



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:16 AM UTC

PDB ID : 2VZA / pdb_00002vza
Title : Type IV secretion system effector protein BepA
Authors : Meury, M.; Schirmer, T.
Deposited on : 2008-07-31
Resolution : 3.05 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

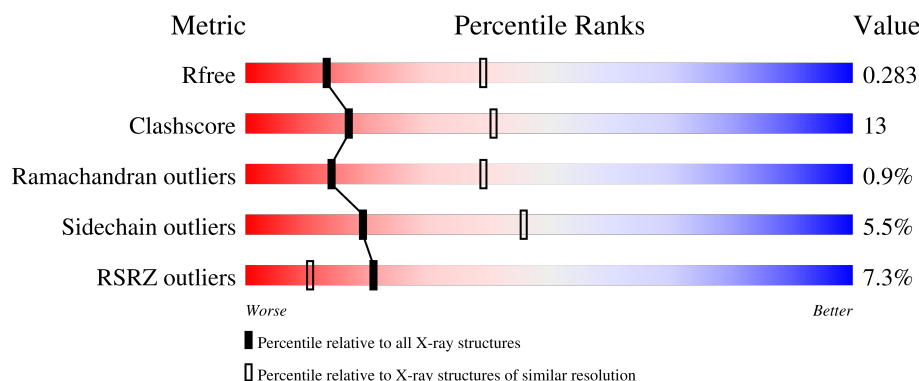
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.05 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	2469 (3.10-3.02)
Clashscore	190562	2569 (3.10-3.02)
Ramachandran outliers	187476	2424 (3.10-3.02)
Sidechain outliers	187428	2423 (3.10-3.02)
RSRZ outliers	180081	2469 (3.10-3.02)

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	298	2% 73% 22% ...
1	B	298	10% 72% 26% ...
1	C	298	15% 69% 27% ...
1	D	298	8% 74% 23% ...
1	E	298	6% 74% 22% ...

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Mol	Chain	Length	Quality of chain
1	F	298	 3% 74% 22% . .
1	G	298	 6% 71% 24% . .
1	H	298	 6% 74% 22% . .

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
2	SO4	G	310[B]	-	-	X	-

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 19098 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 CELL FILAMENTATION PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	296	Total	C	N	O	S	174	0	0
			2376	1507	418	440	11			
1	B	296	Total	C	N	O	S	178	0	0
			2376	1507	418	440	11			
1	C	296	Total	C	N	O	S	193	0	0
			2376	1507	418	440	11			
1	D	296	Total	C	N	O	S	111	0	0
			2376	1507	418	440	11			
1	E	296	Total	C	N	O	S	155	0	0
			2376	1507	418	440	11			
1	F	296	Total	C	N	O	S	157	0	0
			2376	1507	418	440	11			
1	G	296	Total	C	N	O	S	97	0	0
			2376	1507	418	440	11			
1	H	296	Total	C	N	O	S	155	0	0
			2376	1507	418	440	11			

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

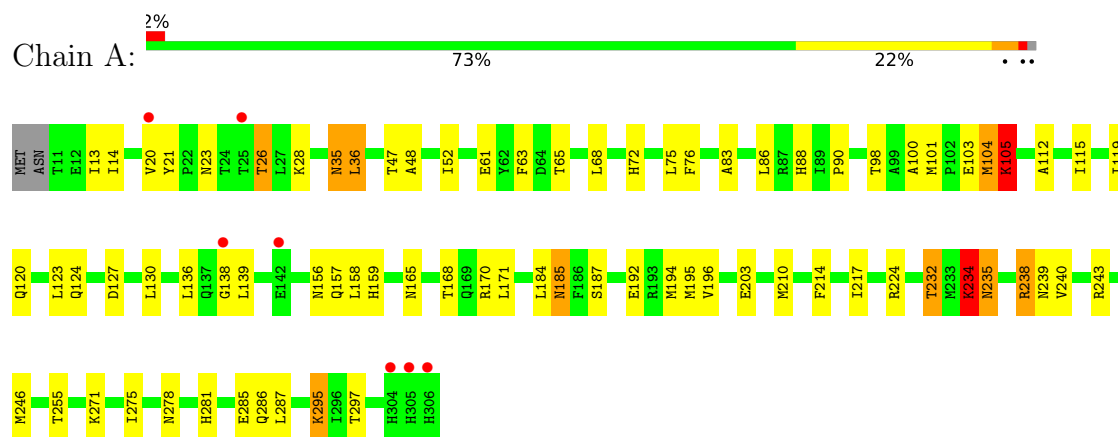


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	1
			10	8	2		
2	B	1	Total	O	S	0	1
			10	8	2		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	1
			10	8	2		
2	D	1	Total	O	S	0	1
			10	8	2		
2	E	1	Total	O	S	0	1
			10	8	2		
2	F	1	Total	O	S	0	1
			10	8	2		
2	F	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	1
			10	8	2		
2	H	1	Total	O	S	0	1
			10	8	2		

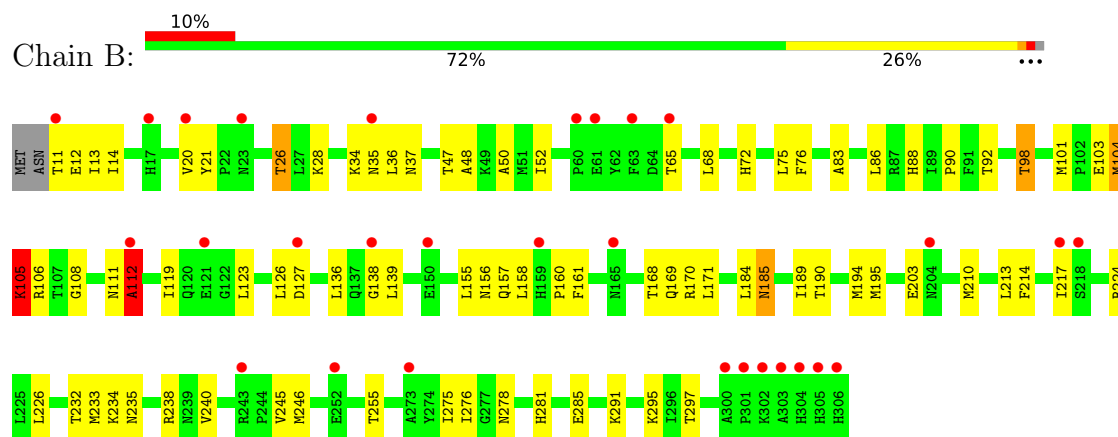
3 Residue-property plots [i](#)

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

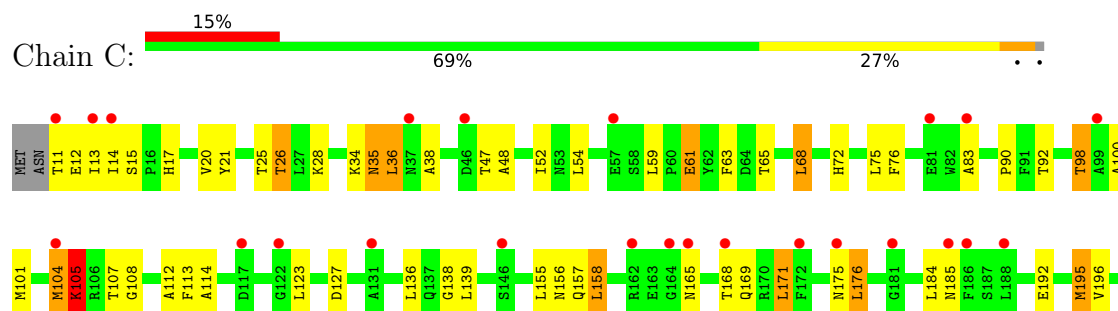
• Molecule 1: CELL FILAMENTATION PROTEIN



• Molecule 1: CELL FILAMENTATION PROTEIN

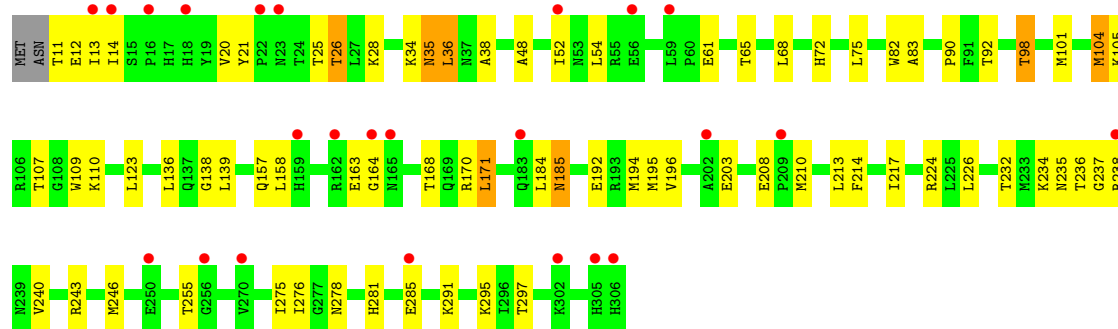
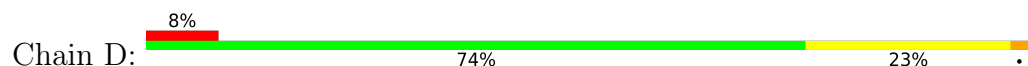


