



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:14 AM UTC

PDB ID : 1Z7M / pdb_00001z7m
Title : ATP Phosphoribosyl transferase (HisZG ATP-PRTase) from *Lactococcus lactis*
Authors : Champagne, K.S.; Sissler, M.; Larrabee, Y.; Doublié, S.; Francklyn, C.S.
Deposited on : 2005-03-25
Resolution : 2.90 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

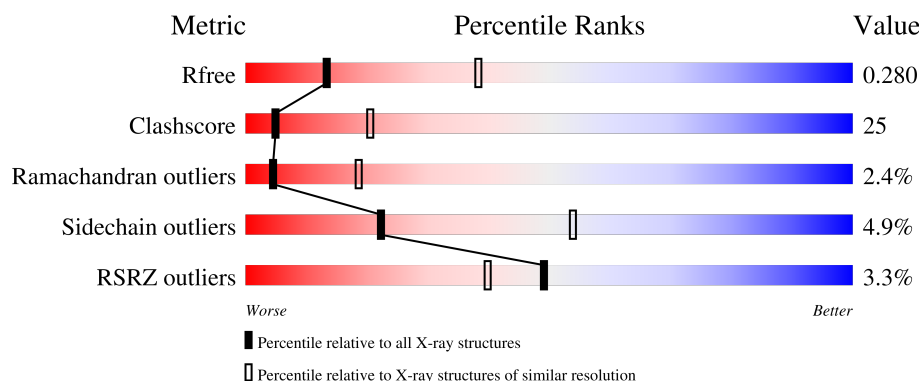
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	344	3% 55% 29% 6% 10%
1	B	344	2% 53% 33% 5% 8%
1	C	344	3% 55% 30% • 12%
1	D	344	2% 52% 34% 5% 9%
2	E	208	4% 52% 37% 7% •

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Mol	Chain	Length	Quality of chain
2	F	208	
2	G	208	
2	H	208	

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
4	PO4	B	329	-	X	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16609 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 ATP phosphoribosyltransferase regulatory subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	311	Total	C	N	O	S	12	0	0
			2526	1624	408	483	11			
1	B	318	Total	C	N	O	S	22	0	0
			2584	1657	424	492	11			
1	C	302	Total	C	N	O	S	11	0	0
			2455	1579	396	469	11			
1	D	314	Total	C	N	O	S	16	0	0
			2557	1642	418	486	11			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	MET	-	cloning artifact	UNP Q02147
A	-14	ARG	-	cloning artifact	UNP Q02147
A	-13	GLY	-	cloning artifact	UNP Q02147
A	-12	SER	-	cloning artifact	UNP Q02147
A	-11	HIS	-	expression tag	UNP Q02147
A	-10	HIS	-	expression tag	UNP Q02147
A	-9	HIS	-	expression tag	UNP Q02147
A	-8	HIS	-	expression tag	UNP Q02147
A	-7	HIS	-	expression tag	UNP Q02147
A	-6	HIS	-	expression tag	UNP Q02147
A	-5	GLY	-	cloning artifact	UNP Q02147
A	-4	SER	-	cloning artifact	UNP Q02147
A	-3	ILE	-	cloning artifact	UNP Q02147
A	-2	GLU	-	cloning artifact	UNP Q02147
A	-1	GLY	-	cloning artifact	UNP Q02147
A	0	ARG	-	cloning artifact	UNP Q02147
B	-15	MET	-	cloning artifact	UNP Q02147
B	-14	ARG	-	cloning artifact	UNP Q02147
B	-13	GLY	-	cloning artifact	UNP Q02147
B	-12	SER	-	cloning artifact	UNP Q02147
B	-11	HIS	-	expression tag	UNP Q02147

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-10	HIS	-	expression tag	UNP Q02147
B	-9	HIS	-	expression tag	UNP Q02147
B	-8	HIS	-	expression tag	UNP Q02147
B	-7	HIS	-	expression tag	UNP Q02147
B	-6	HIS	-	expression tag	UNP Q02147
B	-5	GLY	-	cloning artifact	UNP Q02147
B	-4	SER	-	cloning artifact	UNP Q02147
B	-3	ILE	-	cloning artifact	UNP Q02147
B	-2	GLU	-	cloning artifact	UNP Q02147
B	-1	GLY	-	cloning artifact	UNP Q02147
B	0	ARG	-	cloning artifact	UNP Q02147
C	-15	MET	-	cloning artifact	UNP Q02147
C	-14	ARG	-	cloning artifact	UNP Q02147
C	-13	GLY	-	cloning artifact	UNP Q02147
C	-12	SER	-	cloning artifact	UNP Q02147
C	-11	HIS	-	expression tag	UNP Q02147
C	-10	HIS	-	expression tag	UNP Q02147
C	-9	HIS	-	expression tag	UNP Q02147
C	-8	HIS	-	expression tag	UNP Q02147
C	-7	HIS	-	expression tag	UNP Q02147
C	-6	HIS	-	expression tag	UNP Q02147
C	-5	GLY	-	cloning artifact	UNP Q02147
C	-4	SER	-	cloning artifact	UNP Q02147
C	-3	ILE	-	cloning artifact	UNP Q02147
C	-2	GLU	-	cloning artifact	UNP Q02147
C	-1	GLY	-	cloning artifact	UNP Q02147
C	0	ARG	-	cloning artifact	UNP Q02147
D	-15	MET	-	cloning artifact	UNP Q02147
D	-14	ARG	-	cloning artifact	UNP Q02147
D	-13	GLY	-	cloning artifact	UNP Q02147
D	-12	SER	-	cloning artifact	UNP Q02147
D	-11	HIS	-	expression tag	UNP Q02147
D	-10	HIS	-	expression tag	UNP Q02147
D	-9	HIS	-	expression tag	UNP Q02147
D	-8	HIS	-	expression tag	UNP Q02147
D	-7	HIS	-	expression tag	UNP Q02147
D	-6	HIS	-	expression tag	UNP Q02147
D	-5	GLY	-	cloning artifact	UNP Q02147
D	-4	SER	-	cloning artifact	UNP Q02147
D	-3	ILE	-	cloning artifact	UNP Q02147
D	-2	GLU	-	cloning artifact	UNP Q02147
D	-1	GLY	-	cloning artifact	UNP Q02147

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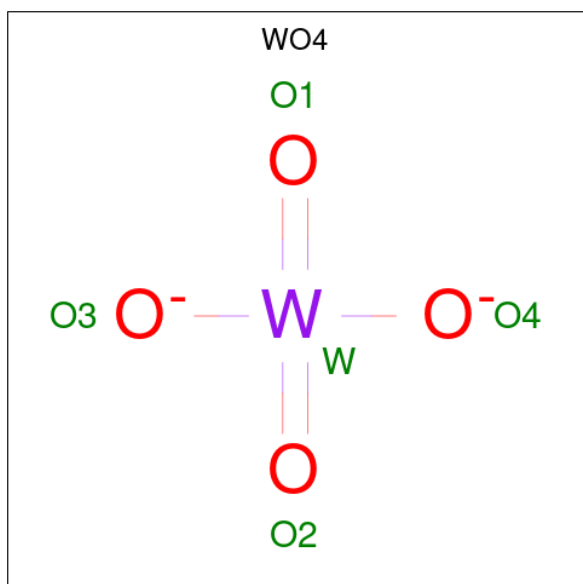
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Chain	Residue	Modelled	Actual	Comment	Reference
D	0	ARG	-	cloning artifact	UNP Q02147

- Molecule 2 is a protein called ATP phosphoribosyltransferase.

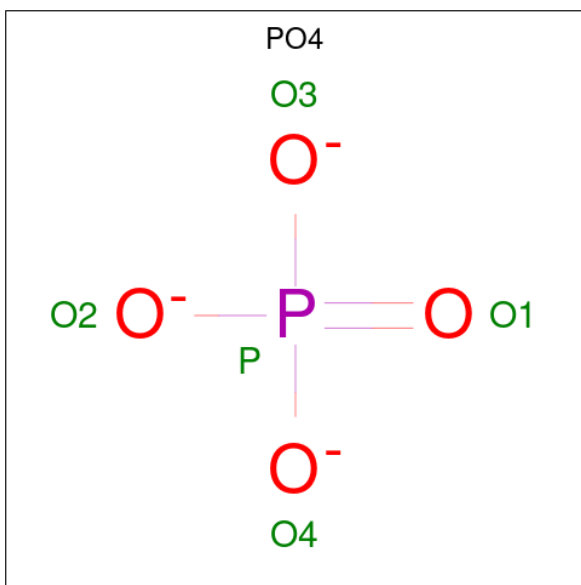
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	200	Total	C	N	O	S	5	0	0
			1610	1034	263	309	4			
2	F	201	Total	C	N	O	S	0	0	0
			1611	1035	263	309	4			
2	G	203	Total	C	N	O	S	5	0	0
			1632	1048	267	313	4			
2	H	199	Total	C	N	O	S	4	0	0
			1594	1025	259	306	4			

- Molecule 3 is TUNGSTATE(VI)ION (CCD ID: WO4) (formula: O₄W).

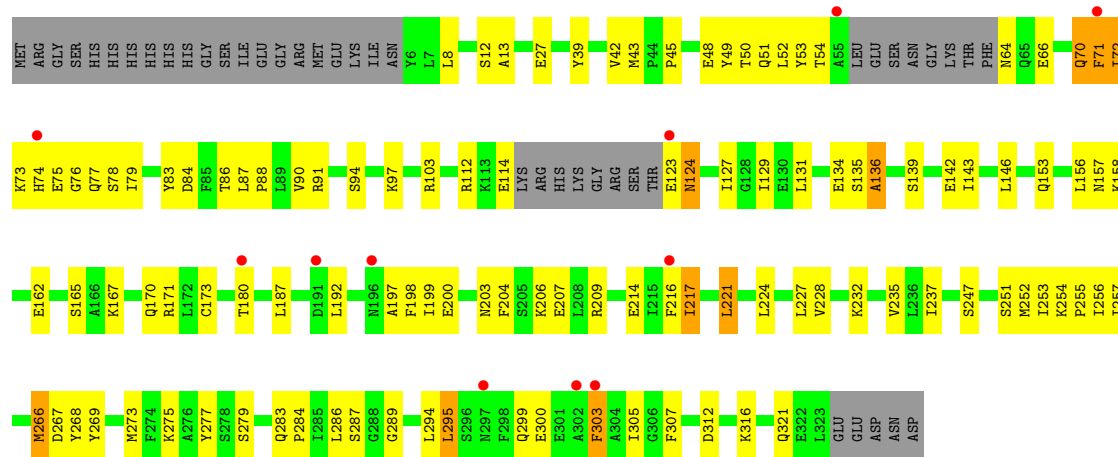


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	O W	0	0
			5 4 1			
3	F	1	Total	O W	0	0
			5 4 1			

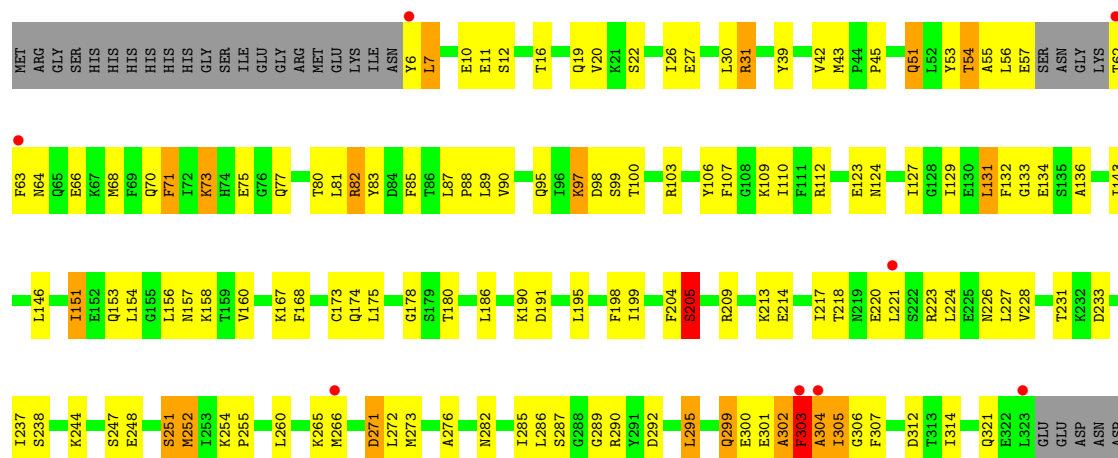
- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



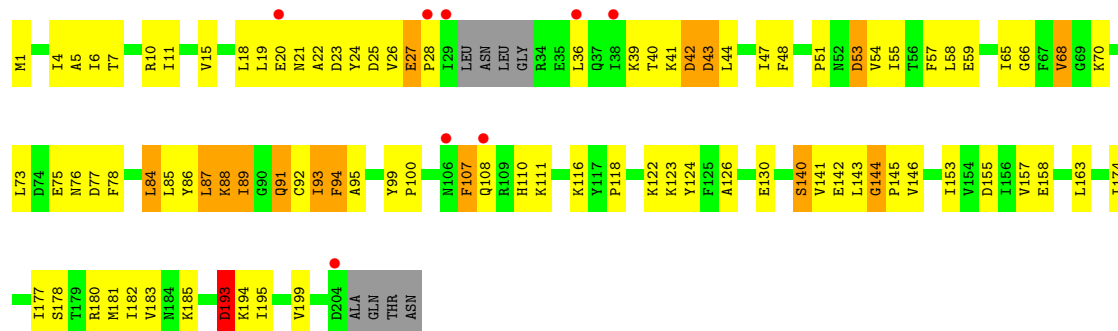
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	P	0	0
			5	4	1		
4	D	1	Total	O	P	0	0
			5	4	1		
4	E	1	Total	O	P	0	0
			5	4	1		
4	F	1	Total	O	P	0	0
			5	4	1		
4	G	1	Total	O	P	0	0
			5	4	1		
4	H	1	Total	O	P	0	0
			5	4	1		



