4:GLN:CD	1:C:9:LYS:HD2	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:250:LEU:HD13	1:C:288:LEU:HD13	2.00	0.44
1:C:250:LEU:HD22	1:C:309:ILE:CG2	2.48	0.44
1:A:42:LEU:HD12	1:A:154:LEU:HB2	2.00	0.44
1:A:245:ASP:HB2	1:A:248:GLN:HG3	1.99	0.44
1:C:248:GLN:HA	1:C:251:SER:OG	2.17	0.44
1:C:360:HIS:CD2	1:C:361:PRO:HD2	2.52	0.44
2:D:315:ASP:CB	2:D:318:GLN:CG	2.82	0.44
1:A:290:HIS:CE1	1:C:347:MET:HG3	2.53	0.44
1:B:135:SER:O	1:B:138:ALA:HB3	2.17	0.44
1:B:191:LEU:HD12	1:B:203:LEU:HD21	1.99	0.44
1:C:256:MET:HE2	1:C:332:LEU:HD21	1.99	0.44
1:A:167:LEU:HB3	1:A:172:GLN:NE2	2.33	0.43
1:B:94:ASP:O	1:B:100:LYS:CE	2.65	0.43
2:D:56:ASP:HB3	2:D:58:ASN:H	1.83	0.43
3:E:30:GLN:O	3:E:30:GLN:HG3	2.18	0.43
1:C:304:ASN:OD1	1:C:304:ASN:C	2.60	0.43
2:D:100:LEU:O	2:D:103:LEU:HB3	2.18	0.43
1:B:246:ASP:C	1:B:248:GLN:H	2.26	0.43
2:D:3:ARG:HG2	2:D:136:GLN:NE2	2.33	0.43
1:C:63:ASN:O	1:C:64:CYS:C	2.61	0.43
1:C:104:THR:HG22	1:C:108:LEU:HG	1.99	0.43
1:C:243:THR:CG2	1:C:244:LEU:N	2.81	0.43
1:C:340:PRO:HB3	1:C:345:ARG:HH21	1.83	0.43
2:D:325:GLU:O	2:D:329:LEU:HG	2.18	0.43
3:E:117:ALA:HB2	3:E:143:LEU:CD1	2.47	0.43
1:C:21:GLN:HE22	1:C:49:VAL:CG1	2.32	0.43
1:C:42:LEU:HD11	1:C:156:THR:HG22	2.01	0.43
1:C:244:LEU:HD23	1:C:247:ASP:OD2	2.17	0.43
2:D:50:HIS:O	2:D:51:HIS:CD2	2.72	0.43
3:E:7:LEU:HD22	3:E:40:LEU:HB2	2.00	0.43
1:B:265:MET:CE	3:E:257:LYS:HE2	2.49	0.43
1:A:10:TRP:CZ2	1:A:190:ILE:HG23	2.54	0.43
1:A:264:VAL:O	1:A:268:ILE:HG13	2.18	0.43
1:A:345:ARG:O	1:A:349:VAL:HG23	2.19	0.43
1:B:257:VAL:O	1:B:257:VAL:HG12	2.17	0.43
2:D:29:LEU:O	2:D:33:GLU:HG3	2.19	0.43
3:E:51:GLN:HG2	3:E:62:CYS:SG	2.58	0.43
3:E:165:ALA:HA	3:E:166:PRO:HD3	1.89	0.43
1:A:94:ASP:N	1:A:100:LYS:HZ3	2.17	0.43
1:B:2021:GLN:O	1:B:2022:GLU:C	2.62	0.43
1:B:269:ASN:ND2	3:E:264:GLN:HG3	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:337:LYS:O	1:B:340:PRO:HD2	2.19	0.43
2:D:191:LEU:O	2:D:193:PRO:HD3	2.18	0.43
1:B:309:ILE:O	1:B:310:GLU:C	2.61	0.43
2:D:119:LYS:HD3	2:D:119:LYS:N	2.11	0.43
1:B:282:LEU:HD23	1:B:285:MET:HE3	2.01	0.42
1:C:278:TRP:CE3	1:C:349:VAL:HG21	2.53	0.42
1:B:321:PRO:HA	1:B:322:PRO:HD2	1.92	0.42