• Molecule 1: CELL FILAMENTATION PROTEIN

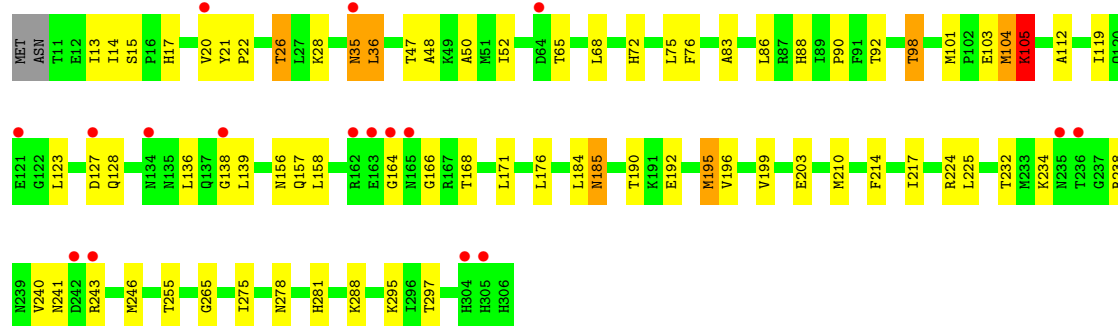
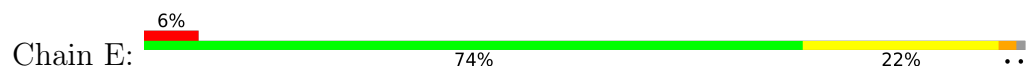




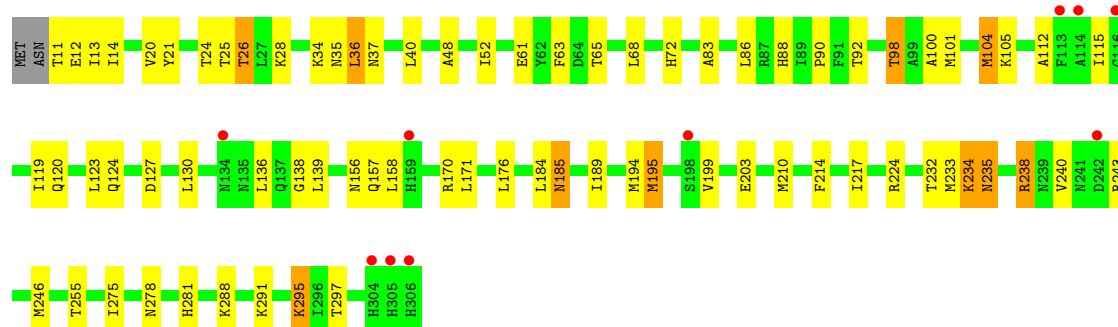
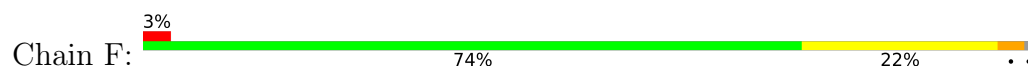
● Molecule 1: CELL FILAMENTATION PROTEIN



● Molecule 1: CELL FILAMENTATION PROTEIN

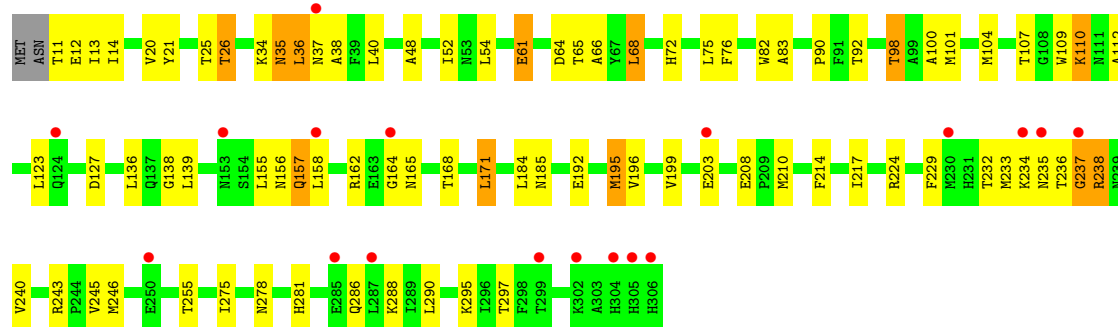


● Molecule 1: CELL FILAMENTATION PROTEIN



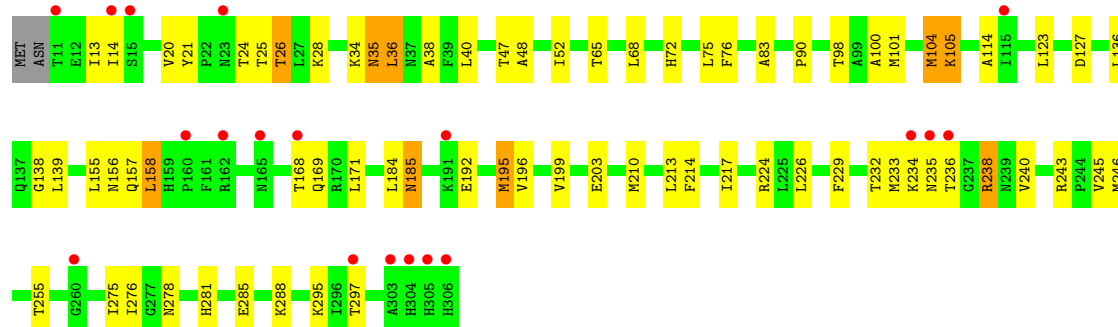
● Molecule 1: CELL FILAMENTATION PROTEIN

Chain G: 



● Molecule 1: CELL FILAMENTATION PROTEIN

Chain H: 



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	229.90Å 229.90Å 308.99Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 3.05 30.00 – 3.05	Depositor EDS
% Data completeness (in resolution range)	92.1 (30.00-3.05) 81.7 (30.00-3.05)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 3.07Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.244 , 0.277 0.248 , 0.283	Depositor DCC
R_{free} test set	2512 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	71.3	Xtrriage
Anisotropy	0.036	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 107.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	19098	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 19.87 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.8587e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	1.11	9/2432 (0.4%)	1.08	11/3285 (0.3%)
1	B	0.89	10/2432 (0.4%)	1.35	17/3285 (0.5%)
1	C	1.40	9/2432 (0.4%)	1.06	17/3285 (0.5%)
1	D	1.19	9/2432 (0.4%)	0.97	13/3285 (0.4%)
1	E	0.89	10/2432 (0.4%)	0.87	9/3285 (0.3%)
1	F	1.17	11/2432 (0.5%)	1.06	13/3285 (0.4%)
1	G	0.77	7/2432 (0.3%)	0.86	8/3285 (0.2%)
1	H	0.89	9/2432 (0.4%)	0.81	7/3285 (0.2%)
All	All	1.06	74/19456 (0.4%)	1.02	95/26280 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	1	2
1	E	0	1
All	All	1	6

All (74) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	105	LYS	C-N	41.87	1.87	1.33
1	F	105	LYS	C-N	38.43	1.85	1.33
1	C	233	MET	C-N	35.96	1.82	1.33
1	A	234	LYS	C-N	-29.19	0.93	1.33
1	D	234	LYS	CG-CD	29.09	2.39	1.52
1	D	237	GLY	C-N	27.31	1.70	1.33
1	B	233	MET	C-N	24.39	1.67	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	105	LYS	C-N	22.99	1.67	1.33
1	D	234	LYS	C-N	22.79	1.65	1.33
1	A	238	ARG	C-N	22.36	1.65	1.33
1	E	105	LYS	C-N	21.40	1.65	1.33
1	C	105	LYS	CA-CB	-20.19	1.19	1.53
1	A	234	LYS	CG-CD	18.54	2.08	1.52
1	F	105	LYS	CB-CG	17.95	2.06	1.52
1	D	238	ARG	CB-CG	17.30	2.04	1.52
1	E	234	LYS	CG-CD	16.71	2.02	1.52
1	G	288	LYS	CA-CB	-15.79	1.28	1.53
1	H	105	LYS	CA-CB	-14.83	1.28	1.53
1	C	285	GLU	CA-CB	14.20	1.77	1.53
1	H	238	ARG	CB-CG	12.60	1.90	1.52
1	B	112	ALA	CA-C	12.59	1.69	1.52
1	C	112	ALA	C-N	-12.08	1.16	1.33
1	F	288	LYS	CA-CB	-11.68	1.35	1.53
1	A	195	MET	CA-CB	-11.31	1.35	1.53
1	F	235	ASN	CB-CG	-11.13	1.24	1.52
1	H	285	GLU	CA-CB	10.51	1.71	1.53
1	E	288	LYS	CA-CB	-10.34	1.37	1.53
1	F	238	ARG	CB-CG	-10.02	1.22	1.52
1	F	234	LYS	CG-CD	9.48	1.80	1.52
1	F	224	ARG	CA-CB	-9.44	1.38	1.53
1	E	112	ALA	C-N	9.36	1.46	1.33
1	B	111	ASN	C-N	9.34	1.46	1.33
1	F	195	MET	CA-CB	-8.71	1.39	1.53
1	F	203	GLU	CA-CB	-8.68	1.39	1.53
1	E	195	MET	CA-CB	-8.60	1.40	1.53
1	H	234	LYS	CG-CD	-8.46	1.27	1.52
1	G	195	MET	CA-CB	-8.43	1.40	1.53
1	D	285	GLU	CA-CB	8.24	1.67	1.53
1	A	224	ARG	CA-CB	-8.04	1.40	1.53
1	H	243	ARG	CA-CB	-7.82	1.43	1.53
1	B	105	LYS	C-N	-7.81	1.22	1.33
1	A	203	GLU	CA-CB	-7.73	1.40	1.53
1	B	203	GLU	CA-CB	-7.69	1.40	1.53
1	C	195	MET	CA-CB	-7.61	1.41	1.53
1	G	243	ARG	CA-CB	-7.54	1.42	1.53
1	A	243	ARG	CA-CB	-7.51	1.42	1.53
1	F	112	ALA	C-N	7.50	1.44	1.33
1	E	224	ARG	CA-CB	-7.32	1.41	1.53
1	B	195	MET	CA-CB	-7.25	1.42	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	224	ARG	CA-CB	-7.22	1.41	1.53
1	E	238	ARG	CB-CG	-7.22	1.30	1.52
1	D	208	GLU	CA-CB	-7.08	1.42	1.53
1	A	112	ALA	C-N	7.03	1.42	1.33
1	H	224	ARG	CA-CB	-6.98	1.42	1.53
1	C	208	GLU	CA-CB	-6.98	1.42	1.53
1	E	203	GLU	CA-CB	-6.91	1.42	1.53
1	G	208	GLU	CA-CB	-6.88	1.42	1.53
1	A	285	GLU	CA-CB	-6.88	1.42	1.53
1	D	243	ARG	CA-CB	-6.63	1.43	1.53
1	E	243	ARG	CA-CB	-6.33	1.45	1.53
1	G	61	GLU	CA-CB	6.33	1.63	1.53
1	D	195	MET	CA-CB	-6.30	1.43	1.53
1	B	285	GLU	CA-CB	6.25	1.63	1.53
1	F	291	LYS	CA-CB	-6.17	1.43	1.53
1	C	203	GLU	CA-CB	-6.05	1.43	1.53
1	C	61	GLU	CA-CB	6.02	1.62	1.53
1	E	105	LYS	CA-CB	-5.97	1.43	1.53
1	H	195	MET	CA-CB	-5.76	1.44	1.53
1	G	224	ARG	CA-CB	-5.74	1.44	1.53
1	G	234	LYS	CG-CD	-5.72	1.35	1.52
1	B	224	ARG	CA-CB	-5.67	1.44	1.53
1	H	288	LYS	CA-CB	-5.44	1.44	1.53
1	B	112	ALA	C-N	-5.28	1.25	1.33
1	B	295	LYS	CA-CB	-5.20	1.44	1.53