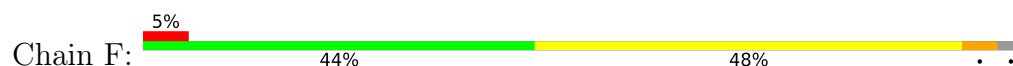
• Molecule 1: ATP phosphoribosyltransferase regulatory subunit

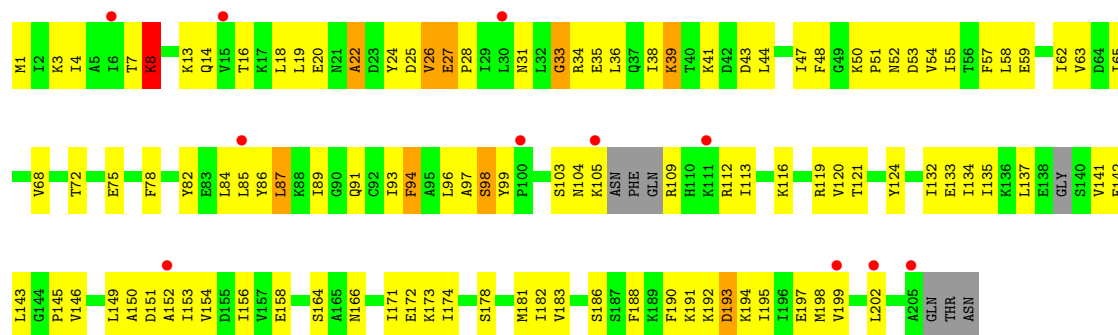


• Molecule 2: ATP phosphoribosyltransferase

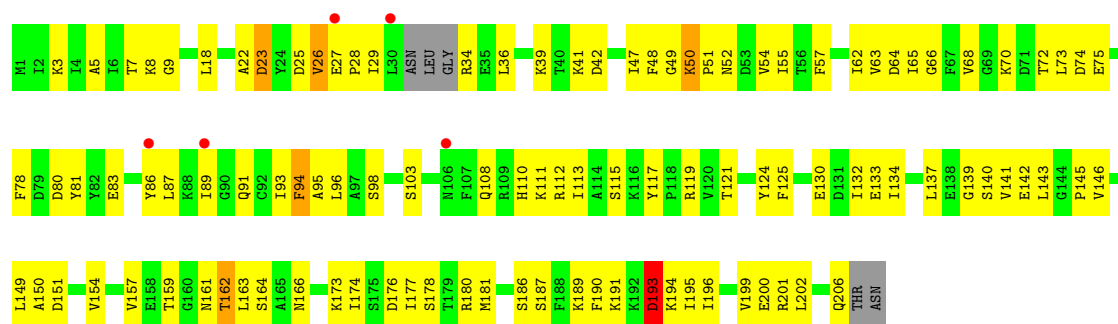


• Molecule 2: ATP phosphoribosyltransferase

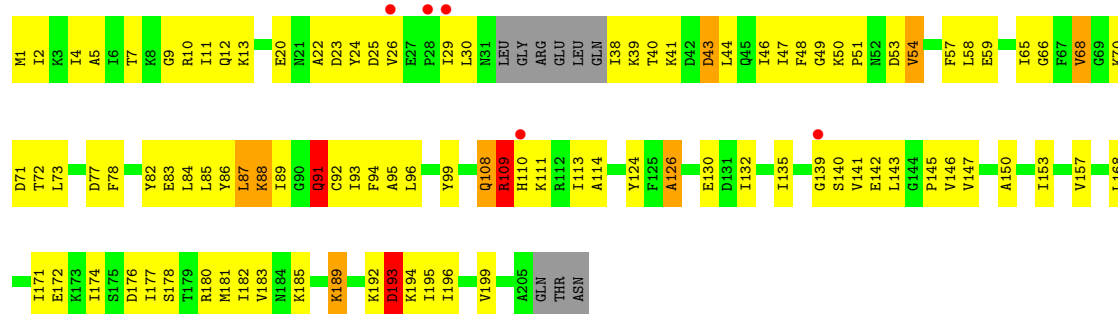




• Molecule 2: ATP phosphoribosyltransferase



• Molecule 2: ATP phosphoribosyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	151.68Å 222.94Å 86.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.90 40.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-2.90) 88.1 (40.00-2.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 2.90Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.245 , 0.285 0.243 , 0.280	Depositor DCC
R_{free} test set	2820 reflections (4.39%)	wwPDB-VP
Wilson B-factor (Å ²)	60.1	Xtriage
Anisotropy	0.385	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 32.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	16609	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% 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: WO4, PO4

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	0.71	5/2567 (0.2%)	1.04	13/3446 (0.4%)
1	B	0.64	0/2627	1.00	13/3526 (0.4%)
1	C	0.66	4/2494 (0.2%)	1.01	8/3348 (0.2%)
1	D	0.64	4/2599 (0.2%)	0.99	12/3488 (0.3%)
2	E	0.51	0/1632	0.98	6/2193 (0.3%)
2	F	0.48	0/1631	0.92	5/2191 (0.2%)
2	G	0.51	0/1654	0.97	7/2223 (0.3%)
2	H	0.61	2/1616 (0.1%)	1.08	12/2173 (0.6%)
All	All	0.62	15/16820 (0.1%)	1.00	76/22588 (0.3%)

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	D	0	1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	110	HIS	C-N	-12.73	1.16	1.33
1	D	205	SER	C-N	-12.11	1.16	1.33
1	D	303	PHE	C-O	8.21	1.33	1.23
1	D	302	ALA	N-CA	-7.65	1.36	1.45
1	A	222	SER	CA-C	7.54	1.62	1.52
1	C	74	HIS	N-CA	-7.29	1.37	1.46
1	A	222	SER	C-N	6.78	1.42	1.33
1	C	70	GLN	C-N	-5.52	1.26	1.33
1	A	114	GLU	CA-C	5.50	1.58	1.53
2	H	108	GLN	C-N	5.43	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	305	ILE	N-CA	-5.25	1.40	1.46
1	A	223	ARG	N-CA	5.20	1.52	1.46
1	D	151	ILE	CA-C	5.17	1.58	1.52
1	C	70	GLN	CA-C	-5.15	1.46	1.52
1	C	71	PHE	CA-C	5.11	1.59	1.52

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	89	ILE	N-CA-C	11.28	122.11	110.72
2	H	110	HIS	CA-C-N	11.00	136.78	121.05
2	H	110	HIS	C-N-CA	11.00	136.78	121.05
1	D	153	GLN	OE1-CD-NE2	-10.34	112.26	122.60
2	H	110	HIS	N-CA-C	10.12	124.91	110.23
1	B	70	GLN	OE1-CD-NE2	-9.91	112.69	122.60
1	A	95	GLN	OE1-CD-NE2	-9.80	112.80	122.60
1	D	51	GLN	OE1-CD-NE2	-9.80	112.80	122.60
1	B	51	GLN	OE1-CD-NE2	-9.76	112.84	122.60
1	D	95	GLN	OE1-CD-NE2	-9.75	112.85	122.60
1	C	70	GLN	OE1-CD-NE2	-9.70	112.90	122.60
2	G	108	GLN	OE1-CD-NE2	-8.94	113.66	122.60
2	H	108	GLN	OE1-CD-NE2	-8.80	113.80	122.60
2	H	109	ARG	CB-CA-C	8.74	125.13	109.83
1	B	56	LEU	N-CA-C	8.66	123.85	107.75
1	C	70	GLN	N-CA-C	7.95	119.72	108.74
2	H	109	ARG	N-CA-C	-7.68	99.15	110.52
2	H	126	ALA	N-CA-C	-7.55	102.73	110.97
1	D	43	MET	CA-C-N	7.49	125.13	119.66
1	D	43	MET	C-N-CA	7.49	125.13	119.66
1	D	153	GLN	CG-CD-NE2	7.33	127.40	116.40
1	C	43	MET	CA-C-N	7.25	124.95	119.66
1	C	43	MET	C-N-CA	7.25	124.95	119.66
1	D	205	SER	O-C-N	-6.92	114.52	122.68
1	A	157	ASN	N-CA-C	6.88	118.57	111.14
1	B	122	THR	N-CA-C	-6.74	105.21	113.50
1	A	64	ASN	N-CA-C	6.74	120.44	109.59
1	C	70	GLN	CG-CD-NE2	6.70	126.45	116.40
1	D	51	GLN	CG-CD-NE2	6.69	126.44	116.40
1	D	95	GLN	CG-CD-NE2	6.66	126.38	116.40
1	A	222	SER	CA-C-N	6.65	129.52	120.54
1	A	222	SER	C-N-CA	6.65	129.52	120.54
1	B	51	GLN	CG-CD-NE2	6.63	126.35	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	108	GLN	CG-CD-NE2	6.63	126.34	116.40
1	A	95	GLN	CG-CD-NE2	6.62	126.33	116.40
1	B	70	GLN	CG-CD-NE2	6.59	126.29	116.40
1	A	62	THR	N-CA-C	6.56	120.00	110.42
2	G	108	GLN	N-CA-C	-6.44	105.28	113.01
2	G	108	GLN	CG-CD-NE2	6.39	125.98	116.40
1	B	59	ASN	N-CA-C	6.37	124.37	110.80
2	H	110	HIS	CB-CA-C	-6.33	99.21	109.72
1	A	206	LYS	N-CA-C	-6.18	104.62	111.36
1	C	74	HIS	O-C-N	6.17	129.19	122.15
1	B	32	LYS	N-CA-C	-6.01	104.42	110.97
2	E	108	GLN	N-CA-C	-5.89	105.67	112.92
2	E	84	LEU	N-CA-C	5.86	117.46	111.14
2	F	62	ILE	N-CA-C	-5.82	104.48	113.16
2	H	46	ILE	N-CA-C	5.79	116.93	108.53
1	B	202	ASN	N-CA-C	5.72	118.81	110.17
2	F	116	LYS	N-CA-C	-5.72	106.34	113.38
2	E	54	VAL	N-CA-C	-5.68	104.97	110.42
2	F	22	ALA	N-CA-C	-5.60	106.12	113.17
2	E	116	LYS	N-CA-C	-5.57	106.49	113.28
2	F	26	VAL	N-CA-C	5.56	115.33	106.88
1	A	75	GLU	N-CA-C	-5.54	106.36	113.01
1	A	217	ILE	N-CA-C	5.54	120.87	109.34
2	F	8	LYS	N-CA-C	5.50	122.52	110.80
1	A	63	PHE	CA-C-N	-5.48	114.98	122.93
1	A	63	PHE	C-N-CA	-5.48	114.98	122.93
1	B	59	ASN	CB-CA-C	-5.46	99.56	110.42
1	C	153	GLN	N-CA-C	-5.36	106.67	114.12
2	G	26	VAL	N-CA-C	5.31	116.06	106.61
2	H	108	GLN	O-C-N	5.26	129.07	122.23
2	E	185	LYS	N-CA-C	5.25	117.00	111.28
2	G	110	HIS	CB-CA-C	5.25	118.39	109.84
2	H	54	VAL	N-CA-C	-5.25	105.42	110.72
1	C	217	ILE	N-CA-C	5.21	120.17	109.34
1	D	217	ILE	N-CA-C	5.19	120.14	109.34
1	B	217	ILE	N-CA-C	5.09	119.93	109.34
1	D	304	ALA	N-CA-C	5.09	118.05	110.52
2	G	50	LYS	CA-C-N	5.09	124.53	119.24
2	G	50	LYS	C-N-CA	5.09	124.53	119.24
1	D	301	GLU	O-C-N	5.04	129.13	122.93
1	B	270	THR	N-CA-C	5.03	116.45	110.97
1	A	304	ALA	CA-C-O	5.01	125.72	120.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	168	PHE	N-CA-C	-5.00	105.91	111.36

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	205	SER	Mainchain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2526	0	2554	124	0
1	B	2584	0	2616	122	0
1	C	2455	0	2480	126	0
1	D	2557	0	2588	123	0
2	E	1610	0	1655	91	0
2	F	1611	0	1664	108	0
2	G	1632	0	1679	100	0
2	H	1594	0	1638	92	0
3	A	5	0	0	0	0
3	F	5	0	0	0	0
4	B	5	0	0	1	0
4	D	5	0	0	0	0
4	E	5	0	0	0	0
4	F	5	0	0	1	0
4	G	5	0	0	0	0
4	H	5	0	0	0	0
All	All	16609	0	16874	841	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 25.