1:C:37:ILE:HG12	1:C:62:LEU:HD21	2.02	0.42
1:A:136:PHE:CZ	1:A:166:ILE:HD12	2.54	0.42
1:B:131:LEU:HB2	1:B:136:PHE:HD1	1.85	0.42
1:C:276:ILE:CG2	1:C:277:GLU:N	2.82	0.42
1:B:76:CYS:SG	1:B:78:ASN:HB2	2.59	0.42
3:E:245:LEU:HB2	3:E:297:ARG:HG3	2.01	0.42
1:A:333:LEU:O	1:A:336:ARG:N	2.49	0.42
1:B:347:MET:O	1:B:351:MET:CG	2.65	0.42
1:C:104:THR:HG22	1:C:108:LEU:CD1	2.50	0.42
3:E:92:ALA:O	3:E:96:VAL:HG23	2.19	0.42
1:A:351:MET:HE3	1:A:354:LEU:HB2	2.01	0.42
1:B:271:ALA:O	1:B:276:ILE:HG13	2.20	0.42
1:C:214:LEU:O	1:C:215:ARG:C	2.61	0.42
3:E:149:GLU:C	3:E:151:LEU:N	2.71	0.42
1:A:147:PRO:HB2	1:A:149:HIS:NE2	2.35	0.42
1:A:333:LEU:HD22	1:C:338:GLU:HB3	2.02	0.42
2:D:311:THR:O	2:D:318:GLN:NE2	2.53	0.42
1:A:333:LEU:HD11	1:C:341:TYR:C	2.45	0.42
1:B:2050:GLY:O	1:B:2051:LYS:C	2.63	0.42
1:B:119:ARG:H	1:B:119:ARG:HG3	1.65	0.42
3:E:18:TYR:HB3	3:E:48:LEU:HD21	2.00	0.42
1:C:342:ALA:HB1	1:C:343:PRO:HD2	2.01	0.42
2:D:243:PRO:HG2	2:D:244:VAL:H	1.85	0.42
2:D:264:SER:O	2:D:265:ALA:CB	2.68	0.42
1:B:244:LEU:CD1	1:B:276:ILE:HD13	2.48	0.41
1:B:333:LEU:O	1:B:334:ILE:C	2.63	0.41
1:A:156:THR:HG22	1:A:157:THR:N	2.34	0.41
1:A:210:ALA:HB1	1:A:213:SER:OG	2.20	0.41
1:A:237:VAL:C	1:A:239:ALA:N	2.76	0.41
1:A:265:MET:HE2	1:B:294:MET:SD	2.61	0.41
1:B:351:MET:SD	3:E:290:LEU:HD13	2.59	0.41
2:D:79:THR:HG22	2:D:80:LEU:N	2.34	0.41
2:D:124:ALA:O	2:D:125:ALA:C	2.63	0.41
2:D:142:PRO:CD	2:D:178:LEU:HD11	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:223:MET:HE2	2:D:288:GLU:O	2.20	0.41
2:D:253:GLU:OE1	2:D:286:MET:HE1	2.19	0.41
3:E:197:SER:HA	3:E:198:PRO:HD3	1.87	0.41
1:A:215:ARG:NH2	5:A:1500:SO4:O1	2.53	0.41
1:A:265:MET:HE2	1:B:294:MET:HE1	2.02	0.41
2:D:64:ILE:HG12	2:D:96:GLN:HB3	2.02	0.41
1:B:351:MET:SD	3:E:290:LEU:HD22	2.60	0.41
1:A:78:ASN:O	1:A:82:ILE:HG13	2.20	0.41
1:A:320:ILE:HA	1:A:321:PRO:HD3	1.89	0.41
2:D:4:LEU:CD1	2:D:137:VAL:HG22	2.50	0.41
3:E:225:PRO:HB3	3:E:276:GLU:OE2	2.20	0.41
1:A:18:VAL:HG12	1:A:19:VAL:N	2.35	0.41
1:A:215:ARG:NH2	5:A:1500:SO4:S	2.94	0.41
1:B:244:LEU:HD11	1:B:276:ILE:HG21	2.02	0.41
1:C:140:LEU:HD23	1:C:140:LEU:HA	1.84	0.41
1:A:283:VAL:HA	1:A:286:LEU:HD12	2.03	0.41