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	234	LYS	O-C-N	-34.00	77.37	122.59
1	B	105	LYS	O-C-N	-30.99	81.38	122.59
1	B	112	ALA	CB-CA-C	-28.45	53.79	110.42
1	F	105	LYS	O-C-N	26.56	157.91	122.59
1	B	112	ALA	N-CA-C	24.42	162.81	110.80
1	B	111	ASN	CA-C-N	-22.53	78.50	121.54
1	B	111	ASN	C-N-CA	-22.53	78.50	121.54
1	D	238	ARG	CA-CB-CG	-18.02	78.06	114.10
1	C	105	LYS	O-C-N	-16.30	100.91	122.59
1	C	105	LYS	CB-CA-C	-14.41	81.73	110.42
1	F	235	ASN	CA-CB-CG	13.73	126.33	112.60
1	E	234	LYS	CB-CG-CD	-11.75	84.28	111.30
1	C	239	ASN	CA-C-N	11.57	142.79	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	239	ASN	C-N-CA	11.57	142.79	121.97
1	C	112	ALA	CA-C-N	10.67	141.91	121.54
1	C	112	ALA	C-N-CA	10.67	141.91	121.54
1	C	239	ASN	O-C-N	-10.64	110.29	123.27
1	D	234	LYS	CB-CG-CD	-10.60	86.91	111.30
1	D	234	LYS	CA-C-N	-10.39	101.70	121.54
1	D	234	LYS	C-N-CA	-10.39	101.70	121.54
1	F	105	LYS	CA-C-N	-10.13	104.92	123.05
1	F	105	LYS	C-N-CA	-10.13	104.92	123.05
1	C	105	LYS	CA-CB-CG	-10.09	93.92	114.10
1	C	105	LYS	N-CA-CB	9.71	126.90	110.49
1	B	112	ALA	CA-C-O	-8.92	107.75	120.51
1	A	203	GLU	N-CA-CB	8.77	123.11	110.13
1	C	203	GLU	N-CA-CB	8.14	122.17	110.13
1	A	234	LYS	CB-CG-CD	-8.10	92.67	111.30
1	B	291	LYS	N-CA-CB	-8.09	100.36	109.74
1	B	203	GLU	N-CA-CB	7.78	121.65	110.13
1	E	203	GLU	N-CA-CB	7.63	121.42	110.13
1	F	105	LYS	CB-CG-CD	7.62	128.83	111.30
1	F	203	GLU	N-CA-CB	7.62	121.41	110.13
1	G	288	LYS	N-CA-CB	7.58	121.27	110.12
1	B	111	ASN	O-C-N	7.56	132.32	123.02
1	B	224	ARG	N-CA-CB	7.53	121.36	110.06
1	F	224	ARG	N-CA-CB	7.51	121.16	110.12
1	B	105	LYS	CA-C-N	7.45	135.77	121.54
1	B	105	LYS	C-N-CA	7.45	135.77	121.54
1	A	195	MET	N-CA-CB	7.36	120.69	110.01
1	H	105	LYS	N-CA-CB	7.11	122.50	110.49
1	F	234	LYS	CB-CG-CD	-7.06	95.06	111.30
1	D	238	ARG	CB-CG-CD	-7.05	95.09	111.30
1	C	112	ALA	O-C-N	-6.95	114.33	122.87
1	H	238	ARG	CA-CB-CG	-6.86	100.37	114.10
1	C	105	LYS	CA-C-N	6.84	132.41	122.16
1	C	105	LYS	C-N-CA	6.84	132.41	122.16
1	E	105	LYS	O-C-N	6.79	131.62	122.59
1	A	234	LYS	CG-CD-CE	6.78	126.90	111.30
1	A	243	ARG	CB-CA-C	6.75	118.01	108.76
1	A	195	MET	CB-CA-C	6.75	121.47	110.88
1	A	224	ARG	N-CA-CB	6.70	119.97	110.12
1	H	203	GLU	N-CA-CB	6.67	119.73	110.07
1	A	158	LEU	N-CA-C	-6.65	100.44	110.28
1	A	235	ASN	N-CA-C	6.57	119.53	108.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	224	ARG	N-CA-CB	6.51	119.69	110.12
1	E	288	LYS	N-CA-CB	6.50	119.68	110.12
1	F	243	ARG	CB-CA-C	6.48	117.64	108.76
1	B	291	LYS	CB-CA-C	6.40	119.55	109.37
1	D	203	GLU	N-CA-CB	6.35	119.53	110.13
1	G	243	ARG	CB-CA-C	6.34	118.31	108.61
1	E	243	ARG	CB-CA-C	6.31	118.34	108.63
1	F	238	ARG	CA-CB-CG	6.29	126.67	114.10
1	D	243	ARG	CB-CA-C	6.28	118.22	108.61
1	F	291	LYS	CB-CA-C	6.28	119.35	109.37
1	A	105	LYS	O-C-N	-6.15	114.41	122.59
1	B	112	ALA	CA-C-N	6.08	134.29	122.07
1	B	112	ALA	C-N-CA	6.08	134.29	122.07
1	E	158	LEU	N-CA-C	-6.07	100.86	109.96
1	G	61	GLU	N-CA-CB	-5.91	101.42	110.16
1	B	238	ARG	O-C-N	5.90	130.88	122.74
1	H	158	LEU	N-CA-C	-5.89	101.13	109.96
1	B	158	LEU	N-CA-C	-5.80	101.26	109.96
1	C	158	LEU	N-CA-C	-5.80	101.70	110.28
1	F	158	LEU	N-CA-C	-5.67	101.45	109.96
1	H	224	ARG	N-CA-CB	5.66	118.43	110.12
1	E	105	LYS	N-CA-CB	5.63	120.01	110.49
1	D	237	GLY	CA-C-N	-5.53	115.02	122.86
1	D	237	GLY	C-N-CA	-5.53	115.02	122.86
1	F	235	ASN	CB-CG-OD1	5.51	131.82	120.80
1	G	158	LEU	N-CA-C	-5.43	101.81	109.96
1	G	203	GLU	N-CA-CB	5.38	118.21	110.20
1	C	291	LYS	N-CA-CB	-5.35	103.53	109.74
1	G	195	MET	CB-CA-C	5.35	119.27	110.88
1	G	234	LYS	CG-CD-CE	5.33	123.56	111.30
1	C	61	GLU	N-CA-CB	-5.30	102.31	110.16
1	H	243	ARG	CB-CA-C	5.30	116.79	108.63
1	H	285	GLU	CB-CA-C	-5.25	100.27	110.46
1	D	158	LEU	N-CA-C	-5.25	102.08	109.96
1	G	224	ARG	CB-CA-C	5.25	119.61	110.68
1	D	224	ARG	N-CA-CB	5.16	118.16	110.22
1	D	291	LYS	N-CA-CB	-5.09	103.83	109.74
1	D	237	GLY	O-C-N	5.07	128.42	122.38
1	E	195	MET	N-CA-CB	5.03	117.31	110.01
1	C	243	ARG	CB-CA-C	5.01	116.28	108.61

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	112	ALA	CA

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	105	LYS	Mainchain
1	A	234	LYS	Mainchain
1	A	238	ARG	Mainchain
1	B	105	LYS	Mainchain
1	B	112	ALA	Mainchain
1	E	105	LYS	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	2376	0	2329	55	2
1	B	2376	0	2330	59	1
1	C	2376	0	2327	63	1
1	D	2376	0	2329	58	2
1	E	2376	0	2330	53	1
1	F	2376	0	2329	67	0
1	G	2376	0	2330	68	1
1	H	2376	0	2330	63	2
2	A	10	0	0	1	0
2	B	15	0	0	1	0
2	C	10	0	0	1	0
2	D	10	0	0	0	0
2	E	10	0	0	1	0
2	F	15	0	0	1	0
2	G	10	0	0	2	0
2	H	10	0	0	0	0
All	All	19098	0	18634	444	5

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 13.