All (841) 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:A:71:PHE:CE1	1:A:79:ILE:HD11	1.26	1.59
1:C:73:LYS:HE2	1:C:77:GLN:CB	1.39	1.51
1:B:58:SER:HB3	1:B:267:ASP:CB	1.53	1.36
1:C:73:LYS:CE	1:C:77:GLN:HB2	1.52	1.36
1:A:71:PHE:CE1	1:A:79:ILE:CD1	2.14	1.30
1:B:266:MET:HE2	1:B:266:MET:HA	1.19	1.17
1:B:58:SER:CB	1:B:267:ASP:HB2	1.75	1.17
1:A:73:LYS:HE2	1:A:77:GLN:CB	1.80	1.12
1:D:299:GLN:HG2	1:D:300:GLU:H	1.06	1.12
1:B:59:ASN:OD1	1:B:59:ASN:C	1.91	1.12
1:C:299:GLN:HG2	1:C:300:GLU:H	0.93	1.10
1:A:73:LYS:HE2	1:A:77:GLN:HB2	1.33	1.10
2:E:36:LEU:HD13	2:F:143:LEU:HD11	1.35	1.08
1:A:73:LYS:HE2	1:A:77:GLN:CG	1.83	1.08
1:D:292:ASP:OD2	1:D:303:PHE:HA	1.57	1.05
1:C:135:SER:HA	1:C:303:PHE:CE2	1.92	1.05
1:C:157:ASN:H	1:C:321:GLN:NE2	1.55	1.05
1:A:73:LYS:HG2	1:A:77:GLN:H	1.22	1.03
1:C:73:LYS:HE2	1:C:77:GLN:CG	1.87	1.03
1:D:173:CYS:HB3	1:D:180:THR:HG22	1.37	1.02
1:C:73:LYS:NZ	1:C:77:GLN:HG3	1.72	1.02
2:H:111:LYS:HD2	2:H:130:GLU:OE2	1.63	0.98
1:D:205:SER:O	1:D:209:ARG:HG3	1.63	0.97
1:C:303:PHE:CD1	1:C:303:PHE:N	2.24	0.97
1:C:299:GLN:CG	1:C:300:GLU:H	1.79	0.95
1:A:73:LYS:HE3	1:A:75:GLU:HB3	1.49	0.95
1:A:157:ASN:H	1:A:321:GLN:NE2	1.63	0.95
1:A:157:ASN:H	1:A:321:GLN:HE22	1.13	0.95
1:A:109:LYS:NZ	1:A:123:GLU:HG3	1.81	0.94
1:B:157:ASN:H	1:B:321:GLN:NE2	1.65	0.94
1:D:157:ASN:H	1:D:321:GLN:NE2	1.65	0.94
1:D:133:GLY:O	1:D:303:PHE:CE1	2.20	0.94
1:C:157:ASN:H	1:C:321:GLN:HE22	1.05	0.93
1:C:72:ILE:HA	1:C:77:GLN:O	1.69	0.92
1:C:73:LYS:CE	1:C:77:GLN:CG	2.46	0.92
1:C:299:GLN:HG2	1:C:300:GLU:N	1.77	0.92
1:B:266:MET:HA	1:B:266:MET:CE	1.99	0.92
1:C:303:PHE:N	1:C:303:PHE:HD1	1.60	0.92
1:A:199:ILE:HG21	1:A:209:ARG:HG3	1.49	0.92
1:B:157:ASN:H	1:B:321:GLN:HE22	1.12	0.92
1:C:134:GLU:O	1:C:303:PHE:CD2	2.23	0.92
2:F:50:LYS:HB3	2:F:51:PRO:HD2	1.51	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:173:CYS:HB3	1:C:180:THR:HG22	1.54	0.90
2:G:18:LEU:HD23	2:G:202:LEU:HD22	1.50	0.89
1:C:70:GLN:O	1:C:71:PHE:HB3	1.71	0.89
1:C:73:LYS:CE	1:C:77:GLN:CB	2.26	0.89
1:D:7:LEU:HD23	1:D:7:LEU:H	1.36	0.88
1:D:157:ASN:H	1:D:321:GLN:HE22	1.17	0.88
1:C:135:SER:HA	1:C:303:PHE:HE2	1.35	0.88
1:A:109:LYS:HZ3	1:A:123:GLU:HG3	1.35	0.88
1:C:73:LYS:HZ3	1:C:77:GLN:HG3	1.39	0.87
1:D:299:GLN:HG2	1:D:300:GLU:N	1.87	0.87
1:A:73:LYS:HE2	1:A:77:GLN:HG3	1.56	0.87
1:B:58:SER:CB	1:B:267:ASP:CB	2.41	0.87
2:G:27:GLU:N	2:G:28:PRO:HD2	1.89	0.87
1:A:73:LYS:CE	1:A:77:GLN:HB2	2.04	0.86
1:B:173:CYS:HB3	1:B:180:THR:HG22	1.56	0.86
1:C:73:LYS:HE2	1:C:77:GLN:HB2	0.88	0.86
2:H:40:THR:HG22	2:H:44:LEU:H	1.41	0.86
1:D:71:PHE:N	1:D:71:PHE:CD1	2.42	0.84
2:G:50:LYS:HB3	2:G:51:PRO:HD2	1.59	0.84
1:B:71:PHE:N	1:B:71:PHE:CD1	2.45	0.84
1:A:173:CYS:HB3	1:A:180:THR:HG22	1.59	0.83
1:A:73:LYS:CE	1:A:77:GLN:HG3	2.08	0.82
2:E:40:THR:HG22	2:E:44:LEU:H	1.45	0.82
1:A:266:MET:HG2	1:A:269:TYR:CE1	2.15	0.81
1:A:71:PHE:HE1	1:A:79:ILE:CD1	1.72	0.81
1:C:157:ASN:N	1:C:321:GLN:HE22	1.79	0.81
2:G:112:ARG:HG3	2:G:150:ALA:HA	1.62	0.80
2:E:20:GLU:HB2	2:E:26:VAL:HG21	1.62	0.80
2:G:181:MET:HE1	2:G:199:VAL:HG22	1.63	0.78
1:B:54:THR:O	1:B:55:ALA:C	2.26	0.78
2:H:1:MET:HE1	2:H:39:LYS:HE3	1.64	0.78
1:C:12:SER:HB2	1:D:45:PRO:HB2	1.64	0.78
1:B:58:SER:HB3	1:B:267:ASP:HB2	0.80	0.78
2:F:145:PRO:HB3	2:F:151:ASP:O	1.82	0.78
2:G:36:LEU:HD13	2:H:143:LEU:HD12	1.66	0.77
2:H:65:ILE:HD13	2:H:181:MET:HE2	1.65	0.77
1:D:70:GLN:C	1:D:71:PHE:CD1	2.63	0.77
1:B:70:GLN:C	1:B:71:PHE:CD1	2.62	0.77
2:E:86:TYR:HE1	2:E:178:SER:HB3	1.50	0.77
2:H:93:ILE:HG22	2:H:176:ASP:HA	1.68	0.76
1:C:73:LYS:CD	1:C:77:GLN:HB2	2.15	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:112:ARG:HG3	2:F:150:ALA:HA	1.67	0.76
1:B:73:LYS:HD3	1:B:77:GLN:HB2	1.67	0.76
1:C:73:LYS:HG3	1:C:77:GLN:H	1.51	0.76
2:F:51:PRO:HG2	2:F:52:ASN:H	1.50	0.76
2:G:113:ILE:HG21	2:G:154:VAL:HG23	1.66	0.75
1:B:54:THR:O	1:B:56:LEU:N	2.18	0.75
1:C:73:LYS:CG	1:C:77:GLN:H	2.00	0.75
2:G:195:ILE:O	2:G:199:VAL:HG23	1.85	0.75
2:F:31:ASN:OD1	2:F:35:GLU:HG3	1.87	0.75
1:B:157:ASN:N	1:B:321:GLN:HE22	1.84	0.74
1:A:71:PHE:CZ	1:A:79:ILE:CD1	2.70	0.74
2:F:195:ILE:O	2:F:199:VAL:HG23	1.86	0.74
2:F:113:ILE:HG21	2:F:154:VAL:HG23	1.69	0.74
1:D:73:LYS:NZ	1:D:75:GLU:HB3	2.01	0.74
2:G:27:GLU:H	2:G:28:PRO:HD2	1.50	0.74
2:F:14:GLN:HB3	2:F:89:ILE:HD12	1.70	0.73
1:C:73:LYS:NZ	1:C:77:GLN:CG	2.49	0.73
1:D:7:LEU:HD23	1:D:7:LEU:N	2.03	0.73
2:F:59:GLU:HG3	2:F:78:PHE:CE1	2.23	0.73
1:B:73:LYS:HZ2	1:B:77:GLN:HG3	1.54	0.73
2:E:36:LEU:HD13	2:F:143:LEU:CD1	2.17	0.73
1:A:12:SER:HB2	1:B:45:PRO:HB2	1.71	0.72
2:H:193:ASP:OD1	2:H:194:LYS:HG3	1.89	0.72
1:B:16:THR:CG2	2:H:109:ARG:HB2	2.19	0.72
1:A:56:LEU:HD22	1:A:297:ASN:HD22	1.53	0.72
1:D:83:TYR:CE1	1:D:112:ARG:HG2	2.25	0.72
2:H:86:TYR:HE1	2:H:178:SER:HB3	1.54	0.72
2:E:86:TYR:HE1	2:E:178:SER:CB	2.02	0.72
1:B:282:ASN:HA	2:G:186:SER:HB2	1.70	0.71
1:D:98:ASP:O	1:D:100:THR:HG22	1.89	0.71
1:A:157:ASN:N	1:A:321:GLN:HE22	1.87	0.71
1:A:73:LYS:NZ	1:A:77:GLN:HG3	2.05	0.71
1:D:265:LYS:CE	1:D:266:MET:HE2	2.21	0.71
2:G:115:SER:HB2	2:G:154:VAL:O	1.89	0.71
2:G:149:LEU:HD22	2:H:57:PHE:HE2	1.56	0.71
1:B:73:LYS:NZ	1:B:75:GLU:HB2	2.06	0.71
1:B:58:SER:HB3	1:B:267:ASP:HB3	1.68	0.70
1:B:98:ASP:O	1:B:100:THR:HG22	1.90	0.70
2:G:86:TYR:CE1	2:G:178:SER:HB3	2.26	0.70
1:D:299:GLN:CG	1:D:300:GLU:H	1.93	0.70
1:B:39:TYR:CD2	1:B:103:ARG:HB3	2.26	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:134:GLU:O	1:C:303:PHE:CG	2.44	0.70
2:E:55:ILE:HD11	2:E:73:LEU:HD23	1.71	0.70
1:D:56:LEU:O	1:D:63:PHE:HB2	1.92	0.70
2:G:18:LEU:CD2	2:G:202:LEU:HD22	2.21	0.70
1:B:71:PHE:N	1:B:71:PHE:HD1	1.86	0.70
2:E:57:PHE:CE2	2:F:149:LEU:HD22	2.28	0.69
1:C:73:LYS:HE3	1:C:75:GLU:HB3	1.74	0.69
2:H:86:TYR:HE1	2:H:178:SER:CB	2.04	0.69
2:E:59:GLU:HG3	2:E:78:PHE:CE1	2.28	0.69
1:B:59:ASN:ND2	1:B:184:THR:HG21	2.06	0.69
2:H:24:TYR:O	2:H:26:VAL:HG23	1.93	0.69
1:A:114:GLU:O	1:A:115:LYS:C	2.36	0.69
1:D:173:CYS:CB	1:D:180:THR:HG22	2.16	0.68
1:B:16:THR:HG21	2:H:109:ARG:HB2	1.74	0.68
2:F:93:ILE:HD12	2:F:173:LYS:HG3	1.75	0.68
1:D:190:LYS:HG3	2:F:82:TYR:CE2	2.29	0.68
1:D:292:ASP:HB3	1:D:302:ALA:O	1.93	0.68
1:A:73:LYS:CE	1:A:75:GLU:HB3	2.23	0.68
1:B:206:LYS:HA	1:B:209:ARG:NH1	2.09	0.68
1:C:39:TYR:CD2	1:C:103:ARG:HB3	2.29	0.68
1:D:133:GLY:O	1:D:303:PHE:HE1	1.77	0.68
1:A:39:TYR:CD2	1:A:103:ARG:HB3	2.28	0.68
1:C:73:LYS:HE2	1:C:77:GLN:CA	2.23	0.68
2:G:142:GLU:O	2:G:145:PRO:HD2	1.94	0.68
2:G:86:TYR:HE1	2:G:178:SER:HB3	1.57	0.68
1:A:52:LEU:O	1:A:56:LEU:HG	1.95	0.67
1:C:214:GLU:HG2	1:C:227:LEU:HD11	1.76	0.67
2:F:97:ALA:O	2:F:152:ALA:HB1	1.94	0.67
2:F:58:LEU:HD22	2:F:182:ILE:HD12	1.76	0.67
1:D:157:ASN:N	1:D:321:GLN:HE22	1.92	0.67
1:D:290:ARG:HG3	1:D:304:ALA:O	1.95	0.67
2:G:23:ASP:HB2	2:G:201:ARG:HH21	1.60	0.67
2:G:193:ASP:OD1	2:G:194:LYS:HG2	1.95	0.66
1:C:135:SER:CA	1:C:303:PHE:CE2	2.76	0.66
1:C:199:ILE:HG21	1:C:209:ARG:HG3	1.76	0.66
2:F:181:MET:HE1	2:F:199:VAL:HG22	1.77	0.66
1:D:73:LYS:HZ3	1:D:75:GLU:HB3	1.58	0.66
2:H:124:TYR:CD1	2:H:174:ILE:HD12	2.31	0.66
2:F:188:PHE:CZ	2:F:192:LYS:HD3	2.31	0.66
2:G:87:LEU:HA	2:G:206:GLN:HE22	1.61	0.66
1:C:90:VAL:HG13	1:C:295:LEU:HD22	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:111:LYS:HD2	2:E:130:GLU:OE2	1.96	0.65
1:B:90:VAL:HG13	1:B:295:LEU:HD22	1.78	0.65
1:C:45:PRO:HB2	1:D:12:SER:HB2	1.78	0.65
2:G:8:LYS:HG2	2:G:48:PHE:HB3	1.77	0.65
2:F:58:LEU:HD22	2:F:182:ILE:CD1	2.25	0.65
1:B:118:LYS:C	1:B:120:ARG:H	2.04	0.65
2:E:57:PHE:HE2	2:F:149:LEU:HD22	1.60	0.65
2:E:58:LEU:HD13	2:E:182:ILE:HG13	1.78	0.65
2:F:191:LYS:O	2:F:195:ILE:HG12	1.97	0.64
1:A:220:GLU:OE2	1:A:223:ARG:HG3	1.97	0.64
1:A:103:ARG:HG2	1:A:103:ARG:HH11	1.62	0.64
1:D:6:TYR:HD1	1:D:7:LEU:H	1.46	0.64
1:D:286:LEU:HD23	1:D:287:SER:N	2.13	0.64
1:B:58:SER:CB	1:B:267:ASP:HB3	2.25	0.64
1:D:247:SER:O	1:D:251:SER:HB3	1.98	0.64
2:E:195:ILE:O	2:E:199:VAL:HG23	1.98	0.64
2:F:84:LEU:HD12	2:F:183:VAL:HG21	1.79	0.64
1:D:186:LEU:HD23	1:D:191:ASP:HB3	1.78	0.63
2:F:27:GLU:N	2:F:28:PRO:CD	2.60	0.63
2:E:124:TYR:CD1	2:E:174:ILE:HD12	2.34	0.63
2:F:142:GLU:O	2:F:145:PRO:HD2	1.99	0.63
1:A:73:LYS:HE3	1:A:75:GLU:CB	2.26	0.63
1:A:252:MET:HG2	1:A:253:ILE:N	2.13	0.63
1:B:109:LYS:HD3	1:B:123:GLU:HG2	1.81	0.63
2:F:36:LEU:O	2:F:47:ILE:HA	1.99	0.63
1:A:295:LEU:HG	1:A:302:ALA:HB3	1.80	0.63
1:C:73:LYS:CE	1:C:77:GLN:HG3	2.20	0.63
1:A:73:LYS:HG2	1:A:77:GLN:N	2.05	0.63
2:F:27:GLU:N	2:F:28:PRO:HD2	2.14	0.62
1:C:187:LEU:HD23	1:C:216:PHE:CE1	2.34	0.62
1:B:11:GLU:HA	1:B:122:THR:HG21	1.80	0.62
1:D:62:THR:OG1	1:D:266:MET:HE1	1.99	0.62
2:G:27:GLU:N	2:G:28:PRO:CD	2.61	0.62
2:F:55:ILE:HD11	2:F:72:THR:HG22	1.80	0.62
1:D:124:ASN:HA	1:D:312:ASP:OD2	1.99	0.62
2:G:94:PHE:HB3	2:G:174:ILE:HB	1.82	0.62
2:G:96:LEU:HD22	2:G:124:TYR:HE2	1.64	0.62
1:C:129:ILE:HD11	1:C:307:PHE:CE2	2.35	0.62
2:H:92:CYS:HB2	2:H:177:ILE:HB	1.82	0.62
1:C:286:LEU:C	1:C:286:LEU:HD23	2.25	0.61
1:C:303:PHE:HD1	1:C:303:PHE:H	0.76	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:GLU:HB3	1:A:223:ARG:HB2	1.82	0.61
2:H:86:TYR:CE2	2:H:88:LYS:HG2	2.35	0.61