1:A:250:LEU:HD23	1:A:312:ARG:CZ	2.51	0.41
1:B:343:PRO:CG	1:B:347:MET:SD	3.09	0.41
1:B:360:HIS:HB2	1:B:363:MET:HE3	2.02	0.41
1:C:281:LEU:O	1:C:285:MET:HG3	2.20	0.41
3:E:329:LEU:HD23	3:E:329:LEU:N	2.34	0.41
1:A:291:ARG:HD2	1:A:306:MET:HE2	2.02	0.41
1:A:362:ARG:HA	1:A:362:ARG:HD3	1.95	0.41
1:B:302:LEU:HD13	1:B:310:GLU:HA	2.03	0.41
1:C:259:ALA:HB3	1:C:363:MET:HE1	2.02	0.41
2:D:310:LEU:HD23	2:D:310:LEU:HA	1.61	0.41
3:E:121:THR:O	3:E:124:ALA:HB3	2.21	0.41
3:E:170:GLN:H	3:E:170:GLN:HG2	1.65	0.41
3:E:239:GLU:HA	3:E:308:ARG:CZ	2.51	0.41
2:D:310:LEU:HB3	2:D:314:GLN:NE2	2.35	0.41
1:A:257:VAL:O	1:A:257:VAL:HG12	2.21	0.40
2:D:270:ARG:HG2	2:D:283:ARG:NH2	2.36	0.40
3:E:73:HIS:HA	3:E:74:PRO:HD3	1.77	0.40
3:E:321:HIS:O	3:E:327:VAL:HG21	2.22	0.40
1:A:276:ILE:H	1:A:276:ILE:HG13	1.66	0.40
1:A:347:MET:O	1:A:348:GLY:C	2.64	0.40
1:B:311:LEU:HD12	1:B:311:LEU:HA	1.88	0.40
2:D:281:ASN:O	2:D:281:ASN:OD1	2.40	0.40
3:E:73:HIS:CE1	3:E:106:LEU:HD22	2.56	0.40
1:B:297:LEU:HD12	1:B:297:LEU:HA	1.90	0.40
1:C:248:GLN:CD	1:C:267:LEU:HD22	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:256:LEU:HD12	3:E:290:LEU:HD12	2.03	0.40
1:A:137:ASN:HA	1:A:140:LEU:HD12	2.02	0.40
1:B:250:LEU:CD2	1:B:309:ILE:HG23	2.51	0.40
1:C:82:ILE:HG23	1:C:90:LEU:HD23	2.03	0.40
2:D:39:ARG:CZ	2:D:50:HIS:HB3	2.51	0.40
3:E:163:TYR:CE2	3:E:165:ALA:HB2	2.57	0.40
1:A:49:VAL:O	5:A:1500:SO4:O1	2.40	0.40
1:A:322:PRO:HG3	1:C:365:LEU:HB2	2.03	0.40
1:B:365:LEU:HB3	1:B:366:PRO:HD2	2.04	0.40
1:C:32:LEU:HD23	1:C:32:LEU:HA	1.94	0.40
3:E:171:TYR:N	3:E:171:TYR:CD2	2.88	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:C:117:ARG:NH2	2:D:281:ASN:ND2[4_486]	1.70	0.50

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	364/373 (98%)	335 (92%)	23 (6%)	6 (2%)	7	20
1	B	363/373 (97%)	325 (90%)	28 (8%)	10 (3%)	4	9
1	C	364/373 (98%)	334 (92%)	22 (6%)	8 (2%)	5	14
2	D	336/343 (98%)	307 (91%)	22 (6%)	7 (2%)	5	15
3	E	332/334 (99%)	301 (91%)	29 (9%)	2 (1%)	21	44
All	All	1759/1796 (98%)	1602 (91%)	124 (7%)	33 (2%)	6	17

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	20	GLY
1	A	104	THR
1	A	111	VAL
1	A	364	PRO