All (444) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:86:LEU:HD12	1:H:25:THR:CG2	1.56	1.34
1:B:86:LEU:HD12	1:D:25:THR:CG2	1.58	1.33
1:E:86:LEU:HD12	1:G:25:THR:CG2	1.60	1.30
1:F:86:LEU:HD12	1:H:25:THR:HG21	1.28	1.10
1:E:86:LEU:HD12	1:G:25:THR:HG21	1.14	1.10
1:B:86:LEU:HD12	1:D:25:THR:HG21	1.18	1.09
1:A:86:LEU:HD12	1:C:25:THR:CG2	1.84	1.07
1:F:86:LEU:HD12	1:H:25:THR:HG23	1.43	1.00
1:G:75:LEU:HD12	1:G:168:THR:HG22	1.44	0.96
1:G:246:MET:HE3	1:G:275:ILE:CD1	1.97	0.94
1:E:86:LEU:CD1	1:G:25:THR:HG21	2.02	0.90
1:B:86:LEU:CD1	1:D:25:THR:CG2	2.48	0.90
1:F:65:THR:HG21	1:F:123:LEU:HB3	1.54	0.90
1:C:75:LEU:HD12	1:C:168:THR:HG22	1.54	0.88
1:H:233:MET:HE3	1:H:238:ARG:HB2	1.55	0.88
1:C:65:THR:HG21	1:C:123:LEU:HB3	1.54	0.87
1:F:124:GLN:HG3	1:H:36:LEU:HD13	1.54	0.87
1:E:86:LEU:CD1	1:G:25:THR:CG2	2.48	0.86
1:G:65:THR:HG21	1:G:123:LEU:HB3	1.58	0.86
1:H:65:THR:HG21	1:H:123:LEU:HB3	1.56	0.86
1:A:65:THR:HG21	1:A:123:LEU:HB3	1.56	0.85
1:F:86:LEU:CD1	1:H:25:THR:CG2	2.50	0.85
1:B:65:THR:HG21	1:B:123:LEU:HB3	1.60	0.84
1:H:75:LEU:HD12	1:H:168:THR:HG22	1.62	0.82
1:A:86:LEU:HD12	1:C:25:THR:HG21	1.62	0.81
1:C:246:MET:HE3	1:C:275:ILE:CD1	2.10	0.80
1:B:86:LEU:CD1	1:D:25:THR:HG21	2.07	0.80
1:B:86:LEU:HD12	1:D:25:THR:HG23	1.62	0.80
1:D:75:LEU:HD12	1:D:168:THR:HG22	1.64	0.80
1:F:233:MET:HE3	1:F:238:ARG:HB2	1.64	0.80
1:F:255:THR:HG22	1:F:297:THR:OG1	1.80	0.80
1:D:65:THR:HG21	1:D:123:LEU:HB3	1.63	0.79
1:F:124:GLN:CG	1:H:36:LEU:HD13	2.13	0.79
1:D:246:MET:HE3	1:D:275:ILE:CD1	2.14	0.78
1:C:246:MET:HE3	1:C:275:ILE:HD12	1.65	0.78
1:E:246:MET:HE3	1:E:275:ILE:CD1	2.13	0.78
1:F:86:LEU:CD1	1:H:25:THR:HG21	2.12	0.78
1:B:255:THR:HG22	1:B:297:THR:OG1	1.84	0.78
1:B:72:HIS:ND1	1:B:83:ALA:O	2.17	0.76
1:H:65:THR:HG22	1:H:123:LEU:HD22	1.66	0.76
1:E:72:HIS:ND1	1:E:83:ALA:O	2.19	0.75
1:E:86:LEU:HD12	1:G:25:THR:HG23	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:72:HIS:ND1	1:F:83:ALA:O	2.21	0.74
1:G:107:THR:HG21	1:G:109:TRP:CE2	2.23	0.74
1:F:88:HIS:HB3	1:F:119:ILE:HD12	1.68	0.74
1:G:210:MET:HE1	1:G:214:PHE:CE2	2.24	0.72
1:F:86:LEU:CD1	1:H:25:THR:HG23	2.17	0.72
1:F:255:THR:HG22	1:F:297:THR:CB	2.18	0.72
1:A:255:THR:HG22	1:A:297:THR:OG1	1.90	0.71
1:H:246:MET:HE3	1:H:275:ILE:CD1	2.19	0.71
1:E:65:THR:HG21	1:E:123:LEU:HB3	1.72	0.71
1:D:226:LEU:HD23	1:D:276:ILE:HD12	1.72	0.71
1:C:92:THR:HG23	1:C:98:THR:HG22	1.73	0.71
1:B:255:THR:HG22	1:B:297:THR:CB	2.21	0.71
1:G:246:MET:HE3	1:G:275:ILE:HD11	1.73	0.70
1:F:124:GLN:HG2	1:H:36:LEU:HD22	1.75	0.69
1:A:255:THR:HG22	1:A:297:THR:CB	2.21	0.69
1:F:120:GLN:OE1	1:H:25:THR:HB	1.93	0.69
1:H:72:HIS:ND1	1:H:83:ALA:O	2.24	0.69
1:D:65:THR:HG22	1:D:123:LEU:HD22	1.75	0.69
1:F:124:GLN:HG3	1:H:36:LEU:CD1	2.21	0.69
1:H:20:VAL:HG12	1:H:21:TYR:O	1.93	0.69
1:G:65:THR:HG23	1:G:127:ASP:OD1	1.94	0.68
1:D:54:LEU:HD13	1:D:171:LEU:CD1	2.24	0.68
1:D:246:MET:HE3	1:D:275:ILE:HD12	1.75	0.68
1:C:255:THR:HG22	1:C:297:THR:CB	2.25	0.68
1:A:86:LEU:HD12	1:C:25:THR:HG23	1.71	0.67
1:H:65:THR:CG2	1:H:123:LEU:HD22	2.24	0.67
1:A:72:HIS:ND1	1:A:83:ALA:O	2.26	0.67
1:C:65:THR:HG22	1:C:123:LEU:HD22	1.76	0.67
1:D:255:THR:HG22	1:D:297:THR:CB	2.25	0.67
1:C:246:MET:CE	1:C:275:ILE:CD1	2.73	0.67
1:C:72:HIS:ND1	1:C:83:ALA:O	2.27	0.66
1:G:255:THR:HG22	1:G:297:THR:CB	2.26	0.66
1:A:246:MET:HE3	1:A:275:ILE:CD1	2.27	0.65
1:D:20:VAL:HG12	1:D:21:TYR:O	1.96	0.65
1:B:65:THR:HG22	1:B:123:LEU:HD22	1.77	0.65
1:G:72:HIS:HA	1:G:168:THR:HG21	1.79	0.64
1:B:246:MET:HE3	1:B:275:ILE:CD1	2.27	0.64
1:F:240:VAL:HG12	1:F:240:VAL:O	1.98	0.64
1:G:246:MET:CE	1:G:275:ILE:HD11	2.27	0.64
1:F:246:MET:HE3	1:F:275:ILE:CD1	2.27	0.64
1:D:170:ARG:HD2	1:D:194:MET:HE2	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:101:MET:HG2	1:C:104:MET:HE3	1.79	0.64
1:H:210:MET:HE1	1:H:214:PHE:CE2	2.33	0.64
1:A:65:THR:HG22	1:A:123:LEU:HD22	1.80	0.63
1:D:54:LEU:HD13	1:D:171:LEU:HD13	1.80	0.63
1:E:128:GLN:N	1:G:37:ASN:HD21	1.97	0.62
1:D:255:THR:HG22	1:D:297:THR:HB	1.82	0.62
1:E:92:THR:HG23	1:E:98:THR:HG22	1.82	0.62
1:E:86:LEU:CD1	1:G:25:THR:HG23	2.27	0.62
1:B:86:LEU:CD1	1:D:25:THR:HG23	2.24	0.61
1:E:255:THR:HG22	1:E:297:THR:CB	2.30	0.61
1:H:255:THR:HG22	1:H:297:THR:CB	2.30	0.61
1:G:20:VAL:HG12	1:G:21:TYR:O	1.99	0.61
1:G:240:VAL:HG12	1:G:240:VAL:O	2.00	0.61
1:D:72:HIS:CD2	1:D:168:THR:HG21	2.35	0.61
1:C:136:LEU:C	1:C:139:LEU:HD13	2.25	0.61
1:C:255:THR:HG22	1:C:297:THR:HB	1.81	0.61
1:A:240:VAL:HG12	1:A:240:VAL:O	2.00	0.61
1:E:136:LEU:C	1:E:139:LEU:HD13	2.26	0.61
1:E:246:MET:HE3	1:E:275:ILE:HD12	1.82	0.61
1:E:26:THR:HG22	1:E:36:LEU:HG	1.82	0.60
1:C:226:LEU:HD23	1:C:276:ILE:HD12	1.81	0.60
1:B:101:MET:SD	1:B:104:MET:CE	2.89	0.60
1:G:246:MET:CE	1:G:275:ILE:CD1	2.78	0.60
1:A:124:GLN:HG2	1:C:36:LEU:HD13	1.84	0.60
1:A:185:ASN:O	1:A:217:ILE:HD12	2.02	0.59
1:C:240:VAL:HG12	1:C:240:VAL:O	2.02	0.59
1:A:101:MET:SD	1:A:104:MET:CE	2.90	0.59
1:B:75:LEU:HD12	1:B:168:THR:HG22	1.83	0.59
1:C:20:VAL:HG12	1:C:21:TYR:O	2.01	0.59
1:D:72:HIS:ND1	1:D:83:ALA:O	2.35	0.59
1:D:240:VAL:HG12	1:D:240:VAL:O	2.03	0.59
1:G:255:THR:HG22	1:G:297:THR:HB	1.83	0.59
1:B:65:THR:CG2	1:B:123:LEU:HD22	2.32	0.59
1:A:75:LEU:HD12	1:A:168:THR:HG22	1.83	0.58
1:A:101:MET:HE2	1:A:104:MET:HA	1.84	0.58
1:B:246:MET:HE3	1:B:275:ILE:HD12	1.84	0.58
1:F:136:LEU:C	1:F:139:LEU:HD13	2.28	0.58
1:D:82:TRP:HH2	1:D:163:GLU:HB3	1.67	0.58
1:A:65:THR:HG23	1:A:127:ASP:OD1	2.03	0.58
1:B:20:VAL:HG12	1:B:21:TYR:O	2.03	0.58
1:F:65:THR:HG22	1:F:123:LEU:HD22	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:14:ILE:HD13	1:E:90:PRO:HB3	1.86	0.58
1:C:246:MET:CE	1:C:275:ILE:HD11	2.34	0.58
1:D:246:MET:CE	1:D:275:ILE:CD1	2.81	0.57
1:E:138:GLY:C	1:E:139:LEU:HD12	2.28	0.57
1:F:101:MET:HE2	1:F:104:MET:HA	1.87	0.57
1:G:72:HIS:ND1	1:G:83:ALA:O	2.37	0.57
1:D:255:THR:HG22	1:D:297:THR:OG1	2.04	0.57
1:H:26:THR:HG21	1:H:34:LYS:O	2.03	0.57
1:B:14:ILE:HD13	1:B:90:PRO:HB3	1.86	0.57
1:A:88:HIS:HB3	1:A:119:ILE:HD12	1.87	0.57
1:B:101:MET:SD	1:B:104:MET:HE2	2.45	0.57
1:F:101:MET:SD	1:F:104:MET:CE	2.93	0.57
1:B:184:LEU:HA	1:B:217:ILE:HG22	1.87	0.57
1:G:236:THR:O	1:G:238:ARG:N	2.38	0.57
1:G:246:MET:HE3	1:G:275:ILE:HD12	1.82	0.57
1:A:246:MET:HE3	1:A:275:ILE:HD12	1.87	0.56
1:B:26:THR:HG22	1:B:36:LEU:HG	1.86	0.56
1:B:136:LEU:C	1:B:139:LEU:HD13	2.31	0.56
1:E:255:THR:HG22	1:E:297:THR:HB	1.86	0.56
1:H:65:THR:HG23	1:H:127:ASP:OD1	2.06	0.56
1:A:86:LEU:CD1	1:C:25:THR:CG2	2.74	0.56
1:A:138:GLY:C	1:A:139:LEU:HD12	2.30	0.56
1:B:47:THR:HG21	1:B:76:PHE:CE1	2.41	0.56