2:H:94:PHE:CD1	2:H:177:ILE:HD11	2.36	0.61
1:B:118:LYS:O	1:B:120:ARG:N	2.34	0.61
1:D:73:LYS:HD3	1:D:77:GLN:HB2	1.82	0.61
1:D:303:PHE:CD1	1:D:303:PHE:N	2.69	0.61
2:F:84:LEU:CD1	2:F:183:VAL:HG21	2.31	0.61
1:A:16:THR:HG23	1:A:19:GLN:OE1	2.01	0.60
1:D:265:LYS:HE2	1:D:266:MET:HE2	1.81	0.60
1:D:282:ASN:HA	2:F:186:SER:HB2	1.83	0.60
1:B:73:LYS:NZ	1:B:77:GLN:HG3	2.16	0.60
2:F:145:PRO:HA	2:F:150:ALA:O	2.01	0.60
2:G:149:LEU:HD22	2:H:57:PHE:CE2	2.34	0.60
2:E:24:TYR:CE2	2:E:44:LEU:HD11	2.36	0.60
2:G:93:ILE:HD12	2:G:173:LYS:HG3	1.83	0.60
1:B:262:MET:HG2	1:B:273:MET:HE3	1.82	0.60
1:C:73:LYS:HG3	1:C:76:GLY:H	1.67	0.60
1:C:91:ARG:O	1:C:94:SER:HB2	2.01	0.59
1:C:73:LYS:HZ3	1:C:77:GLN:CG	2.11	0.59
1:C:206:LYS:O	1:C:206:LYS:HD3	2.02	0.59
2:F:134:ILE:N	2:F:134:ILE:HD12	2.18	0.59
2:G:145:PRO:HB3	2:G:151:ASP:O	2.01	0.59
2:G:7:THR:HG22	2:G:51:PRO:HA	1.83	0.59
1:C:266:MET:HG2	1:C:269:TYR:CE1	2.38	0.59
1:D:205:SER:O	1:D:209:ARG:CG	2.46	0.59
2:F:193:ASP:OD1	2:F:194:LYS:HG2	2.02	0.59
2:G:95:ALA:HB3	2:G:157:VAL:CG2	2.33	0.59
1:D:272:LEU:HD12	1:D:273:MET:H	1.66	0.59
1:D:199:ILE:HD12	1:D:213:LYS:NZ	2.18	0.59
2:G:134:ILE:HD12	2:G:134:ILE:N	2.17	0.59
1:C:136:ALA:N	1:C:303:PHE:HD2	2.00	0.59
2:G:75:GLU:OE2	2:G:119:ARG:HB2	2.03	0.59
1:A:73:LYS:CG	1:A:77:GLN:H	2.08	0.58
1:C:214:GLU:HG2	1:C:227:LEU:CD1	2.32	0.58
2:H:86:TYR:CE1	2:H:178:SER:OG	2.55	0.58
1:A:265:LYS:HB3	1:A:266:MET:SD	2.43	0.58
1:D:167:LYS:HB2	1:D:271:ASP:OD2	2.02	0.58
1:D:214:GLU:HG2	1:D:227:LEU:HD11	1.84	0.58
1:A:195:LEU:O	1:A:198:PHE:HB3	2.03	0.58
1:B:129:ILE:HD13	1:B:146:LEU:HD13	1.84	0.58
1:D:85:PHE:O	1:D:88:PRO:HG2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:25:ASP:HB3	2:E:42:ASP:OD1	2.04	0.58
2:F:8:LYS:HG3	2:F:48:PHE:HB3	1.85	0.58
1:A:7:LEU:HD12	1:A:7:LEU:H	1.68	0.58
1:A:200:GLU:O	1:A:200:GLU:HG3	2.03	0.58
1:B:214:GLU:HG2	1:B:227:LEU:CD1	2.33	0.58
1:D:190:LYS:HG3	2:F:82:TYR:CD2	2.38	0.58
1:D:31:ARG:HH11	1:D:31:ARG:HG3	1.69	0.58
1:D:265:LYS:HE2	1:D:266:MET:CE	2.34	0.58
2:H:58:LEU:HD13	2:H:182:ILE:HG13	1.84	0.57
2:F:7:THR:HG22	2:F:51:PRO:HA	1.87	0.57
2:F:121:THR:HG23	2:F:154:VAL:HG21	1.84	0.57
1:A:289:GLY:O	1:A:305:ILE:HG13	2.04	0.57
1:D:98:ASP:O	1:D:100:THR:N	2.37	0.57
2:F:50:LYS:O	2:F:54:VAL:HG23	2.04	0.57
2:F:96:LEU:HD22	2:F:124:TYR:HE2	1.68	0.57
2:H:96:LEU:HD12	2:H:153:ILE:O	2.05	0.57
1:D:214:GLU:HG2	1:D:227:LEU:CD1	2.35	0.57
1:C:173:CYS:CB	1:C:180:THR:HG22	2.32	0.57
2:G:111:LYS:HE2	2:G:130:GLU:OE2	2.05	0.56
1:B:262:MET:CG	1:B:273:MET:HE3	2.35	0.56
1:B:286:LEU:HD23	1:B:286:LEU:C	2.29	0.56
2:G:55:ILE:HD11	2:G:72:THR:HG22	1.87	0.56
1:B:129:ILE:CD1	1:B:146:LEU:HD13	2.34	0.56
1:D:265:LYS:NZ	1:D:266:MET:HE2	2.20	0.56
2:F:94:PHE:HB3	2:F:174:ILE:HB	1.87	0.56
2:G:91:GLN:O	2:G:91:GLN:HG2	2.05	0.56
2:H:7:THR:HG22	2:H:51:PRO:HA	1.86	0.56
1:B:103:ARG:NH1	1:B:142:GLU:OE2	2.39	0.56
2:E:65:ILE:HD13	2:E:181:MET:CE	2.35	0.56
2:G:5:ALA:HB3	2:G:54:VAL:HG13	1.87	0.56
2:H:7:THR:HA	2:H:49:GLY:O	2.05	0.56
2:H:108:GLN:HA	2:H:108:GLN:OE1	2.06	0.56
1:A:299:GLN:HG3	1:A:300:GLU:N	2.20	0.56
1:B:224:LEU:O	1:B:228:VAL:HG23	2.06	0.56
1:C:206:LYS:HD3	1:C:206:LYS:C	2.31	0.56
2:F:51:PRO:HG2	2:F:52:ASN:ND2	2.21	0.56
2:E:193:ASP:OD1	2:E:194:LYS:HG3	2.07	0.55
2:G:143:LEU:HA	2:G:146:VAL:HB	1.87	0.55
2:H:87:LEU:C	2:H:89:ILE:H	2.13	0.55
1:B:73:LYS:HZ1	1:B:75:GLU:HB2	1.71	0.55
1:C:12:SER:HB2	1:D:45:PRO:CB	2.34	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:LEU:O	1:B:145:SER:HB2	2.06	0.55
1:C:167:LYS:NZ	1:C:235:VAL:HG13	2.21	0.55
2:E:143:LEU:O	2:E:144:GLY:C	2.49	0.55
2:E:84:LEU:HD12	2:E:183:VAL:HG21	1.87	0.55
1:A:45:PRO:HB2	1:B:12:SER:HB2	1.88	0.55
1:C:49:TYR:O	1:C:50:THR:C	2.50	0.55
2:E:65:ILE:HG22	2:E:66:GLY:N	2.22	0.55
2:G:25:ASP:OD2	2:G:41:LYS:HG3	2.07	0.55
2:H:22:ALA:O	2:H:23:ASP:HB2	2.06	0.55
2:H:40:THR:CG2	2:H:44:LEU:H	2.16	0.55
1:A:233:ASP:O	1:A:237:ILE:HG23	2.06	0.55
1:D:204:PHE:O	1:D:209:ARG:NE	2.40	0.55
2:H:86:TYR:CE1	2:H:178:SER:HB3	2.39	0.55
2:F:86:TYR:CE1	2:F:178:SER:HB3	2.42	0.55
2:G:57:PHE:O	2:G:62:ILE:HB	2.06	0.55
1:C:157:ASN:N	1:C:321:GLN:NE2	2.39	0.55
2:E:4:ILE:HG22	2:E:5:ALA:N	2.22	0.55
2:G:27:GLU:OE1	2:G:39:LYS:O	2.24	0.55
2:E:20:GLU:C	2:E:22:ALA:H	2.15	0.55
1:A:73:LYS:HD2	1:B:116:ARG:HH12	1.72	0.54
1:B:85:PHE:O	1:B:89:LEU:HG	2.07	0.54
1:C:52:LEU:C	1:C:54:THR:H	2.14	0.54
1:C:268:TYR:CE1	1:C:294:LEU:HD11	2.43	0.54
1:D:6:TYR:HB2	1:D:7:LEU:HD23	1.89	0.54
1:D:173:CYS:O	1:D:178:GLY:HA2	2.07	0.54
1:A:90:VAL:HG13	1:A:295:LEU:HD22	1.88	0.54
2:H:4:ILE:HG22	2:H:5:ALA:N	2.22	0.54
1:A:53:TYR:O	1:A:54:THR:C	2.51	0.54
2:F:93:ILE:HG21	2:F:173:LYS:HE3	1.90	0.54
2:H:1:MET:HE1	2:H:39:LYS:CE	2.34	0.54
2:H:86:TYR:CE1	2:H:178:SER:CB	2.89	0.54
2:H:95:ALA:HA	2:H:174:ILE:HG12	1.88	0.54
2:F:7:THR:CG2	2:F:68:VAL:HG12	2.38	0.54
2:G:87:LEU:CA	2:G:206:GLN:HE22	2.21	0.54
1:C:103:ARG:NH1	1:C:142:GLU:OE2	2.41	0.54
2:H:145:PRO:HA	2:H:150:ALA:O	2.08	0.54
1:A:81:LEU:O	1:A:82:ARG:C	2.51	0.54
1:D:186:LEU:CD2	1:D:191:ASP:HB3	2.37	0.54
1:B:81:LEU:O	1:B:82:ARG:C	2.50	0.54
2:H:85:LEU:HD12	2:H:86:TYR:H	1.73	0.54
2:E:85:LEU:HB3	2:E:181:MET:HB3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:139:GLY:O	2:G:141:VAL:N	2.40	0.53
2:H:68:VAL:HG21	2:H:73:LEU:HD21	1.89	0.53
1:A:206:LYS:HD3	1:A:206:LYS:C	2.32	0.53
2:G:65:ILE:HG22	2:G:66:GLY:N	2.23	0.53
2:G:95:ALA:HB3	2:G:157:VAL:HG23	1.89	0.53
1:D:156:LEU:HA	1:D:321:GLN:HE22	1.72	0.53
1:D:71:PHE:N	1:D:71:PHE:HD1	2.03	0.53
1:A:64:ASN:HB2	1:A:66:GLU:HG3	1.90	0.53
2:H:51:PRO:HB2	2:H:72:THR:HG21	1.90	0.53
1:A:129:ILE:CD1	1:A:146:LEU:HD13	2.38	0.53
1:B:74:HIS:CG	1:B:75:GLU:N	2.76	0.53
1:B:247:SER:O	1:B:251:SER:HB3	2.08	0.53
1:C:45:PRO:CB	1:D:12:SER:HB2	2.38	0.53
2:E:41:LYS:C	2:E:43:ASP:H	2.17	0.53
2:F:91:GLN:HG3	2:F:91:GLN:O	2.08	0.53
2:G:191:LYS:O	2:G:195:ILE:HG12	2.08	0.53
1:B:131:LEU:HB2	1:B:143:ILE:HD11	1.91	0.53
1:C:73:LYS:NZ	1:C:77:GLN:HB2	2.21	0.53
2:E:87:LEU:C	2:E:89:ILE:H	2.17	0.53
2:H:87:LEU:N	2:H:87:LEU:HD23	2.24	0.53
1:A:71:PHE:HE1	1:A:79:ILE:HD11	0.80	0.52
1:A:73:LYS:CD	1:A:77:GLN:HB2	2.38	0.52
1:C:27:GLU:HG2	1:C:127:ILE:HD11	1.90	0.52
1:D:224:LEU:O	1:D:228:VAL:HG23	2.08	0.52
2:E:86:TYR:CE2	2:E:88:LYS:HG2	2.44	0.52
2:H:1:MET:O	2:H:2:ILE:HD13	2.10	0.52
1:B:59:ASN:HD21	1:B:184:THR:HG21	1.73	0.52
1:D:27:GLU:OE2	1:D:107:PHE:HB3	2.09	0.52
2:E:65:ILE:HD13	2:E:181:MET:HE2	1.91	0.52
2:G:70:LYS:HE3	2:G:74:ASP:OD1	2.09	0.52
1:D:73:LYS:HZ2	1:D:77:GLN:HG3	1.74	0.52
2:F:16:THR:HG22	2:F:28:PRO:HG3	1.92	0.52
1:B:286:LEU:HD23	1:B:287:SER:N	2.25	0.52
1:B:214:GLU:HG2	1:B:227:LEU:HD11	1.91	0.52
1:B:227:LEU:O	1:B:231:THR:HG23	2.09	0.52
2:G:125:PHE:CD1	2:G:132:ILE:HD13	2.44	0.52
1:A:53:TYR:O	1:A:57:GLU:HG2	2.09	0.52
1:A:71:PHE:CE1	1:A:79:ILE:CG1	2.92	0.52
1:A:207:GLU:CD	1:A:207:GLU:H	2.18	0.52
1:C:247:SER:O	1:C:251:SER:HB3	2.10	0.52
1:D:233:ASP:O	1:D:237:ILE:HG12	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:207:GLU:CD	1:C:207:GLU:N	2.68	0.52
2:E:94:PHE:CD1	2:E:177:ILE:HD11	2.45	0.52
2:H:86:TYR:HE1	2:H:178:SER:OG	1.91	0.52
2:H:139:GLY:O	2:H:141:VAL:N	2.43	0.52
1:D:64:ASN:ND2	1:D:66:GLU:HB2	2.25	0.52
2:H:93:ILE:HG13	2:H:157:VAL:O	2.09	0.52
2:G:7:THR:CG2	2:G:51:PRO:HA	2.39	0.51
1:A:71:PHE:CD1	1:A:71:PHE:C	2.88	0.51
1:A:276:ALA:HB3	1:A:286:LEU:HB3	1.92	0.51
1:B:8:LEU:HD11	1:B:14:GLU:CD	2.35	0.51
1:B:204:PHE:CD2	1:B:208:LEU:HD23	2.46	0.51
1:B:221:LEU:HD23	1:B:221:LEU:O	2.10	0.51
1:B:10:GLU:HB2	1:B:116:ARG:HH21	1.74	0.51
1:A:21:LYS:HE2	1:B:40:GLN:OE1	2.11	0.51
1:C:71:PHE:O	1:C:79:ILE:N	2.37	0.51
1:C:103:ARG:HG2	1:C:103:ARG:HH11	1.75	0.51
1:C:124:ASN:HA	1:C:312:ASP:OD2	2.10	0.51
1:D:70:GLN:C	1:D:71:PHE:CG	2.89	0.51
1:D:129:ILE:HD11	1:D:307:PHE:CE2	2.44	0.51
1:D:175:LEU:HD11	1:D:233:ASP:OD2	2.11	0.51
2:H:12:GLN:HG3	2:H:48:PHE:HE2	1.76	0.51
2:H:41:LYS:C	2:H:43:ASP:H	2.18	0.51
1:D:97:LYS:HD2	1:D:97:LYS:O	2.11	0.51
2:F:98:SER:HB2	2:F:152:ALA:CB	2.41	0.51
1:B:90:VAL:HG22	1:B:132:PHE:CZ	2.46	0.51
4:B:329:PO4:O1	2:G:189:LYS:NZ	2.43	0.51
1:D:220:GLU:OE2	1:D:223:ARG:HB2	2.11	0.51
2:G:51:PRO:HG2	2:G:52:ASN:H	1.75	0.51
2:G:112:ARG:HA	2:G:133:GLU:O	2.10	0.51
2:H:82:TYR:CE2	2:H:185:LYS:HE2	2.46	0.51
2:H:113:ILE:HD12	2:H:113:ILE:N	2.26	0.51
1:C:135:SER:C	1:C:303:PHE:CD2	2.89	0.51
1:B:299:GLN:HG3	1:B:300:GLU:N	2.25	0.50
1:C:48:GLU:OE2	1:C:91:ARG:NH2	2.42	0.50
1:D:39:TYR:CD2	1:D:103:ARG:HB3	2.46	0.50
2:F:134:ILE:HD12	2:F:134:ILE:H	1.75	0.50
1:D:10:GLU:OE2	2:E:122:LYS:HE3	2.10	0.50
1:B:162:GLU:CD	2:G:189:LYS:HZ2	2.19	0.50
1:C:289:GLY:O	1:C:305:ILE:HG13	2.11	0.50
2:E:86:TYR:CE1	2:E:178:SER:HB3	2.39	0.50
2:E:53:ASP:OD2	2:F:137:LEU:HD22	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:THR:OG1	1:B:266:MET:SD	2.70	0.50
2:F:113:ILE:N	2:F:113:ILE:HD12	2.26	0.50
1:A:225:GLU:O	1:A:229:THR:HG23	2.12	0.50
1:C:73:LYS:HE2	1:C:77:GLN:N	2.26	0.50
1:D:16:THR:HG23	1:D:19:GLN:OE1	2.12	0.50
2:E:95:ALA:HA	2:E:174:ILE:HG12	1.94	0.50
1:B:93:TYR:CD2	1:B:295:LEU:HD11	2.47	0.50
1:B:187:LEU:HD23	1:B:216:PHE:CE1	2.46	0.50