1	B	2022	GLU
1	B	104	THR
1	B	261	GLY
1	B	310	GLU
1	C	310	GLU
2	D	279	TRP
1	B	2050	GLY
1	C	104	THR
1	C	303	GLY
2	D	131	ALA
2	D	282	ARG
1	B	111	VAL
1	C	4	GLN
2	D	46	GLY
2	D	269	LEU
3	E	62	CYS
1	C	249	ALA
2	D	125	ALA
3	E	150	ARG
1	A	339	LEU
1	B	7	ALA
1	B	364	PRO
1	C	22	GLU
1	C	278	TRP
1	A	246	ASP
1	B	101	VAL
1	B	299	PRO
2	D	317	GLY
1	C	101	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	303/310 (98%)	287 (95%)	16 (5%)	20	46
1	B	302/310 (97%)	281 (93%)	21 (7%)	14	34
1	C	303/310 (98%)	279 (92%)	24 (8%)	11	28
2	D	287/291 (99%)	258 (90%)	29 (10%)	7	18
3	E	270/270 (100%)	240 (89%)	30 (11%)	6	15
All	All	1465/1491 (98%)	1345 (92%)	120 (8%)	10	27

All (120) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	TYR
1	A	15	PHE
1	A	46	THR
1	A	69	THR
1	A	76	CYS
1	A	117	ARG
1	A	130	MET
1	A	166	ILE
1	A	251	SER
1	A	309	ILE
1	A	318	ARG
1	A	323	THR
1	A	327	LEU
1	A	344	ASP
1	A	357	LEU
1	A	367	GLU
1	B	6	LEU
1	B	2017	ASP
1	B	2042	LEU
1	B	2046	THR
1	B	2047	ARG
1	B	71	THR
1	B	76	CYS
1	B	137	ASN
1	B	160	GLN
1	B	164	VAL
1	B	167	LEU
1	B	194	GLU
1	B	248	GLN
1	B	251	SER
1	B	253	VAL

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Mol	Chain	Res	Type
1	B	298	SER
1	B	318	ARG
1	B	333	LEU
1	B	351	MET
1	B	357	LEU
1	B	363	MET
1	C	3	TYR
1	C	5014	THR
1	C	5017	ASP
1	C	18	VAL
1	C	22	GLU
1	C	47	ARG
1	C	51	LYS
1	C	52	THR
1	C	71	THR
1	C	88	VAL
1	C	97	SER
1	C	128	VAL
1	C	157	THR
1	C	160	GLN
1	C	165	THR
1	C	176	LYS
1	C	219	SER
1	C	240	MET
1	C	251	SER
1	C	252	LEU
1	C	333	LEU
1	C	344	ASP
1	C	351	MET
1	C	357	LEU
2	D	40	GLN
2	D	54	SER
2	D	64	ILE
2	D	84	LEU
2	D	98	LEU
2	D	101	THR
2	D	109	LEU
2	D	113	ARG
2	D	115	ASN
2	D	119	LYS
2	D	133	ARG
2	D	143	GLU

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Mol	Chain	Res	Type
2	D	160	LEU
2	D	162	LEU
2	D	183	GLN
2	D	198	THR
2	D	200	PRO
2	D	208	ASP
2	D	215	PHE
2	D	221	LEU
2	D	223	MET
2	D	228	ARG
2	D	230	LEU
2	D	266	HIS
2	D	279	TRP
2	D	292	ARG
2	D	296	THR
2	D	305	LEU
2	D	330	LEU
3	E	13	LYS
3	E	15	VAL
3	E	35	MET
3	E	68	MET
3	E	91	ASP
3	E	110	LYS
3	E	120	LEU
3	E	147	GLU
3	E	149	GLU
3	E	154	THR
3	E	156	ARG
3	E	159	CYS
3	E	170	GLN