1:C:90:PRO:HA	1:C:100:ALA:HB2	1.87	0.56
1:G:35:ASN:C	1:G:35:ASN:HD22	2.13	0.56
1:A:185:ASN:C	1:A:217:ILE:HG23	2.31	0.56
1:F:48:ALA:O	1:F:52:ILE:HD13	2.05	0.56
1:G:210:MET:HE1	1:G:214:PHE:HE2	1.70	0.56
1:A:26:THR:HG22	1:A:36:LEU:HG	1.87	0.55
1:D:136:LEU:C	1:D:139:LEU:HD13	2.31	0.55
1:A:192:GLU:O	1:A:196:VAL:HG23	2.07	0.55
1:F:101:MET:SD	1:F:104:MET:HE2	2.46	0.55
1:B:138:GLY:C	1:B:139:LEU:HD12	2.32	0.55
1:F:210:MET:HE1	1:F:214:PHE:CE2	2.42	0.55
1:H:255:THR:HG22	1:H:297:THR:HB	1.88	0.55
1:A:255:THR:HG22	1:A:297:THR:HB	1.88	0.55
1:B:255:THR:HG22	1:B:297:THR:HB	1.89	0.55
1:C:54:LEU:HB3	1:C:171:LEU:HD11	1.89	0.55
1:B:88:HIS:HB3	1:B:119:ILE:HD12	1.89	0.55
1:C:192:GLU:O	1:C:196:VAL:HG23	2.08	0.54
1:A:136:LEU:C	1:A:139:LEU:HD13	2.32	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:ASN:HB3	1:A:281:HIS:CD2	2.43	0.54
1:F:184:LEU:HA	1:F:217:ILE:HG22	1.89	0.54
1:G:138:GLY:C	1:G:139:LEU:HD12	2.32	0.54
1:H:233:MET:HE3	1:H:238:ARG:CB	2.32	0.54
1:E:240:VAL:HG12	1:E:240:VAL:O	2.08	0.54
1:F:124:GLN:CD	1:H:40:LEU:HD11	2.32	0.54
1:G:255:THR:HG22	1:G:297:THR:OG1	2.07	0.54
1:B:37:ASN:ND2	2:B:311:SO4:O1	2.41	0.54
1:H:101:MET:HE2	1:H:104:MET:HA	1.89	0.54
1:H:240:VAL:HG12	1:H:240:VAL:O	2.08	0.54
1:A:20:VAL:HG12	1:A:21:TYR:O	2.08	0.54
1:H:255:THR:HG22	1:H:297:THR:OG1	2.07	0.54
1:E:184:LEU:HA	1:E:217:ILE:HG22	1.90	0.53
1:D:65:THR:CG2	1:D:123:LEU:HD22	2.38	0.53
1:C:255:THR:HG22	1:C:297:THR:OG1	2.08	0.53
1:H:246:MET:HE3	1:H:275:ILE:HD12	1.90	0.53
1:A:65:THR:CG2	1:A:123:LEU:HD22	2.38	0.53
1:E:101:MET:SD	1:E:104:MET:HE2	2.49	0.53
1:A:120:GLN:OE1	1:C:25:THR:HB	2.08	0.53
1:D:246:MET:CE	1:D:275:ILE:HD11	2.39	0.53
1:E:103:GLU:OE1	1:G:107:THR:OG1	2.24	0.53
1:H:90:PRO:HA	1:H:100:ALA:HB2	1.90	0.53
1:H:136:LEU:C	1:H:139:LEU:HD13	2.33	0.53
1:C:65:THR:CG2	1:C:123:LEU:HD22	2.39	0.53
1:E:185:ASN:O	1:E:217:ILE:HD12	2.08	0.53
1:C:14:ILE:HD13	1:C:90:PRO:HB3	1.91	0.52
1:C:138:GLY:C	1:C:139:LEU:HD12	2.34	0.52
1:D:54:LEU:HB3	1:D:171:LEU:HD11	1.90	0.52
1:F:185:ASN:O	1:F:217:ILE:HD12	2.09	0.52
1:E:255:THR:HG22	1:E:297:THR:OG1	2.10	0.52
1:G:101:MET:HG2	1:G:104:MET:HE3	1.92	0.52
1:H:226:LEU:HD23	1:H:276:ILE:HD12	1.90	0.52
1:D:14:ILE:HD13	1:D:90:PRO:HB3	1.91	0.52
1:D:72:HIS:HA	1:D:168:THR:HG21	1.91	0.52
1:D:138:GLY:C	1:D:139:LEU:HD12	2.34	0.52
1:E:101:MET:HE2	1:E:104:MET:HA	1.91	0.52
1:F:255:THR:HG22	1:F:297:THR:HB	1.89	0.52
1:A:271:LYS:HA	1:D:109:TRP:CD1	2.44	0.52
1:H:138:GLY:C	1:H:139:LEU:HD12	2.35	0.51
1:B:240:VAL:O	1:B:240:VAL:HG12	2.11	0.51
1:B:101:MET:HG2	1:B:104:MET:HE3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:35:ASN:HB3	1:C:38:ALA:HB3	1.93	0.51
1:F:65:THR:CG2	1:F:123:LEU:HD22	2.41	0.51
1:B:92:THR:HG23	1:B:98:THR:HG22	1.91	0.51
1:G:184:LEU:HA	1:G:217:ILE:HG22	1.93	0.51
1:C:59:LEU:HD22	1:C:175:ASN:HB3	1.92	0.51
1:E:48:ALA:O	1:E:52:ILE:HD13	2.11	0.51
1:B:103:GLU:OE1	1:D:107:THR:OG1	2.13	0.51
1:B:246:MET:CE	1:B:275:ILE:CD1	2.88	0.51
1:D:210:MET:HE1	1:D:214:PHE:CE2	2.45	0.51
1:F:26:THR:HG22	1:F:36:LEU:HG	1.92	0.51
1:F:90:PRO:HA	1:F:100:ALA:HB2	1.93	0.51
1:B:86:LEU:HD22	1:B:160:PRO:HB2	1.93	0.51
1:C:26:THR:HG21	1:C:34:LYS:O	2.11	0.51
1:D:26:THR:HG22	1:D:36:LEU:HG	1.93	0.51
1:A:48:ALA:O	1:A:52:ILE:HD13	2.11	0.50
1:D:72:HIS:HA	1:D:168:THR:CG2	2.41	0.50
1:G:26:THR:HG21	1:G:34:LYS:O	2.11	0.50
1:B:11:THR:HG23	1:B:12:GLU:HG2	1.93	0.50
1:F:92:THR:HG23	1:F:98:THR:HG22	1.93	0.50
1:G:65:THR:HG22	1:G:123:LEU:HD22	1.93	0.50
1:G:72:HIS:HA	1:G:168:THR:CG2	2.40	0.50
1:E:86:LEU:HD13	1:E:123:LEU:CD1	2.42	0.50
1:E:35:ASN:C	1:E:35:ASN:HD22	2.19	0.50
1:E:65:THR:HG22	1:E:123:LEU:HD22	1.93	0.50
1:F:26:THR:HG21	1:F:34:LYS:O	2.12	0.50
1:F:138:GLY:C	1:F:139:LEU:HD12	2.36	0.50
1:B:101:MET:HE2	1:B:104:MET:HA	1.93	0.50
1:F:37:ASN:ND2	2:F:311:SO4:O1	2.41	0.50
1:G:26:THR:HG22	1:G:36:LEU:HG	1.93	0.50
1:G:35:ASN:HB3	1:G:38:ALA:HB3	1.93	0.50
1:H:184:LEU:HA	1:H:217:ILE:HG22	1.94	0.50
1:A:86:LEU:HD13	1:A:123:LEU:CD1	2.41	0.50
1:D:92:THR:HG23	1:D:98:THR:HG22	1.93	0.50
1:C:63:PHE:CG	1:C:176:LEU:HD23	2.47	0.50
1:B:297:THR:HG23	1:B:297:THR:O	2.12	0.50
1:F:195:MET:O	1:F:199:VAL:HG23	2.12	0.49
1:C:184:LEU:HA	1:C:217:ILE:HG22	1.94	0.49
1:F:86:LEU:HD13	1:F:123:LEU:CD1	2.42	0.49
1:G:136:LEU:C	1:G:139:LEU:HD13	2.37	0.49
1:A:210:MET:HE1	1:A:214:PHE:CE2	2.48	0.49
1:E:210:MET:HE1	1:E:214:PHE:CE2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:26:THR:HG22	1:C:36:LEU:HG	1.95	0.49
1:G:101:MET:SD	1:G:104:MET:HE3	2.52	0.49
1:A:101:MET:HG2	1:A:104:MET:HE3	1.93	0.49
1:B:213:LEU:C	1:B:213:LEU:HD23	2.38	0.49
1:F:63:PHE:O	1:F:130:LEU:HD13	2.12	0.49
1:A:297:THR:HG23	1:A:297:THR:O	2.12	0.49
1:H:35:ASN:C	1:H:35:ASN:HD22	2.21	0.49
1:B:155:LEU:HD23	1:B:169:GLN:HG3	1.94	0.48
1:B:226:LEU:HD23	1:B:276:ILE:HD12	1.95	0.48
1:C:278:ASN:HB3	1:C:281:HIS:CD2	2.47	0.48
1:E:47:THR:HG21	1:E:76:PHE:CE1	2.49	0.48
1:G:238:ARG:O	1:G:240:VAL:HG23	2.13	0.48
1:H:14:ILE:HD13	1:H:90:PRO:HB3	1.95	0.48
1:D:101:MET:HG2	1:D:104:MET:HE3	1.95	0.48
1:F:124:GLN:CG	1:H:36:LEU:HD22	2.42	0.48
1:G:90:PRO:HA	1:G:100:ALA:HB2	1.95	0.48
1:A:14:ILE:HD13	1:A:90:PRO:HB3	1.96	0.48
1:F:21:TYR:CE2	1:F:28:LYS:HA	2.48	0.48
1:E:101:MET:SD	1:E:104:MET:CE	3.02	0.48
1:G:64:ASP:OD1	1:G:66:ALA:HB3	2.13	0.48
1:F:115:ILE:N	1:F:115:ILE:HD12	2.29	0.48
1:A:184:LEU:HA	1:A:217:ILE:HG22	1.95	0.48
1:C:68:LEU:HD11	1:C:155:LEU:HD11	1.96	0.48
1:C:155:LEU:HD23	1:C:169:GLN:HG3	1.96	0.48
1:F:233:MET:CE	1:F:238:ARG:HB2	2.40	0.47
1:H:101:MET:HG2	1:H:104:MET:HE3	1.96	0.47
1:B:278:ASN:HB3	1:B:281:HIS:CD2	2.48	0.47
1:C:65:THR:HG23	1:C:127:ASP:OD1	2.14	0.47
1:F:246:MET:HE3	1:F:275:ILE:HD12	1.95	0.47
1:H:236:THR:O	1:H:236:THR:HG22	2.14	0.47
1:A:86:LEU:CD1	1:C:25:THR:HG23	2.41	0.47
1:C:165:ASN:N	2:C:310[B]:SO4:O4	2.47	0.47
1:D:101:MET:SD	1:D:104:MET:HE2	2.55	0.47
1:H:47:THR:HG22	1:H:75:LEU:O	2.15	0.47
1:E:20:VAL:HG12	1:E:21:TYR:O	2.14	0.47
1:B:170:ARG:HD2	1:B:194:MET:HE2	1.95	0.47
1:D:101:MET:HE2	1:D:104:MET:HA	1.96	0.47
1:B:65:THR:HG23	1:B:127:ASP:OD1	2.15	0.47
1:C:54:LEU:HD13	1:C:171:LEU:CD1	2.44	0.47
1:D:184:LEU:HA	1:D:217:ILE:HG22	1.95	0.47
1:G:68:LEU:HD11	1:G:155:LEU:HD11	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:192:GLU:O	1:H:196:VAL:HG23	2.15	0.47
1:D:213:LEU:HD23	1:D:213:LEU:C	2.40	0.47
1:D:226:LEU:HD23	1:D:276:ILE:CD1	2.44	0.47
1:G:20:VAL:HG11	1:G:25:THR:HA	1.96	0.47
1:G:101:MET:SD	1:G:104:MET:CE	3.03	0.47
1:G:278:ASN:HB3	1:G:281:HIS:CD2	2.49	0.47