1:B:199:ILE:HG21	1:B:209:ARG:HG3	1.93	0.50
2:E:141:VAL:HG23	2:E:153:ILE:HD12	1.94	0.50
2:E:143:LEU:CD1	2:F:36:LEU:HD13	2.42	0.50
2:H:111:LYS:CD	2:H:130:GLU:OE2	2.49	0.50
2:E:92:CYS:C	2:E:93:ILE:HG23	2.37	0.49
2:H:20:GLU:C	2:H:22:ALA:H	2.21	0.49
1:C:71:PHE:O	1:C:78:SER:HA	2.11	0.49
2:G:25:ASP:N	2:G:42:ASP:OD2	2.38	0.49
1:B:156:LEU:HA	1:B:321:GLN:HE22	1.77	0.49
1:D:81:LEU:O	1:D:82:ARG:C	2.56	0.49
1:D:131:LEU:HB2	1:D:143:ILE:HD11	1.94	0.49
2:G:159:THR:OG1	2:G:161:ASN:ND2	2.46	0.49
1:C:207:GLU:CD	1:C:207:GLU:H	2.19	0.49
2:E:177:ILE:HG22	2:E:178:SER:N	2.28	0.49
1:B:73:LYS:HZ1	1:B:75:GLU:CB	2.26	0.49
1:B:96:ILE:HG22	1:B:98:ASP:H	1.78	0.49
1:B:157:ASN:N	1:B:321:GLN:NE2	2.48	0.49
1:A:156:LEU:HA	1:A:321:GLN:HE22	1.76	0.49
1:D:26:ILE:O	1:D:30:LEU:HG	2.12	0.49
1:D:109:LYS:HE2	1:D:123:GLU:HB3	1.95	0.49
2:E:6:ILE:HD13	2:E:15:VAL:HG11	1.95	0.49
2:F:51:PRO:HG2	2:F:52:ASN:N	2.24	0.49
1:D:53:TYR:C	1:D:55:ALA:H	2.20	0.49
2:E:7:THR:HG22	2:E:51:PRO:HA	1.94	0.49
2:F:1:MET:HB2	2:F:43:ASP:O	2.12	0.48
2:F:143:LEU:HA	2:F:146:VAL:HB	1.94	0.48
2:H:92:CYS:O	2:H:93:ILE:HG23	2.12	0.48
1:D:55:ALA:C	1:D:56:LEU:HD12	2.38	0.48
2:E:22:ALA:O	2:E:23:ASP:HB2	2.13	0.48
1:C:136:ALA:N	1:C:303:PHE:CD2	2.81	0.48
1:D:154:LEU:HD13	1:D:314:ILE:HD13	1.95	0.48
1:D:199:ILE:HD12	1:D:213:LYS:HZ3	1.78	0.48
1:D:276:ALA:O	1:D:285:ILE:HG12	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:292:ASP:CG	1:D:303:PHE:HA	2.36	0.48
2:E:1:MET:HE1	2:E:39:LYS:HE3	1.94	0.48
2:E:92:CYS:O	2:E:93:ILE:CG2	2.61	0.48
2:H:71:ASP:HB2	2:H:94:PHE:CZ	2.49	0.48
1:B:254:LYS:HG3	1:B:255:PRO:HD2	1.95	0.48
1:D:295:LEU:HG	1:D:302:ALA:HB3	1.96	0.48
2:E:145:PRO:HD3	2:E:153:ILE:CG2	2.44	0.48
1:A:26:ILE:HG21	1:A:311:MET:HE1	1.95	0.48
1:A:109:LYS:HZ2	1:A:123:GLU:HG3	1.75	0.48
2:G:7:THR:HA	2:G:49:GLY:O	2.13	0.48
1:A:224:LEU:HD22	1:A:260:LEU:HD12	1.95	0.48
1:B:58:SER:OG	1:B:267:ASP:HB3	2.12	0.48
1:C:156:LEU:HA	1:C:321:GLN:HE22	1.78	0.48
1:D:227:LEU:O	1:D:231:THR:HG23	2.13	0.48
2:G:23:ASP:HB2	2:G:201:ARG:NH2	2.26	0.48
2:E:143:LEU:HD11	2:F:36:LEU:HB2	1.96	0.48
2:F:98:SER:HB2	2:F:152:ALA:HB2	1.95	0.48
2:F:158:GLU:HB3	4:F:209:PO4:O3	2.14	0.48
2:G:137:LEU:HD22	2:H:53:ASP:OD2	2.14	0.48
1:B:98:ASP:O	1:B:100:THR:N	2.46	0.48
1:D:97:LYS:HD2	1:D:97:LYS:C	2.39	0.48
2:G:164:SER:C	2:G:166:ASN:H	2.21	0.48
1:A:124:ASN:HA	1:A:312:ASP:OD2	2.14	0.48
1:B:93:TYR:HD2	1:B:295:LEU:HD11	1.79	0.48
2:G:26:VAL:HG12	2:G:29:ILE:HG12	1.96	0.48
1:A:53:TYR:O	1:A:55:ALA:N	2.47	0.47
1:A:72:ILE:HG22	1:A:73:LYS:N	2.29	0.47
1:C:162:GLU:OE1	2:H:189:LYS:HE3	2.13	0.47
1:A:160:VAL:HB	1:A:257:ILE:HD12	1.96	0.47
2:F:86:TYR:HE1	2:F:178:SER:HB3	1.79	0.47
2:G:121:THR:HG23	2:G:154:VAL:HG21	1.97	0.47
1:B:160:VAL:HG13	2:G:190:PHE:CE2	2.49	0.47
2:G:8:LYS:HG3	2:G:49:GLY:CA	2.44	0.47
2:H:124:TYR:CG	2:H:174:ILE:HD12	2.49	0.47
1:B:189:LYS:O	1:B:190:LYS:C	2.57	0.47
1:C:71:PHE:CD1	1:C:71:PHE:C	2.91	0.47
1:C:71:PHE:HD1	1:C:72:ILE:O	1.98	0.47
2:E:20:GLU:CB	2:E:26:VAL:HG21	2.40	0.47
2:F:143:LEU:H	2:F:143:LEU:HD12	1.80	0.47
1:D:22:SER:O	1:D:26:ILE:HG13	2.14	0.47
2:G:141:VAL:HG12	2:G:141:VAL:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:86:TYR:CD2	2:H:88:LYS:HG2	2.50	0.47
2:E:36:LEU:O	2:E:47:ILE:HA	2.14	0.47
2:H:50:LYS:HB3	2:H:51:PRO:HD2	1.97	0.47
1:A:71:PHE:CZ	1:A:79:ILE:HD12	2.48	0.47
1:B:262:MET:SD	1:B:273:MET:HG3	2.54	0.47
1:C:167:LYS:HZ2	1:C:235:VAL:HG13	1.79	0.47
1:D:7:LEU:N	1:D:7:LEU:CD2	2.73	0.47
1:D:55:ALA:O	1:D:56:LEU:HD12	2.15	0.47
1:D:110:ILE:HD12	1:D:112:ARG:HH11	1.80	0.47
2:E:36:LEU:CD1	2:F:143:LEU:HD11	2.26	0.47
2:E:86:TYR:CE1	2:E:178:SER:CB	2.92	0.47
2:F:4:ILE:HA	2:F:65:ILE:O	2.15	0.47
2:G:73:LEU:HD22	2:G:81:TYR:CZ	2.49	0.47
2:H:113:ILE:HD13	2:H:132:ILE:HB	1.95	0.47
1:A:316:LYS:HB2	1:A:316:LYS:HE3	1.77	0.47
1:C:187:LEU:CD2	1:C:216:PHE:CE1	2.97	0.47
2:H:40:THR:HG22	2:H:44:LEU:N	2.20	0.47
1:B:167:LYS:HB2	1:B:271:ASP:OD2	2.15	0.47
1:D:75:GLU:HA	1:D:75:GLU:OE1	2.14	0.47
2:E:65:ILE:HG22	2:E:66:GLY:H	1.79	0.47
2:E:86:TYR:HE1	2:E:178:SER:OG	1.98	0.47
2:E:86:TYR:CD1	2:E:180:ARG:HD3	2.50	0.47
2:E:91:GLN:HE21	2:E:91:GLN:HB2	1.58	0.47
1:A:173:CYS:O	1:A:178:GLY:HA2	2.15	0.47
2:E:42:ASP:HB2	2:E:44:LEU:HG	1.95	0.47
1:C:73:LYS:HZ1	1:C:77:GLN:HG3	1.70	0.46
1:C:123:GLU:O	1:C:124:ASN:HB2	2.14	0.46
1:D:90:VAL:HG22	1:D:132:PHE:CZ	2.50	0.46
2:E:93:ILE:HD12	2:E:95:ALA:HB2	1.95	0.46
2:F:109:ARG:HH22	2:F:112:ARG:HD3	1.81	0.46
2:H:195:ILE:O	2:H:199:VAL:HG23	2.14	0.46
1:A:214:GLU:HG2	1:A:227:LEU:HD11	1.96	0.46
2:E:143:LEU:O	2:E:146:VAL:N	2.49	0.46
1:A:11:GLU:OE1	1:B:73:LYS:HB2	2.15	0.46
1:D:195:LEU:O	1:D:198:PHE:HB3	2.15	0.46
2:F:113:ILE:HG23	2:F:153:ILE:HA	1.97	0.46
1:D:160:VAL:HG13	2:F:190:PHE:CE2	2.50	0.46
2:F:44:LEU:HD21	2:F:198:MET:HE1	1.97	0.46
1:A:62:THR:HG22	1:A:63:PHE:O	2.16	0.46
2:E:4:ILE:HG22	2:E:5:ALA:H	1.80	0.46
2:E:143:LEU:HD11	2:F:36:LEU:HD13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:THR:C	1:B:56:LEU:N	2.74	0.46
1:D:85:PHE:O	1:D:89:LEU:HG	2.16	0.46
1:B:214:GLU:OE1	1:B:223:ARG:HD3	2.16	0.46
2:G:87:LEU:HA	2:G:206:GLN:NE2	2.30	0.46
2:G:113:ILE:HD12	2:G:113:ILE:N	2.31	0.46
2:H:113:ILE:HD13	2:H:132:ILE:CD1	2.46	0.46
1:A:199:ILE:HD12	1:A:213:LYS:NZ	2.31	0.46
2:E:24:TYR:CD2	2:E:44:LEU:HD11	2.50	0.46
1:C:49:TYR:O	1:C:51:GLN:N	2.49	0.46
2:F:22:ALA:HB3	2:F:24:TYR:HD1	1.81	0.46
2:F:26:VAL:HG13	2:F:28:PRO:HD2	1.98	0.46
2:G:196:ILE:O	2:G:200:GLU:HG2	2.16	0.46
2:F:31:ASN:CG	2:F:35:GLU:HG3	2.39	0.46
2:F:113:ILE:HD13	2:F:132:ILE:CD1	2.46	0.46
2:H:54:VAL:HG11	2:H:68:VAL:HG13	1.97	0.46
1:A:45:PRO:O	1:A:82:ARG:HG3	2.16	0.45
1:D:214:GLU:O	1:D:218:THR:HG22	2.15	0.45
2:G:18:LEU:HD21	2:G:202:LEU:HB3	1.97	0.45
2:G:22:ALA:O	2:G:23:ASP:CB	2.64	0.45
1:C:73:LYS:HG2	1:C:77:GLN:H	1.80	0.45
1:C:221:LEU:O	1:C:221:LEU:HD23	2.17	0.45
1:D:304:ALA:O	1:D:305:ILE:HB	2.16	0.45
2:E:75:GLU:OE2	2:E:118:PRO:HD2	2.16	0.45
2:H:25:ASP:OD2	2:H:41:LYS:HG2	2.17	0.45
1:A:98:ASP:O	1:A:100:THR:HG22	2.16	0.45
1:D:103:ARG:HH11	1:D:103:ARG:HG2	1.81	0.45
1:A:73:LYS:CE	1:A:77:GLN:CG	2.65	0.45
2:F:98:SER:HB3	2:F:171:ILE:HD11	1.98	0.45
1:A:227:LEU:O	1:A:231:THR:HG23	2.17	0.45
1:D:158:LYS:HG2	2:F:190:PHE:CE2	2.52	0.45
2:H:145:PRO:HD3	2:H:153:ILE:CG2	2.47	0.45
1:A:43:MET:SD	1:B:20:VAL:HG13	2.56	0.45
1:A:154:LEU:HD13	1:A:314:ILE:HD13	1.99	0.45
1:A:265:LYS:HE3	1:A:275:LYS:NZ	2.31	0.45
1:C:286:LEU:HD23	1:C:287:SER:N	2.32	0.45
2:E:18:LEU:HD22	2:E:87:LEU:HD22	1.98	0.45
2:G:112:ARG:O	2:G:150:ALA:HB1	2.16	0.45
1:C:252:MET:HG2	1:C:253:ILE:H	1.81	0.45
2:E:40:THR:HG22	2:E:44:LEU:N	2.21	0.45
2:F:20:GLU:HB2	2:F:26:VAL:HG21	1.98	0.45
2:F:75:GLU:OE1	2:F:120:VAL:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:78:PHE:CE1	2:G:80:ASP:HB2	2.52	0.45
1:A:87:LEU:HA	1:A:87:LEU:HD23	1.69	0.45
1:C:49:TYR:C	1:C:51:GLN:N	2.73	0.45
2:E:7:THR:OG1	2:E:11:ILE:HB	2.17	0.45
2:G:34:ARG:O	2:G:34:ARG:HG3	2.16	0.45
1:A:7:LEU:C	1:A:8:LEU:HD12	2.42	0.45
1:A:57:GLU:OE2	1:A:57:GLU:HA	2.17	0.45
1:A:131:LEU:HB2	1:A:143:ILE:HD11	1.98	0.45
1:A:189:LYS:O	1:A:190:LYS:C	2.59	0.45
1:B:74:HIS:CG	1:B:75:GLU:H	2.35	0.45
1:B:136:ALA:O	1:B:140:GLU:HG3	2.16	0.45
2:E:87:LEU:CB	2:E:89:ILE:HG12	2.46	0.45
2:E:99:TYR:HB3	2:E:100:PRO:HD2	1.98	0.45
1:B:89:LEU:HD11	1:B:106:TYR:HD2	1.81	0.45
1:B:191:ASP:HA	2:G:83:GLU:O	2.16	0.45
1:C:252:MET:CG	1:C:253:ILE:N	2.80	0.45
2:E:11:ILE:HD12	2:E:11:ILE:N	2.32	0.45
2:F:18:LEU:HD23	2:F:202:LEU:HD22	1.97	0.45
2:G:70:LYS:HD3	2:G:180:ARG:CZ	2.46	0.45
1:A:48:GLU:HG2	1:A:52:LEU:HD23	1.99	0.44
1:C:83:TYR:CE1	1:C:112:ARG:HG2	2.51	0.44
1:C:123:GLU:HB2	1:C:312:ASP:OD1	2.18	0.44
1:C:135:SER:C	1:C:303:PHE:HD2	2.25	0.44
1:D:11:GLU:CD	1:D:11:GLU:H	2.25	0.44
2:F:3:LYS:HB2	2:F:63:VAL:HA	1.98	0.44
2:H:65:ILE:HG22	2:H:66:GLY:N	2.32	0.44
1:A:115:LYS:HG2	1:A:115:LYS:O	2.16	0.44
1:C:129:ILE:CD1	1:C:146:LEU:HD13	2.47	0.44
1:D:151:ILE:HG22	1:D:151:ILE:O	2.16	0.44
2:F:133:GLU:OE1	2:F:135:ILE:HD11	2.17	0.44
2:G:5:ALA:CB	2:G:54:VAL:HG13	2.48	0.44
2:H:47:ILE:HG22	2:H:48:PHE:N	2.31	0.44
2:H:171:ILE:O	2:H:172:GLU:HB2	2.16	0.44
1:C:228:VAL:HG12	1:C:237:ILE:HG22	1.98	0.44
1:D:305:ILE:HG12	1:D:306:GLY:N	2.31	0.44
1:A:7:LEU:O	1:A:8:LEU:HD12	2.17	0.44
1:A:39:TYR:CG	1:A:103:ARG:HB3	2.52	0.44
1:B:75:GLU:HA	1:B:75:GLU:OE1	2.18	0.44
2:G:51:PRO:HG2	2:G:52:ASN:ND2	2.32	0.44
2:G:143:LEU:HD12	2:G:143:LEU:N	2.32	0.44
2:E:40:THR:CG2	2:E:44:LEU:H	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:19:LEU:O	2:F:24:TYR:HB2	2.18	0.44
2:F:44:LEU:CD2	2:F:198:MET:HE1	2.47	0.44
2:G:36:LEU:HD22	2:H:143:LEU:HD11	1.98	0.44
1:B:16:THR:HG23	1:B:19:GLN:OE1	2.17	0.44
1:B:39:TYR:CG	1:B:103:ARG:HB3	2.53	0.44
1:C:143:ILE:HG13	1:C:305:ILE:HG23	2.00	0.44
2:F:58:LEU:CD2	2:F:182:ILE:HD12	2.48	0.44
2:F:143:LEU:HD12	2:F:143:LEU:N	2.32	0.44
2:G:139:GLY:O	2:G:141:VAL:HG23	2.17	0.44
1:A:224:LEU:O	1:A:228:VAL:HG23	2.18	0.44
1:B:7:LEU:HD11	2:H:126:ALA:HA	1.98	0.44
1:C:73:LYS:NZ	1:C:77:GLN:CB	2.74	0.44
1:C:124:ASN:CA	1:C:312:ASP:OD2	2.65	0.44