3	E	175	TRP
3	E	202	LEU
3	E	206	GLN
3	E	216	LEU
3	E	220	LEU
3	E	245	LEU
3	E	252	LEU
3	E	256	LEU
3	E	274	VAL
3	E	277	LEU
3	E	285	ARG
3	E	290	LEU

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Mol	Chain	Res	Type
3	E	296	ILE
3	E	299	GLN
3	E	310	LEU
3	E	315	LEU
3	E	329	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	ASN
1	A	78	ASN
1	A	198	HIS
1	A	360	HIS
1	B	2023	HIS
1	B	2038	HIS
1	B	110	ASN
1	B	129	HIS
1	B	185	HIS
1	B	198	HIS
1	B	223	GLN
1	B	248	GLN
1	B	269	ASN
1	B	326	GLN
1	B	330	GLN
1	B	360	HIS
1	C	137	ASN
1	C	198	HIS
1	C	360	HIS
2	D	32	GLN
2	D	40	GLN
2	D	51	HIS
2	D	94	ASN
2	D	105	HIS
2	D	136	GLN
2	D	168	GLN
2	D	183	GLN
2	D	211	HIS
2	D	216	HIS
2	D	266	HIS
2	D	276	HIS
2	D	295	GLN
2	D	297	GLN

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Mol	Chain	Res	Type
2	D	314	GLN
2	D	318	GLN
3	E	73	HIS
3	E	162	HIS
3	E	237	ASN
3	E	240	GLN
3	E	299	GLN
3	E	307	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](#)

Of 7 ligands modelled in this entry, 4 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	SO4	A	1500	-	4,4,4	1.83	2 (50%)	6,6,6	0.96	0
5	SO4	B	2500	-	4,4,4	1.85	2 (50%)	6,6,6	0.83	0
5	SO4	C	5500	-	4,4,4	1.84	2 (50%)	6,6,6	0.85	0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	2500	SO4	O1-S	2.99	1.62	1.44
5	C	5500	SO4	O1-S	2.87	1.61	1.44
5	A	1500	SO4	O1-S	2.76	1.61	1.44
5	A	1500	SO4	O3-S	-2.34	1.28	1.48
5	C	5500	SO4	O3-S	-2.28	1.29	1.48
5	B	2500	SO4	O3-S	-2.16	1.30	1.48

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1500	SO4	7	0
5	B	2500	SO4	2	0
5	C	5500	SO4	3	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	366/373 (98%)	1.13	75 (20%) 2 2	32, 76, 152, 173	0
1	B	365/373 (97%)	1.21	82 (22%) 2 2	27, 75, 159, 190	0
1	C	366/373 (98%)	0.91	51 (13%) 6 5	27, 62, 129, 156	0
2	D	338/343 (98%)	1.10	60 (17%) 4 3	38, 69, 121, 142	0
3	E	334/334 (100%)	1.15	77 (23%) 2 2	30, 67, 156, 161	0
All	All	1769/1796 (98%)	1.10	345 (19%) 3 2	27, 69, 151, 190	0

All (345) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	359	PHE	8.5
3	E	79	LEU	6.2
2	D	280	GLN	5.5
1	B	132	SER	5.5
1	B	306	MET	5.5
2	D	281	ASN	5.5
1	B	242	GLY	5.3