1:D:21:TYR:CE2	1:D:28:LYS:HA	2.49	0.47
1:D:26:THR:HG21	1:D:34:LYS:O	2.14	0.47
1:A:246:MET:CE	1:A:275:ILE:CD1	2.92	0.46
1:D:185:ASN:C	1:D:217:ILE:HG23	2.40	0.46
1:G:14:ILE:HD13	1:G:90:PRO:HB3	1.98	0.46
1:G:107:THR:HG21	1:G:109:TRP:NE1	2.31	0.46
1:H:48:ALA:O	1:H:52:ILE:HD13	2.14	0.46
1:E:88:HIS:HB3	1:E:119:ILE:HD12	1.96	0.46
1:G:35:ASN:C	1:G:35:ASN:ND2	2.74	0.46
1:B:210:MET:HE1	1:B:214:PHE:CE2	2.51	0.46
1:H:24:THR:HB	1:H:26:THR:HG23	1.98	0.46
1:H:246:MET:CE	1:H:275:ILE:CD1	2.91	0.46
1:F:278:ASN:HB3	1:F:281:HIS:CD2	2.50	0.46
1:H:195:MET:O	1:H:199:VAL:HG23	2.16	0.46
1:A:159:HIS:CE1	1:A:165:ASN:ND2	2.84	0.46
1:F:246:MET:CE	1:F:275:ILE:HD11	2.46	0.46
1:F:255:THR:CG2	1:F:297:THR:OG1	2.60	0.46
1:G:107:THR:HG22	1:G:110:LYS:HE2	1.98	0.46
1:C:286:GLN:O	1:C:290:LEU:HD13	2.16	0.46
1:E:75:LEU:HD12	1:E:168:THR:HG22	1.98	0.46
1:B:190:THR:HG21	1:B:245:VAL:HG23	1.97	0.46
1:G:92:THR:HG23	1:G:98:THR:HG22	1.98	0.46
1:G:112:ALA:O	1:G:157:GLN:NE2	2.49	0.46
1:H:210:MET:HE1	1:H:214:PHE:HE2	1.79	0.46
1:B:246:MET:CE	1:B:275:ILE:HD11	2.46	0.45
1:F:233:MET:O	1:F:234:LYS:C	2.58	0.45
1:F:14:ILE:HD13	1:F:90:PRO:HB3	1.99	0.45
1:A:47:THR:HG21	1:A:76:PHE:CE1	2.51	0.45
1:D:107:THR:HG22	1:D:110:LYS:HD2	1.97	0.45
1:E:225:LEU:HD22	1:E:265:GLY:HA3	1.97	0.45
1:F:11:THR:HG23	1:F:12:GLU:HG2	1.98	0.45
1:F:20:VAL:HG11	1:F:25:THR:HA	1.97	0.45
1:G:195:MET:O	1:G:199:VAL:HG23	2.17	0.45
1:A:21:TYR:CE2	1:A:28:LYS:HA	2.51	0.45
1:B:86:LEU:HD13	1:B:123:LEU:CD1	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:ASN:C	1:A:35:ASN:HD22	2.24	0.45
1:E:246:MET:CE	1:E:275:ILE:CD1	2.90	0.45
1:C:213:LEU:C	1:C:213:LEU:HD23	2.41	0.45
1:G:76:PHE:CZ	1:G:164:GLY:HA3	2.52	0.45
1:D:35:ASN:C	1:D:35:ASN:HD22	2.24	0.45
1:A:115:ILE:N	1:A:115:ILE:HD12	2.32	0.45
1:D:185:ASN:O	1:D:217:ILE:HD12	2.17	0.45
1:C:210:MET:HE1	1:C:214:PHE:CE2	2.52	0.45
1:A:101:MET:SD	1:A:104:MET:HE3	2.56	0.44
1:B:255:THR:CG2	1:B:297:THR:OG1	2.60	0.44
1:D:101:MET:SD	1:D:104:MET:CE	3.05	0.44
1:F:36:LEU:HD22	1:F:40:LEU:HD11	1.99	0.44
1:H:278:ASN:HB3	1:H:281:HIS:CD2	2.51	0.44
1:B:86:LEU:HD23	1:B:161:PHE:CE1	2.52	0.44
1:E:192:GLU:O	1:E:196:VAL:HG23	2.18	0.44
1:G:54:LEU:HD13	1:G:171:LEU:HD13	1.99	0.44
1:A:124:GLN:CG	1:C:36:LEU:HD13	2.45	0.44
1:C:114:ALA:HB2	1:C:158:LEU:HD23	1.99	0.44
1:F:185:ASN:C	1:F:217:ILE:HG23	2.42	0.44
1:G:36:LEU:HD22	1:G:40:LEU:HD11	1.99	0.44
1:G:72:HIS:CD2	1:G:168:THR:HG21	2.52	0.44
1:F:246:MET:CE	1:F:275:ILE:CD1	2.93	0.44
1:H:246:MET:CE	1:H:275:ILE:HD11	2.47	0.44
1:A:90:PRO:HA	1:A:100:ALA:HB2	2.00	0.44
1:F:20:VAL:HG12	1:F:21:TYR:O	2.18	0.44
1:D:72:HIS:CG	1:D:168:THR:HG21	2.53	0.44
1:G:164:GLY:N	2:G:310[B]:SO4:O2	2.50	0.44
1:B:26:THR:HG21	1:B:34:LYS:O	2.18	0.44
1:B:48:ALA:O	1:B:52:ILE:HD13	2.18	0.44
1:E:50:ALA:HB1	1:E:75:LEU:HA	2.00	0.44
1:E:65:THR:CG2	1:E:123:LEU:HD22	2.47	0.44
1:C:11:THR:HG23	1:C:12:GLU:HG2	1.99	0.43
1:E:20:VAL:HG13	1:E:26:THR:O	2.18	0.43
1:E:21:TYR:CE2	1:E:28:LYS:HA	2.53	0.43
1:E:246:MET:CE	1:E:275:ILE:HD11	2.48	0.43
1:H:233:MET:HE2	1:H:240:VAL:HG21	2.00	0.43
1:A:185:ASN:N	1:A:217:ILE:CG2	2.81	0.43
1:A:286:GLN:O	1:A:287:LEU:C	2.61	0.43
1:G:165:ASN:N	2:G:310[B]:SO4:O2	2.37	0.43
1:C:35:ASN:HD22	1:C:38:ALA:H	1.66	0.43
1:F:124:GLN:HG2	1:H:36:LEU:HD13	1.95	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:54:LEU:HB3	1:G:171:LEU:HD11	2.00	0.43
1:G:192:GLU:O	1:G:196:VAL:HG23	2.18	0.43
1:C:101:MET:HE2	1:C:104:MET:HA	1.99	0.43
1:H:26:THR:HG22	1:H:36:LEU:HG	2.01	0.43
1:F:124:GLN:CG	1:H:36:LEU:CD1	2.87	0.43
1:D:278:ASN:HB3	1:D:281:HIS:CD2	2.54	0.43
1:E:127:ASP:C	1:G:37:ASN:HD21	2.26	0.43
1:F:185:ASN:N	1:F:217:ILE:HG23	2.34	0.43
1:A:63:PHE:O	1:A:130:LEU:HD13	2.18	0.43
1:A:185:ASN:ND2	1:A:187:SER:OG	2.52	0.43
1:B:185:ASN:C	1:B:185:ASN:HD22	2.27	0.43
1:C:63:PHE:CZ	1:C:176:LEU:HA	2.53	0.43
1:H:229:PHE:CD2	1:H:245:VAL:HG11	2.54	0.43
1:D:48:ALA:O	1:D:52:ILE:HD13	2.19	0.42
1:A:232:THR:C	1:A:234:LYS:H	2.27	0.42
1:C:15:SER:OG	1:C:17:HIS:CD2	2.72	0.42
1:C:72:HIS:CD2	1:C:168:THR:HG21	2.54	0.42
1:C:228:GLU:OE2	1:C:263:LEU:N	2.52	0.42
1:H:155:LEU:HD23	1:H:169:GLN:HG3	2.01	0.42
1:C:54:LEU:HD13	1:C:171:LEU:HD13	1.99	0.42
1:E:190:THR:HB	1:E:241:ASN:HA	2.02	0.42
1:F:170:ARG:HD2	1:F:194:MET:HE2	2.01	0.42
1:G:286:GLN:O	1:G:290:LEU:HD13	2.19	0.42
1:B:185:ASN:N	1:B:217:ILE:CG2	2.83	0.42
1:G:54:LEU:HD13	1:G:171:LEU:CD1	2.50	0.42
1:A:103:GLU:HB2	1:A:115:ILE:HG23	2.01	0.42
1:D:164:GLY:O	1:D:168:THR:HG23	2.18	0.42
1:H:21:TYR:CE2	1:H:28:LYS:HA	2.55	0.42
1:A:170:ARG:HD2	1:A:194:MET:HE2	2.02	0.42
1:C:136:LEU:O	1:C:139:LEU:HD13	2.18	0.42
1:F:88:HIS:HE1	1:H:25:THR:HG21	1.85	0.42
1:G:48:ALA:O	1:G:52:ILE:HD13	2.20	0.42
1:B:189:ILE:HG21	1:B:194:MET:HG2	2.01	0.42
1:C:101:MET:SD	1:C:104:MET:CE	3.08	0.42
1:C:47:THR:HG21	1:C:76:PHE:CE1	2.55	0.42
1:E:278:ASN:HB3	1:E:281:HIS:CD2	2.54	0.42
1:G:82:TRP:CH2	1:G:162:ARG:HB3	2.54	0.42
1:F:185:ASN:N	1:F:217:ILE:CG2	2.82	0.42
1:A:165:ASN:ND2	2:A:310[B]:SO4:O2	2.51	0.41
1:C:72:HIS:HA	1:C:168:THR:HG21	2.02	0.41
1:G:233:MET:C	1:G:235:ASN:N	2.77	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:THR:HG23	1:B:12:GLU:N	2.35	0.41
1:B:21:TYR:CE2	1:B:28:LYS:HA	2.55	0.41
1:C:48:ALA:O	1:C:52:ILE:HD13	2.20	0.41
1:E:65:THR:HG23	1:E:127:ASP:OD1	2.20	0.41
1:F:101:MET:HG2	1:F:104:MET:HE3	2.02	0.41
1:C:21:TYR:CE2	1:C:28:LYS:HA	2.56	0.41
1:B:210:MET:HE3	1:B:210:MET:HB3	1.92	0.41
1:H:35:ASN:HB3	1:H:38:ALA:HB3	2.02	0.41
1:E:164:GLY:O	1:E:168:THR:HG23	2.20	0.41
1:E:195:MET:O	1:E:199:VAL:HG23	2.21	0.41
1:H:47:THR:HG21	1:H:76:PHE:CE1	2.55	0.41
1:B:50:ALA:HB1	1:B:75:LEU:HA	2.03	0.41
1:B:185:ASN:N	1:B:217:ILE:HG23	2.36	0.41
1:C:247:VAL:O	1:C:248:ALA:C	2.64	0.41
1:D:192:GLU:O	1:D:196:VAL:HG23	2.21	0.41
1:E:297:THR:O	1:E:297:THR:HG23	2.19	0.41
1:H:114:ALA:HB2	1:H:158:LEU:HD23	2.02	0.41
1:H:185:ASN:C	1:H:185:ASN:HD22	2.28	0.41
1:D:20:VAL:HG11	1:D:25:THR:HA	2.02	0.41
1:E:136:LEU:O	1:E:139:LEU:HD13	2.21	0.41
1:E:166:GLY:N	2:E:310[A]:SO4:O4	2.54	0.41
1:F:24:THR:HB	1:F:26:THR:HG23	2.03	0.40
1:G:11:THR:HG23	1:G:12:GLU:HG2	2.02	0.40
1:B:86:LEU:HD22	1:B:160:PRO:CB	2.51	0.40
1:C:195:MET:O	1:C:199:VAL:HG23	2.21	0.40
1:D:11:THR:HG23	1:D:12:GLU:HG2	2.02	0.40
1:G:229:PHE:CD2	1:G:245:VAL:HG11	2.56	0.40
1:E:15:SER:HG	1:E:17:HIS:CE1	2.39	0.40
1:D:35:ASN:HB3	1:D:38:ALA:HB3	2.02	0.40
1:F:65:THR:HG23	1:F:127:ASP:OD1	2.21	0.40
1:F:189:ILE:HG21	1:F:194:MET:HG2	2.03	0.40
1:H:213:LEU:HD23	1:H:213:LEU:C	2.47	0.40
1:F:124:GLN:OE1	1:H:40:LEU:HD11	2.21	0.40