2:E:40:THR:HG21	2:E:44:LEU:HB2	1.98	0.44
2:G:95:ALA:HB3	2:G:157:VAL:HG21	2.00	0.44
2:H:85:LEU:HG	2:H:86:TYR:N	2.33	0.44
1:B:237:ILE:HG13	1:B:238:SER:N	2.32	0.44
1:D:273:MET:HA	1:D:289:GLY:HA3	1.99	0.44
2:E:27:GLU:O	2:E:27:GLU:OE1	2.36	0.44
2:E:76:ASN:OD1	2:E:77:ASP:N	2.51	0.44
2:G:3:LYS:HB2	2:G:63:VAL:HA	1.99	0.44
2:G:50:LYS:O	2:G:54:VAL:HG23	2.17	0.44
2:G:124:TYR:CG	2:G:174:ILE:HD12	2.53	0.44
1:B:23:LEU:O	1:B:27:GLU:HG3	2.18	0.44
1:B:233:ASP:HB3	1:B:236:LEU:HB2	2.00	0.44
1:C:198:PHE:CE2	1:C:204:PHE:HE1	2.36	0.44
2:F:104:ASN:O	2:F:105:LYS:C	2.61	0.44
1:B:207:GLU:H	1:B:207:GLU:CD	2.26	0.43
1:C:197:ALA:O	1:C:200:GLU:HB3	2.18	0.43
1:C:316:LYS:HE3	1:C:316:LYS:HB2	1.89	0.43
1:D:214:GLU:HG3	1:D:218:THR:CG2	2.47	0.43
2:E:86:TYR:CE1	2:E:180:ARG:CZ	3.01	0.43
2:F:24:TYR:O	2:F:26:VAL:HG23	2.17	0.43
2:F:87:LEU:N	2:F:87:LEU:HD23	2.33	0.43
2:F:113:ILE:HD13	2:F:132:ILE:HD13	2.00	0.43
1:A:143:ILE:HG13	1:A:305:ILE:HG23	2.01	0.43
1:B:211:LEU:HD22	1:B:231:THR:HG21	2.00	0.43
1:D:6:TYR:CD1	1:D:7:LEU:HD23	2.53	0.43
2:H:1:MET:HB2	2:H:43:ASP:O	2.18	0.43
2:H:29:ILE:HG22	2:H:30:LEU:N	2.32	0.43
1:B:16:THR:HG22	2:H:109:ARG:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:158:LYS:HB3	1:C:279:SER:OG	2.18	0.43
1:C:170:GLN:O	1:C:171:ARG:C	2.62	0.43
2:E:19:LEU:O	2:E:24:TYR:HB2	2.18	0.43
2:E:65:ILE:HG21	2:E:181:MET:CE	2.49	0.43
2:E:85:LEU:HB3	2:E:181:MET:CB	2.48	0.43
2:G:176:ASP:O	2:G:177:ILE:HD13	2.18	0.43
1:A:73:LYS:HZ3	1:A:77:GLN:HG3	1.79	0.43
1:B:189:LYS:O	2:G:83:GLU:N	2.47	0.43
1:D:154:LEU:O	1:D:156:LEU:N	2.46	0.43
2:F:53:ASP:O	2:F:57:PHE:CD1	2.71	0.43
1:A:266:MET:CG	1:A:269:TYR:CE1	2.94	0.43
2:G:161:ASN:O	2:G:162:THR:C	2.62	0.43
2:H:84:LEU:HD12	2:H:183:VAL:HG21	1.99	0.43
2:H:114:ALA:HA	2:H:135:ILE:O	2.19	0.43
1:C:73:LYS:HG3	1:C:76:GLY:N	2.30	0.43
1:C:86:THR:O	1:C:90:VAL:HG23	2.19	0.43
1:D:237:ILE:HG13	1:D:238:SER:N	2.32	0.43
2:F:93:ILE:O	2:F:156:ILE:HA	2.19	0.43
1:A:319:GLU:O	1:A:320:ARG:C	2.59	0.43
1:B:129:ILE:HD11	1:B:307:PHE:CE2	2.53	0.43
2:E:10:ARG:HH12	2:E:158:GLU:CD	2.26	0.43
2:E:123:LYS:O	2:E:126:ALA:HB3	2.19	0.43
2:F:26:VAL:C	2:F:28:PRO:HD2	2.43	0.43
2:G:86:TYR:CE1	2:G:178:SER:CB	3.00	0.43
2:G:161:ASN:O	2:G:163:LEU:N	2.51	0.43
1:A:209:ARG:HE	1:A:213:LYS:HE2	1.83	0.43
1:B:316:LYS:HB2	1:B:316:LYS:HE3	1.78	0.43
2:E:40:THR:CG2	2:E:44:LEU:HB2	2.48	0.43
1:A:286:LEU:C	1:A:286:LEU:HD23	2.43	0.43
1:C:165:SER:C	1:C:273:MET:HE2	2.44	0.43
2:E:92:CYS:C	2:E:93:ILE:CG2	2.92	0.43
2:G:96:LEU:HD22	2:G:124:TYR:CE2	2.50	0.43
2:H:7:THR:OG1	2:H:11:ILE:HB	2.19	0.43
1:C:52:LEU:O	1:C:54:THR:N	2.48	0.43
2:E:36:LEU:HB3	2:F:143:LEU:HD21	2.01	0.43
2:E:86:TYR:CE1	2:E:178:SER:OG	2.68	0.43
2:H:12:GLN:O	2:H:12:GLN:HG2	2.17	0.43
1:B:64:ASN:HD21	1:B:66:GLU:CD	2.28	0.42
1:B:187:LEU:CD2	1:B:216:PHE:CE1	3.02	0.42
1:C:124:ASN:N	1:C:312:ASP:OD2	2.49	0.42
1:D:244:LYS:HE2	1:D:248:GLU:OE1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:124:TYR:CE1	2:E:174:ILE:HD12	2.54	0.42
2:F:13:LYS:O	2:F:14:GLN:C	2.62	0.42
2:H:77:ASP:OD1	2:H:77:ASP:C	2.62	0.42
1:C:13:ALA:O	1:D:45:PRO:HB3	2.19	0.42
1:C:48:GLU:HG2	1:C:52:LEU:HD22	2.00	0.42
1:C:199:ILE:O	1:C:199:ILE:HG22	2.18	0.42
1:C:224:LEU:O	1:C:228:VAL:HG23	2.19	0.42
2:E:47:ILE:HG22	2:E:48:PHE:N	2.33	0.42
1:C:254:LYS:HG3	1:C:255:PRO:HD2	2.01	0.42
2:E:141:VAL:HG21	2:E:155:ASP:HB2	2.01	0.42
2:H:10:ARG:HA	2:H:13:LYS:HE2	2.01	0.42
1:C:283:GLN:HB3	1:C:284:PRO:HD2	2.01	0.42
1:D:90:VAL:HG13	1:D:295:LEU:HD22	2.00	0.42
2:F:25:ASP:OD2	2:F:41:LYS:HG3	2.19	0.42
2:F:51:PRO:CG	2:F:52:ASN:H	2.24	0.42
2:H:99:TYR:CD2	2:H:168:LEU:HD23	2.54	0.42
1:A:53:TYR:C	1:A:55:ALA:N	2.76	0.42
1:A:73:LYS:HG3	1:A:76:GLY:N	2.34	0.42
1:A:157:ASN:N	1:A:321:GLN:NE2	2.47	0.42
1:B:143:ILE:HG13	1:B:305:ILE:HG23	2.02	0.42
1:B:206:LYS:HA	1:B:209:ARG:HH12	1.80	0.42
1:D:27:GLU:HG2	1:D:127:ILE:HD11	2.00	0.42
1:B:175:LEU:HD11	1:B:233:ASP:OD2	2.20	0.42
2:F:113:ILE:HG23	2:F:152:ALA:O	2.20	0.42
1:D:204:PHE:C	1:D:205:SER:O	2.63	0.42
1:D:252:MET:H	1:D:252:MET:HG3	1.46	0.42
2:E:193:ASP:CG	2:E:194:LYS:H	2.25	0.42
2:G:117:TYR:CD1	2:G:117:TYR:N	2.88	0.42
2:H:91:GLN:HE21	2:H:91:GLN:HB2	1.54	0.42
1:D:87:LEU:N	1:D:88:PRO:HD2	2.35	0.42
1:D:226:ASN:O	1:D:227:LEU:C	2.62	0.42
2:F:7:THR:HG21	2:F:68:VAL:HG12	2.01	0.42
2:F:133:GLU:O	2:F:133:GLU:HG2	2.18	0.42
1:B:73:LYS:CE	1:B:75:GLU:HB2	2.49	0.42
1:B:100:THR:OG1	1:B:101:SER:N	2.53	0.42
1:D:54:THR:O	1:D:54:THR:HG23	2.20	0.42
1:A:132:PHE:CE2	1:A:304:ALA:HB1	2.55	0.42
1:B:74:HIS:C	1:B:76:GLY:N	2.78	0.42
1:B:81:LEU:HD12	1:B:81:LEU:HA	1.88	0.42
1:C:214:GLU:C	1:C:216:PHE:N	2.75	0.42
1:D:51:GLN:HA	1:D:54:THR:HG22	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:87:LEU:O	2:E:89:ILE:N	2.41	0.42
2:G:113:ILE:CG2	2:G:154:VAL:HG23	2.45	0.42
1:B:195:LEU:O	1:B:198:PHE:HB3	2.20	0.41
1:C:64:ASN:ND2	1:C:66:GLU:HB2	2.36	0.41
1:C:192:LEU:HD12	2:H:84:LEU:HA	2.02	0.41
1:C:217:ILE:HD12	2:H:196:ILE:HD12	2.02	0.41
2:F:55:ILE:CD1	2:F:72:THR:HG22	2.46	0.41
1:A:103:ARG:HG2	1:A:103:ARG:NH1	2.32	0.41
1:A:145:SER:O	1:A:149:GLN:HG3	2.20	0.41
1:A:286:LEU:HD23	1:A:287:SER:N	2.35	0.41
1:A:307:PHE:CD1	1:A:307:PHE:C	2.98	0.41
1:C:87:LEU:O	1:C:88:PRO:C	2.63	0.41
1:C:200:GLU:HA	1:C:200:GLU:OE2	2.20	0.41
2:E:107:PHE:CD1	2:E:107:PHE:N	2.87	0.41
2:G:7:THR:HG21	2:G:68:VAL:HG12	2.02	0.41
2:G:164:SER:C	2:G:166:ASN:N	2.77	0.41
1:A:48:GLU:HG2	1:A:52:LEU:CD2	2.49	0.41
1:A:103:ARG:N	1:A:103:ARG:HD2	2.36	0.41
1:B:117:HIS:C	1:B:118:LYS:HG3	2.45	0.41
2:E:85:LEU:HD12	2:E:86:TYR:H	1.86	0.41
2:H:59:GLU:HG3	2:H:78:PHE:CE1	2.56	0.41
2:H:142:GLU:O	2:H:146:VAL:HG23	2.20	0.41
1:A:124:ASN:HA	1:A:124:ASN:HD22	1.43	0.41
1:C:72:ILE:HG22	1:C:73:LYS:H	1.85	0.41
1:C:256:ILE:HG22	1:C:257:ILE:N	2.34	0.41
1:D:151:ILE:O	1:D:151:ILE:CG2	2.68	0.41
2:E:7:THR:CG2	2:E:68:VAL:HG12	2.50	0.41
2:F:75:GLU:OE2	2:F:119:ARG:HB2	2.20	0.41
2:G:8:LYS:HG3	2:G:49:GLY:N	2.36	0.41
2:H:92:CYS:C	2:H:93:ILE:HG23	2.45	0.41
2:H:93:ILE:HD12	2:H:95:ALA:HB2	2.02	0.41
1:A:82:ARG:HG3	1:A:82:ARG:HH11	1.85	0.41
1:A:193:SER:O	1:A:196:ASN:HB3	2.21	0.41
1:C:129:ILE:HD13	1:C:146:LEU:HD13	2.01	0.41
2:E:65:ILE:HG21	2:E:181:MET:HE3	2.02	0.41
2:G:22:ALA:O	2:G:23:ASP:HB2	2.20	0.41
2:G:87:LEU:HB3	2:G:206:GLN:HE22	1.85	0.41
1:A:31:ARG:HG3	1:A:31:ARG:HH11	1.86	0.41
1:A:264:PRO:HD3	1:A:273:MET:HE1	2.02	0.41
1:B:56:LEU:O	1:B:63:PHE:HB2	2.21	0.41
1:B:73:LYS:NZ	1:B:75:GLU:CB	2.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:68:MET:HB3	1:D:80:THR:HG21	2.02	0.41
1:D:89:LEU:HD11	1:D:106:TYR:HD2	1.84	0.41
1:D:214:GLU:HG3	1:D:218:THR:HG21	2.01	0.41
2:F:39:LYS:HA	2:F:44:LEU:O	2.21	0.41
2:H:58:LEU:CD1	2:H:182:ILE:HG13	2.50	0.41
1:C:275:LYS:HD3	1:C:277:TYR:OH	2.20	0.41
1:D:244:LYS:O	1:D:247:SER:HB3	2.21	0.41
2:F:14:GLN:NE2	2:F:89:ILE:HB	2.36	0.41
2:F:14:GLN:HE21	2:F:89:ILE:HD12	1.86	0.41
1:A:30:LEU:HD21	1:A:150:VAL:HG13	2.02	0.41
1:A:75:GLU:O	1:A:75:GLU:HG3	2.21	0.41
1:C:70:GLN:O	1:C:71:PHE:CB	2.46	0.41
2:F:38:ILE:HD12	2:F:38:ILE:HA	1.91	0.41
2:G:143:LEU:H	2:G:143:LEU:CD1	2.33	0.41
2:G:181:MET:CE	2:G:199:VAL:HG22	2.43	0.41
1:A:83:TYR:CE1	1:A:112:ARG:HG2	2.56	0.41
1:A:209:ARG:HG2	1:A:213:LYS:HE2	2.03	0.41
1:A:214:GLU:HG2	1:A:227:LEU:CD1	2.49	0.41
1:B:126:GLN:HA	1:B:309:CYS:O	2.21	0.41
1:B:158:LYS:HE3	1:B:158:LYS:HB2	1.86	0.41
1:C:214:GLU:OE2	1:C:214:GLU:HA	2.21	0.41
1:D:73:LYS:NZ	1:D:75:GLU:CB	2.80	0.41
2:E:157:VAL:CG2	2:E:163:LEU:HD11	2.51	0.41
2:F:75:GLU:O	2:F:119:ARG:HD3	2.20	0.41
2:F:137:LEU:HD23	2:F:137:LEU:HA	1.89	0.41
2:G:47:ILE:HG22	2:G:48:PHE:N	2.32	0.41
2:H:1:MET:HB3	2:H:43:ASP:OD2	2.20	0.41
1:A:132:PHE:HE2	1:A:304:ALA:HB1	1.85	0.41
2:E:11:ILE:HD12	2:E:11:ILE:H	1.86	0.41
2:E:145:PRO:HD3	2:E:153:ILE:HG23	2.03	0.41
2:H:87:LEU:C	2:H:89:ILE:N	2.79	0.41
1:A:71:PHE:CE2	1:B:69:PHE:HD2	2.39	0.40
1:A:72:ILE:HG22	1:A:73:LYS:O	2.20	0.40
1:C:73:LYS:HZ3	1:C:77:GLN:CB	2.33	0.40
2:F:33:GLY:C	2:F:35:GLU:N	2.79	0.40
2:F:164:SER:C	2:F:166:ASN:N	2.77	0.40
2:G:7:THR:CG2	2:G:68:VAL:HG12	2.50	0.40
2:G:93:ILE:HG21	2:G:173:LYS:HE3	2.03	0.40
2:H:83:GLU:OE1	2:H:180:ARG:HD2	2.21	0.40
2:H:92:CYS:O	2:H:93:ILE:CG2	2.68	0.40
2:H:93:ILE:CD1	2:H:95:ALA:HB2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:TYR:O	1:A:50:THR:C	2.63	0.40
1:A:87:LEU:N	1:A:88:PRO:HD2	2.35	0.40
1:B:10:GLU:HB2	1:B:116:ARG:NH2	2.35	0.40
1:C:134:GLU:HB3	1:C:139:SER:OG	2.20	0.40
2:F:98:SER:OG	2:F:99:TYR:N	2.51	0.40
2:H:41:LYS:C	2:H:43:ASP:N	2.78	0.40
1:B:73:LYS:CD	1:B:77:GLN:HB2	2.46	0.40
1:D:254:LYS:CG	1:D:255:PRO:HD2	2.51	0.40
1:B:31:ARG:HH11	1:B:31:ARG:HG3	1.86	0.40
1:B:214:GLU:HG3	1:B:218:THR:CG2	2.51	0.40
1:D:16:THR:O	1:D:20:VAL:HG23	2.20	0.40
2:F:85:LEU:HD12	2:F:86:TYR:H	1.86	0.40
2:F:164:SER:C	2:F:166:ASN:H	2.28	0.40
2:G:64:ASP:HB3	2:G:187:SER:HB3	2.03	0.40
2:H:143:LEU:O	2:H:147:VAL:HG22	2.21	0.40
1:A:214:GLU:HG3	1:A:218:THR:CG2	2.52	0.40
1:B:256:ILE:HG22	1:B:257:ILE:N	2.37	0.40
1:C:39:TYR:CG	1:C:103:ARG:HB3	2.57	0.40
1:D:168:PHE:CE2	1:D:260:LEU:HB3	2.57	0.40
2:F:172:GLU:HG2	2:F:173:LYS:N	2.37	0.40