1	B	136	PHE	5.2
2	D	316	TYR	5.1
2	D	326	GLY	5.0
1	A	138	ALA	4.9
2	D	338	ASP	4.8
1	C	241	LEU	4.8
3	E	90	VAL	4.7
1	B	365	LEU	4.6
3	E	103	HIS	4.6
1	B	368	PRO	4.6
2	D	337	ALA	4.5
1	B	2023	HIS	4.5
3	E	20	ALA	4.5

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Mol	Chain	Res	Type	RSRZ
3	E	132	LEU	4.4
1	B	364	PRO	4.4
3	E	37	ASP	4.3
1	A	368	PRO	4.3
2	D	275	LYS	4.2
3	E	44	LEU	4.2
3	E	125	ALA	4.2
1	C	238	SER	4.2
1	C	367	GLU	4.2
1	A	119	ARG	4.2
1	B	179	ASP	4.2
1	C	249	ALA	4.2
2	D	317	GLY	4.2
2	D	279	TRP	4.1
1	B	2038	HIS	4.0
1	B	2068	ILE	3.9
3	E	56	HIS	3.9
2	D	225	LYS	3.9
1	A	68	ILE	3.9
2	D	336	LEU	3.9
1	A	367	GLU	3.8
1	B	229	ASP	3.8
3	E	76	TYR	3.8
1	B	300	ALA	3.8
3	E	109	ALA	3.8
1	B	246	ASP	3.8
1	B	366	PRO	3.8
2	D	236	LEU	3.8
2	D	333	HIS	3.7
3	E	92	ALA	3.7
3	E	334	LEU	3.7
2	D	211	HIS	3.7
1	C	247	ASP	3.7
1	A	104	THR	3.6
3	E	307	ASN	3.6
3	E	128	LEU	3.6
1	A	235	GLN	3.6
1	C	244	LEU	3.6
1	A	82	ILE	3.6
1	C	366	PRO	3.6
2	D	264	SER	3.6
3	E	302	SER	3.6

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Mol	Chain	Res	Type	RSRZ
3	E	333	HIS	3.5
1	A	201	ARG	3.5
3	E	112	VAL	3.5
1	A	108	LEU	3.5
1	B	367	GLU	3.5
2	D	278	VAL	3.5
2	D	329	LEU	3.5
1	A	66	THR	3.5
2	D	319	SER	3.4
3	E	108	GLY	3.4
3	E	116	ASP	3.4
1	C	365	LEU	3.4
1	C	307	ALA	3.4
1	C	302	LEU	3.4
1	A	152	PHE	3.4
3	E	113	TRP	3.4
1	C	303	GLY	3.4
1	A	166	ILE	3.3
1	A	366	PRO	3.3
3	E	49	LEU	3.3
1	B	95	ALA	3.3
2	D	332	CYS	3.3
1	B	131	LEU	3.3
3	E	111	VAL	3.3
3	E	24	HIS	3.3
1	A	74	GLY	3.3
1	C	100	LYS	3.3
1	C	330	GLN	3.3
1	B	305	ASP	3.3
1	B	176	LYS	3.2
1	B	230	GLY	3.2
2	D	320	VAL	3.2
3	E	93	VAL	3.2
2	D	36	ASP	3.2
1	A	365	LEU	3.2
1	B	302	LEU	3.2
1	B	361	PRO	3.2
1	C	368	PRO	3.2
1	A	101	VAL	3.2
1	A	168	SER	3.2
3	E	77	TYR	3.2
1	C	298	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	3	TYR	3.1
1	B	139	LEU	3.1
1	C	321	PRO	3.1
1	A	157	THR	3.1
1	B	135	SER	3.1
1	B	304	ASN	3.1
1	B	142	THR	3.1
3	E	83	LYS	3.1
3	E	119	LEU	3.0
1	B	301	ALA	3.0
1	B	358	ALA	3.0
1	C	300	ALA	3.0
1	C	291	ARG	3.0
2	D	296	THR	3.0
1	B	138	ALA	3.0
1	C	308	ALA	3.0
3	E	123	ALA	3.0
1	B	164	VAL	3.0
1	C	260	ASN	3.0
1	A	305	ASP	3.0
1	C	4	GLN	3.0