All (5) 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:A:235:ASN:ND2	1:E:22:PRO:O[8_555]	1.74	0.46
1:C:237:GLY:CA	1:G:237:GLY:N[10_455]	1.89	0.31

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:ASN:ND2	1:B:235:ASN:CA[12_555]	1.97	0.23
1:D:236:THR:O	1:H:235:ASN:N[6_555]	2.06	0.14
1:D:236:THR:O	1:H:235:ASN:CA[6_555]	2.11	0.09

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	294/298 (99%)	278 (95%)	13 (4%)	3 (1%)	12	37
1	B	294/298 (99%)	281 (96%)	9 (3%)	4 (1%)	9	29
1	C	294/298 (99%)	280 (95%)	9 (3%)	5 (2%)	7	25
1	D	294/298 (99%)	281 (96%)	10 (3%)	3 (1%)	12	37
1	E	294/298 (99%)	283 (96%)	9 (3%)	2 (1%)	18	45
1	F	294/298 (99%)	282 (96%)	11 (4%)	1 (0%)	36	63
1	G	294/298 (99%)	279 (95%)	13 (4%)	2 (1%)	18	45
1	H	294/298 (99%)	283 (96%)	9 (3%)	2 (1%)	18	45
All	All	2352/2384 (99%)	2247 (96%)	83 (4%)	22 (1%)	14	39

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	239	ASN
1	C	108	GLY
1	C	113	PHE
1	D	235	ASN
1	G	237	GLY
1	B	112	ALA
1	C	105	LYS
1	C	107	THR
1	D	295	LYS

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Mol	Chain	Res	Type
1	B	106	ARG
1	C	295	LYS
1	H	295	LYS
1	E	295	LYS
1	F	295	LYS
1	G	295	LYS
1	H	105	LYS
1	A	105	LYS
1	A	295	LYS
1	D	105	LYS
1	E	105	LYS
1	B	105	LYS
1	B	108	GLY