There are no symmetry-related clashes.

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	307/344 (89%)	274 (89%)	29 (9%)	4 (1%)	9	32
1	B	316/344 (92%)	286 (90%)	26 (8%)	4 (1%)	9	32
1	C	296/344 (86%)	274 (93%)	16 (5%)	6 (2%)	6	22
1	D	310/344 (90%)	281 (91%)	21 (7%)	8 (3%)	4	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	196/208 (94%)	170 (87%)	20 (10%)	6 (3%)	3	14
2	F	195/208 (94%)	162 (83%)	25 (13%)	8 (4%)	2	9
2	G	199/208 (96%)	167 (84%)	25 (13%)	7 (4%)	3	12
2	H	195/208 (94%)	165 (85%)	24 (12%)	6 (3%)	3	14
All	All	2014/2208 (91%)	1779 (88%)	186 (9%)	49 (2%)	4	18

All (49) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	53	TYR
1	A	299	GLN
1	B	61	LYS
1	D	99	SER
1	D	134	GLU
2	E	140	SER
2	F	8	LYS
2	F	193	ASP
2	G	103	SER
2	G	140	SER
2	G	193	ASP
2	H	140	SER
1	B	55	ALA
1	B	99	SER
1	B	119	GLY
1	C	136	ALA
1	D	299	GLN
2	E	144	GLY
2	E	193	ASP
2	F	103	SER
2	H	9	GLY
2	H	193	ASP
1	A	54	THR
1	A	99	SER
1	C	53	TYR
1	D	54	THR
2	F	34	ARG
2	G	89	ILE
2	H	88	LYS
1	C	97	LYS
1	C	232	LYS
1	D	136	ALA