1	A	136	PHE	3.0
1	A	364	PRO	3.0
3	E	91	ASP	2.9
3	E	55	GLY	2.9
1	C	364	PRO	2.9
1	C	301	ALA	2.9
3	E	124	ALA	2.9
1	A	107	LEU	2.9
1	B	166	ILE	2.9
3	E	107	GLY	2.9
1	A	71	THR	2.9
1	C	243	THR	2.9
1	B	101	VAL	2.9
1	A	134	HIS	2.9
1	A	238	SER	2.8
1	A	260	ASN	2.8
2	D	194	ASP	2.8
3	E	131	THR	2.8
1	C	245	ASP	2.8
1	B	70	ALA	2.8
1	C	101	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
3	E	114	VAL	2.8
1	A	116	ALA	2.8
3	E	104	ALA	2.8
1	C	294	MET	2.8
1	A	219	SER	2.8
2	D	321	TRP	2.8
1	A	103	ASP	2.8
1	B	247	ASP	2.8
1	C	239	ALA	2.8
1	B	133	ARG	2.8
2	D	240	GLY	2.7
1	C	320	ILE	2.7
3	E	67	LEU	2.7
1	C	104	THR	2.7
1	C	292	ILE	2.7
1	B	2025	LEU	2.7
3	E	100	LEU	2.7
1	A	177	ALA	2.7
1	A	239	ALA	2.7
3	E	88	LEU	2.7
1	A	47	ARG	2.7
3	E	146	ARG	2.7
2	D	322	ALA	2.7
3	E	170	GLN	2.6
1	A	73	CYS	2.6
1	C	107	LEU	2.6
1	B	303	GLY	2.6
2	D	224	GLY	2.6
1	B	152	PHE	2.6
1	C	21	GLN	2.6
1	C	248	GLN	2.6
3	E	61	HIS	2.6
1	B	104	THR	2.6
2	D	318	GLN	2.6
1	B	90	LEU	2.6
1	C	5011	ARG	2.6
2	D	123	ASN	2.6
3	E	74	PRO	2.6
3	E	3	TRP	2.6
1	B	107	LEU	2.6
2	D	283	ARG	2.6
3	E	42	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	146	PRO	2.6
1	B	114	ALA	2.6
1	B	163	PRO	2.6
1	C	358	ALA	2.6
3	E	136	PRO	2.6
1	A	62	LEU	2.5
1	B	141	LYS	2.5
3	E	71	GLY	2.5
1	A	147	PRO	2.5
3	E	78	THR	2.5
1	C	276	ILE	2.5
1	A	153	LEU	2.5
2	D	284	GLY	2.5
2	D	268	PRO	2.5
2	D	62	ASN	2.5
1	C	309	ILE	2.5
1	B	244	LEU	2.5
1	C	357	LEU	2.5
3	E	73	HIS	2.5
1	B	113	TYR	2.5
1	B	137	ASN	2.5
2	D	237	ARG	2.5
2	D	86	GLU	2.5
1	A	113	TYR	2.5
1	A	111	VAL	2.5
1	B	100	LYS	2.4
3	E	97	THR	2.4
1	B	2058	LEU	2.4
2	D	324	LEU	2.4
3	E	58	SER	2.4
1	A	72	PRO	2.4
1	A	85	GLY	2.4
3	E	4	TYR	2.4
2	D	234	GLN	2.4
1	A	143	LEU	2.4
3	E	86	ASN	2.4
3	E	129	LEU	2.4
1	C	3	TYR	2.4
2	D	120	ALA	2.4
2	D	145	ALA	2.4
3	E	70	ALA	2.4
1	B	125	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	305	ASP	2.4
3	E	53	PRO	2.4
1	C	293	ALA	2.4
1	B	243	THR	2.4
1	C	211	GLU	2.4
1	A	106	ASP	2.4
3	E	68	MET	2.4
1	B	212	GLY	2.4
1	B	314	ARG	2.4
2	D	39	ARG	2.4
3	E	150	ARG	2.4
3	E	127	ALA	2.4
1	A	142	THR	2.3
3	E	126	ASN	2.3
1	A	205	LEU	2.3
1	B	143	LEU	2.3
2	D	222	LEU	2.3
1	A	149	HIS	2.3