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Mol	Chain	Res	Type
1	D	251	SER
2	E	21	ASN
2	G	162	THR
1	C	203	ASN
1	D	271	ASP
2	E	28	PRO
2	E	88	LYS
2	F	98	SER
2	G	9	GLY
2	G	98	SER
2	H	91	GLN
2	H	192	LYS
1	C	124	ASN
2	F	33	GLY
2	F	141	VAL
2	F	27	GLU
1	D	305	ILE

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	282/311 (91%)	270 (96%)	12 (4%)	26	60
1	B	288/311 (93%)	267 (93%)	21 (7%)	13	38
1	C	274/311 (88%)	263 (96%)	11 (4%)	28	62
1	D	285/311 (92%)	270 (95%)	15 (5%)	20	52
2	E	180/186 (97%)	165 (92%)	15 (8%)	10	32
2	F	180/186 (97%)	176 (98%)	4 (2%)	45	77
2	G	182/186 (98%)	179 (98%)	3 (2%)	55	83
2	H	178/186 (96%)	169 (95%)	9 (5%)	21	53
All	All	1849/1988 (93%)	1759 (95%)	90 (5%)	22	54

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	42	VAL
1	A	56	LEU
1	A	82	ARG
1	A	124	ASN
1	A	131	LEU
1	A	146	LEU
1	A	252	MET
1	A	266	MET
1	A	267	ASP
1	A	295	LEU
1	A	303	PHE
1	B	8	LEU
1	B	10	GLU
1	B	11	GLU
1	B	14	GLU
1	B	25	GLN
1	B	42	VAL
1	B	57	GLU
1	B	59	ASN
1	B	71	PHE
1	B	73	LYS
1	B	82	ARG
1	B	122	THR
1	B	123	GLU
1	B	131	LEU
1	B	145	SER
1	B	146	LEU
1	B	152	GLU
1	B	219	ASN
1	B	221	LEU
1	B	266	MET
1	B	295	LEU
1	C	8	LEU
1	C	42	VAL
1	C	72	ILE
1	C	84	ASP
1	C	114	GLU
1	C	131	LEU
1	C	221	LEU
1	C	266	MET
1	C	267	ASP
1	C	295	LEU

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Mol	Chain	Res	Type
1	C	303	PHE
1	D	7	LEU
1	D	31	ARG
1	D	42	VAL
1	D	57	GLU
1	D	71	PHE
1	D	73	LYS
1	D	82	ARG
1	D	97	LYS
1	D	131	LEU
1	D	146	LEU
1	D	174	GLN
1	D	221	LEU
1	D	252	MET
1	D	295	LEU
1	D	303	PHE
2	E	27	GLU
2	E	42	ASP
2	E	43	ASP
2	E	53	ASP
2	E	68	VAL
2	E	70	LYS
2	E	87	LEU
2	E	91	GLN
2	E	93	ILE
2	E	94	PHE
2	E	107	PHE
2	E	110	HIS
2	E	140	SER
2	E	142	GLU
2	E	193	ASP
2	F	39	LYS
2	F	87	LEU
2	F	94	PHE
2	F	197	GLU
2	G	23	ASP
2	G	94	PHE
2	G	193	ASP
2	H	38	ILE
2	H	43	ASP
2	H	68	VAL
2	H	70	LYS

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Mol	Chain	Res	Type
2	H	87	LEU
2	H	91	GLN
2	H	109	ARG
2	H	189	LYS
2	H	193	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	25	GLN
1	A	70	GLN
1	A	77	GLN
1	A	124	ASN
1	A	226	ASN
1	A	297	ASN
1	A	321	GLN
1	B	64	ASN
1	B	77	GLN
1	B	95	GLN
1	B	202	ASN
1	B	226	ASN
1	B	321	GLN
1	C	18	ASN
1	C	70	GLN
1	C	95	GLN
1	C	124	ASN
1	C	149	GLN
1	C	321	GLN
1	D	18	ASN
1	D	64	ASN
1	D	126	GLN
1	D	282	ASN
1	D	283	GLN
1	D	310	HIS
1	D	321	GLN
2	E	14	GLN
2	E	37	GLN
2	E	45	GLN
2	E	91	GLN
2	E	108	GLN
2	F	12	GLN

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Mol	Chain	Res	Type
2	F	14	GLN
2	F	31	ASN
2	F	52	ASN
2	F	60	HIS
2	G	14	GLN
2	G	37	GLN
2	G	52	ASN
2	G	91	GLN
2	G	108	GLN
2	G	161	ASN
2	G	206	GLN
2	H	14	GLN
2	H	31	ASN
2	H	45	GLN
2	H	91	GLN
2	H	161	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](#)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	WO4	F	210	-	2,4,4	1.25	0	-		
4	PO4	D	329	-	4,4,4	1.67	0	6,6,6	0.47	0
4	PO4	E	209	-	4,4,4	1.72	0	6,6,6	0.46	0
4	PO4	H	209	-	4,4,4	1.66	1 (25%)	6,6,6	0.46	0
4	PO4	F	209	-	4,4,4	1.74	1 (25%)	6,6,6	0.45	0
3	WO4	A	329	-	2,4,4	1.18	0	-		
4	PO4	B	329	-	4,4,4	7.05	3 (75%)	6,6,6	3.68	4 (66%)
4	PO4	G	209	-	4,4,4	1.68	0	6,6,6	0.46	0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	329	PO4	P-O3	10.16	1.84	1.54
4	B	329	PO4	P-O1	-8.09	1.32	1.50
4	B	329	PO4	P-O2	-5.46	1.38	1.54
4	H	209	PO4	P-O4	-2.07	1.48	1.54
4	F	209	PO4	P-O2	-2.06	1.48	1.54

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	329	PO4	O4-P-O3	-5.32	91.35	107.91
4	B	329	PO4	O2-P-O1	4.89	128.24	110.95
4	B	329	PO4	O3-P-O2	-3.63	96.61	107.91
4	B	329	PO4	O3-P-O1	-3.40	98.91	110.95

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
4	F	209	PO4	1	0
4	B	329	PO4	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	1
2	H	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	205:SER	C	206:LYS	N	1.16
1	H	110:HIS	C	111:LYS	N	1.16

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	311/344 (90%)	0.15	12 (3%) 43 35	35, 55, 87, 98	3 (0%)
1	B	317/344 (92%)	0.39	7 (2%) 62 53	39, 65, 87, 99	6 (1%)
1	C	302/344 (87%)	0.35	11 (3%) 46 38	36, 65, 88, 93	3 (0%)
1	D	314/344 (91%)	0.56	8 (2%) 58 48	38, 77, 94, 99	4 (1%)
2	E	200/208 (96%)	0.55	8 (4%) 42 34	42, 77, 94, 99	2 (1%)
2	F	201/208 (96%)	0.69	11 (5%) 30 24	69, 80, 93, 100	0
2	G	203/208 (97%)	0.45	5 (2%) 58 48	43, 75, 91, 98	1 (0%)
2	H	199/208 (95%)	0.43	5 (2%) 58 48	48, 75, 92, 97	1 (0%)
All	All	2047/2208 (92%)	0.43	67 (3%) 49 40	35, 72, 92, 100	20 (0%)

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	59	ASN	4.9
2	F	85	LEU	4.5
1	C	303	PHE	4.3
2	F	205	ALA	4.1
2	E	36	LEU	3.9
1	D	303	PHE	3.7
1	A	6	TYR	3.4
2	F	30	LEU	3.3
1	D	6	TYR	3.2
1	A	303	PHE	3.2
2	F	152	ALA	3.1
1	D	62	THR	3.0
1	D	323	LEU	2.9
1	B	14	GLU	2.9
2	G	89	ILE	2.9
1	C	123	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	74	HIS	2.8
1	A	54	THR	2.7
2	E	108	GLN	2.7
1	C	74	HIS	2.7
2	H	29	ILE	2.6
2	H	26	VAL	2.6
1	A	7	LEU	2.6
1	B	56	LEU	2.6
1	C	297	ASN	2.6
2	E	29	ILE	2.5
1	A	95	GLN	2.5
2	G	30	LEU	2.5
1	C	180	THR	2.5
1	B	63	PHE	2.4
2	E	38	ILE	2.4
2	H	110	HIS	2.4
2	E	28	PRO	2.4
2	E	204	ASP	2.4
1	C	216	PHE	2.4
2	G	106	ASN	2.3
1	A	123	GLU	2.3
1	B	61	LYS	2.3
2	F	105	LYS	2.3
1	A	209	ARG	2.3
1	C	191	ASP	2.3
1	B	62	THR	2.3
1	A	185	GLU	2.2
1	D	304	ALA	2.2
1	A	74	HIS	2.2
1	D	63	PHE	2.2
1	C	55	ALA	2.2
2	F	111	LYS	2.2
2	F	6	ILE	2.2
2	H	28	PRO	2.2
2	G	86	TYR	2.2
2	F	202	LEU	2.2
2	F	100	PRO	2.1
1	D	266	MET	2.1
2	F	199	VAL	2.1
1	D	221	LEU	2.1
1	C	302	ALA	2.1
2	G	27	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
2	E	106	ASN	2.1
2	H	139	GLY	2.1
1	A	302	ALA	2.1
2	F	15	VAL	2.1
1	C	196	ASN	2.1
1	C	71	PHE	2.0
1	A	298	PHE	2.0
1	A	300	GLU	2.0
2	E	20	GLU	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(Å ²)	Q<0.9
3	WO4	A	329	5/5	0.45	0.18	161,161,161,162	5
3	WO4	F	210	5/5	0.55	0.15	162,162,162,162	5
4	PO4	F	209	5/5	0.76	0.10	103,103,104,104	0
4	PO4	G	209	5/5	0.78	0.10	102,102,103,103	0
4	PO4	B	329	5/5	0.81	0.16	103,103,104,127	0
4	PO4	D	329	5/5	0.88	0.11	103,104,104,105	0
4	PO4	E	209	5/5	0.90	0.07	105,105,106,106	0
4	PO4	H	209	5/5	0.92	0.06	84,86,86,86	0

6.5 Other polymers [i](#)

There are no such residues in this entry.