2	D	223	MET	2.3
2	D	323	GLU	2.3
1	B	119	ARG	2.3
1	C	335	GLY	2.3
3	E	69	GLN	2.3
1	A	162	LEU	2.3
1	A	327	LEU	2.3
1	A	125	ILE	2.3
1	A	161	LYS	2.3
1	A	89	ASP	2.3
3	E	51	GLN	2.3
3	E	147	GLU	2.3
1	A	112	GLN	2.3
1	B	108	LEU	2.3
2	D	238	LEU	2.3
3	E	331	VAL	2.3
1	B	7	ALA	2.2
1	C	306	MET	2.2
1	B	117	ARG	2.2
2	D	144	GLN	2.2
1	A	48	GLY	2.2
1	A	90	LEU	2.2
1	B	6	LEU	2.2
1	C	311	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	119	LYS	2.2
1	B	277	GLU	2.2
3	E	121	THR	2.2
3	E	145	THR	2.2
3	E	163	TYR	2.2
1	C	299	PRO	2.2
1	A	21	GLN	2.2
1	A	100	LYS	2.2
2	D	76	SER	2.2
1	A	18	VAL	2.2
1	A	91	ILE	2.2
1	A	96	ALA	2.2
1	A	114	ALA	2.2
1	A	209	ALA	2.2
1	B	96	ALA	2.2
1	B	211	GLU	2.2
1	A	243	THR	2.2
1	B	98	ARG	2.2
1	A	115	PRO	2.2
1	C	161	LYS	2.2
1	B	363	MET	2.2
1	C	242	GLY	2.1
1	A	81	GLU	2.1
1	B	181	GLU	2.1
3	E	95	GLU	2.1
1	A	98	ARG	2.1
3	E	101	ASN	2.1
1	A	245	ASP	2.1
1	B	5	VAL	2.1
1	A	120	PHE	2.1
3	E	223	SER	2.1
1	B	71	THR	2.1
1	B	4	GLN	2.1
1	B	170	CYS	2.1
1	A	61	GLY	2.1
1	B	149	HIS	2.1
3	E	141	PHE	2.1
1	B	2014	THR	2.1
1	B	99	THR	2.1
2	D	214	PRO	2.1
1	C	240	MET	2.1
3	E	54	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	167	LEU	2.1
2	D	331	LEU	2.1
1	A	38	HIS	2.1
3	E	65	CYS	2.1
1	B	82	ILE	2.1
3	E	46	ARG	2.0
2	D	271	ALA	2.0
3	E	45	SER	2.0
3	E	80	ALA	2.0
1	A	99	THR	2.0
1	C	142	THR	2.0
2	D	128	THR	2.0
1	B	130	MET	2.0
1	B	327	LEU	2.0
2	D	235	GLN	2.0
1	B	360	HIS	2.0
2	D	50	HIS	2.0
2	D	287	GLY	2.0
3	E	303	VAL	2.0
2	D	252	ARG	2.0
2	D	273	PHE	2.0
1	A	70	ALA	2.0
1	B	298	SER	2.0
1	B	115	PRO	2.0
1	A	57	LEU	2.0
2	D	40	GLN	2.0
2	D	108	LEU	2.0
2	D	157	GLN	2.0
1	A	80	ARG	2.0
2	D	277	ARG	2.0
1	B	341	TYR	2.0

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

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($\text{\AA}^2$)	Q<0.9
4	ZN	E	400	1/1	0.83	0.11	156,156,156,156	0
5	SO4	A	1500	5/5	0.93	0.10	64,65,66,67	0
5	SO4	B	2500	5/5	0.95	0.07	68,70,70,70	0
5	SO4	C	5500	5/5	0.97	0.08	36,36,39,41	0
4	ZN	A	400	1/1	0.98	0.05	130,130,130,130	0
4	ZN	B	400	1/1	0.98	0.05	105,105,105,105	0
4	ZN	C	400	1/1	0.99	0.03	44,44,44,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.