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	252/254 (99%)	237 (94%)	15 (6%)	17	43
1	B	252/254 (99%)	239 (95%)	13 (5%)	21	48
1	C	252/254 (99%)	236 (94%)	16 (6%)	16	41
1	D	252/254 (99%)	240 (95%)	12 (5%)	23	50
1	E	252/254 (99%)	239 (95%)	13 (5%)	21	48
1	F	252/254 (99%)	236 (94%)	16 (6%)	16	41
1	G	252/254 (99%)	238 (94%)	14 (6%)	19	45
1	H	252/254 (99%)	240 (95%)	12 (5%)	23	50
All	All	2016/2032 (99%)	1905 (94%)	111 (6%)	19	46

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ILE
1	A	26	THR

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Mol	Chain	Res	Type
1	A	35	ASN
1	A	36	LEU
1	A	61	GLU
1	A	68	LEU
1	A	98	THR
1	A	104	MET
1	A	156	ASN
1	A	157	GLN
1	A	171	LEU
1	A	185	ASN
1	A	232	THR
1	A	234	LYS
1	A	295	LYS
1	B	13	ILE
1	B	26	THR
1	B	35	ASN
1	B	68	LEU
1	B	98	THR
1	B	104	MET
1	B	126	LEU
1	B	156	ASN
1	B	157	GLN
1	B	171	LEU
1	B	185	ASN
1	B	232	THR
1	B	234	LYS
1	C	13	ILE
1	C	26	THR
1	C	35	ASN
1	C	36	LEU
1	C	61	GLU
1	C	68	LEU
1	C	98	THR
1	C	104	MET
1	C	105	LYS
1	C	156	ASN
1	C	157	GLN
1	C	171	LEU
1	C	176	LEU
1	C	185	ASN
1	C	232	THR
1	C	234	LYS

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Mol	Chain	Res	Type
1	D	13	ILE
1	D	26	THR
1	D	35	ASN
1	D	36	LEU
1	D	61	GLU
1	D	68	LEU
1	D	98	THR
1	D	104	MET
1	D	157	GLN
1	D	171	LEU
1	D	185	ASN
1	D	232	THR
1	E	13	ILE
1	E	26	THR
1	E	35	ASN
1	E	36	LEU
1	E	68	LEU
1	E	98	THR
1	E	104	MET
1	E	156	ASN
1	E	157	GLN
1	E	171	LEU
1	E	176	LEU
1	E	185	ASN
1	E	232	THR
1	F	13	ILE
1	F	26	THR
1	F	35	ASN
1	F	36	LEU
1	F	61	GLU
1	F	68	LEU
1	F	98	THR
1	F	104	MET
1	F	156	ASN
1	F	157	GLN
1	F	171	LEU
1	F	176	LEU
1	F	185	ASN
1	F	232	THR
1	F	235	ASN
1	F	295	LYS
1	G	13	ILE

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Mol	Chain	Res	Type
1	G	26	THR
1	G	35	ASN
1	G	36	LEU
1	G	61	GLU
1	G	68	LEU
1	G	98	THR
1	G	110	LYS
1	G	156	ASN
1	G	157	GLN
1	G	171	LEU
1	G	185	ASN
1	G	232	THR
1	G	238	ARG
1	H	13	ILE
1	H	26	THR
1	H	35	ASN
1	H	36	LEU
1	H	68	LEU
1	H	98	THR
1	H	104	MET
1	H	156	ASN
1	H	157	GLN
1	H	171	LEU
1	H	185	ASN
1	H	232	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (97) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	ASN
1	A	74	GLN
1	A	124	GLN
1	A	135	ASN
1	A	169	GLN
1	A	175	ASN
1	A	183	GLN
1	A	185	ASN
1	A	305	HIS
1	B	17	HIS
1	B	35	ASN
1	B	70	HIS
1	B	74	GLN

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Mol	Chain	Res	Type
1	B	124	GLN
1	B	135	ASN
1	B	157	GLN
1	B	169	GLN
1	B	183	GLN
1	B	185	ASN
1	B	269	ASN
1	B	305	HIS
1	C	17	HIS
1	C	18	HIS
1	C	35	ASN
1	C	70	HIS
1	C	124	GLN
1	C	135	ASN
1	C	137	GLN
1	C	157	GLN
1	C	159	HIS
1	C	169	GLN
1	C	175	ASN
1	C	185	ASN
1	C	269	ASN
1	C	281	HIS
1	C	286	GLN
1	C	305	HIS
1	D	17	HIS
1	D	35	ASN
1	D	70	HIS
1	D	135	ASN
1	D	169	GLN
1	D	175	ASN
1	D	183	GLN
1	D	185	ASN
1	D	269	ASN
1	D	286	GLN
1	D	305	HIS
1	E	35	ASN
1	E	70	HIS
1	E	124	GLN
1	E	137	GLN
1	E	157	GLN
1	E	169	GLN
1	E	183	GLN

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Mol	Chain	Res	Type
1	E	185	ASN
1	E	239	ASN
1	E	269	ASN
1	E	281	HIS
1	F	17	HIS
1	F	35	ASN
1	F	137	GLN
1	F	157	GLN
1	F	169	GLN
1	F	175	ASN
1	F	183	GLN
1	F	185	ASN
1	F	212	HIS
1	F	269	ASN
1	F	281	HIS
1	F	305	HIS
1	G	17	HIS
1	G	35	ASN
1	G	37	ASN
1	G	70	HIS
1	G	135	ASN
1	G	157	GLN
1	G	159	HIS
1	G	169	GLN
1	G	175	ASN
1	G	185	ASN
1	G	269	ASN
1	G	286	GLN
1	G	305	HIS
1	H	17	HIS
1	H	18	HIS
1	H	35	ASN
1	H	70	HIS
1	H	124	GLN
1	H	135	ASN
1	H	157	GLN
1	H	159	HIS
1	H	169	GLN
1	H	185	ASN
1	H	239	ASN
1	H	269	ASN
1	H	305	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

18 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	H	310[A]	-	4,4,4	0.26	0	6,6,6	0.21	0
2	SO4	F	310[B]	-	4,4,4	0.23	0	6,6,6	0.15	0
2	SO4	B	310[A]	-	4,4,4	0.25	0	6,6,6	0.25	0
2	SO4	A	310[B]	-	4,4,4	0.22	0	6,6,6	0.17	0
2	SO4	C	310[A]	-	4,4,4	0.23	0	6,6,6	0.15	0
2	SO4	D	310[B]	-	4,4,4	0.33	0	6,6,6	0.20	0
2	SO4	E	310[B]	-	4,4,4	0.23	0	6,6,6	0.25	0
2	SO4	G	310[B]	-	4,4,4	0.24	0	6,6,6	0.24	0
2	SO4	F	310[A]	-	4,4,4	0.31	0	6,6,6	0.16	0
2	SO4	E	310[A]	-	4,4,4	0.27	0	6,6,6	0.18	0
2	SO4	B	310[B]	-	4,4,4	0.25	0	6,6,6	0.19	0
2	SO4	B	311	-	4,4,4	0.25	0	6,6,6	0.27	0
2	SO4	C	310[B]	-	4,4,4	0.25	0	6,6,6	0.11	0
2	SO4	F	311	-	4,4,4	0.18	0	6,6,6	0.27	0
2	SO4	G	310[A]	-	4,4,4	0.25	0	6,6,6	0.33	0
2	SO4	H	310[B]	-	4,4,4	0.28	0	6,6,6	0.27	0
2	SO4	A	310[A]	-	4,4,4	0.28	0	6,6,6	0.28	0
2	SO4	D	310[A]	-	4,4,4	0.26	0	6,6,6	0.10	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	310[B]	SO4	1	0
2	G	310[B]	SO4	2	0
2	E	310[A]	SO4	1	0
2	B	311	SO4	1	0
2	C	310[B]	SO4	1	0
2	F	311	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	3
1	D	2
1	A	2
1	F	1
1	H	1
1	B	1
1	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	105:LYS	C	106:ARG	N	1.87
1	F	105:LYS	C	106:ARG	N	1.85
1	C	233:MET	C	234:LYS	N	1.82
1	D	237:GLY	C	238:ARG	N	1.70
1	H	105:LYS	C	106:ARG	N	1.67
1	B	233:MET	C	234:LYS	N	1.66

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	238:ARG	C	239:ASN	N	1.65
1	D	234:LYS	C	235:ASN	N	1.65
1	E	105:LYS	C	106:ARG	N	1.65
1	C	112:ALA	C	113:PHE	N	1.16
1	A	234:LYS	C	235:ASN	N	0.93

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	285/298 (95%)	0.54	7 (2%) 58 35	28, 77, 78, 80	18 (6%)
1	B	285/298 (95%)	0.87	29 (10%) 12 6	28, 77, 78, 80	18 (6%)
1	C	283/298 (94%)	1.19	45 (15%) 5 2	28, 77, 78, 80	18 (6%)
1	D	293/298 (98%)	0.67	24 (8%) 17 9	28, 77, 78, 80	19 (6%)
1	E	289/298 (96%)	0.58	17 (5%) 28 14	28, 77, 78, 80	20 (6%)
1	F	289/298 (96%)	0.52	10 (3%) 47 26	28, 77, 78, 80	21 (7%)
1	G	296/298 (99%)	0.74	18 (6%) 27 14	28, 77, 78, 80	20 (6%)
1	H	289/298 (96%)	0.65	19 (6%) 24 12	28, 77, 78, 80	20 (6%)
All	All	2309/2384 (96%)	0.72	169 (7%) 21 10	28, 77, 78, 80	154 (6%)

All (169) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	112	ALA	6.4
1	B	304	HIS	5.0
1	G	306	HIS	4.9
1	H	306	HIS	4.9
1	C	256	GLY	4.8
1	E	236	THR	4.5
1	H	235	ASN	4.4
1	B	60	PRO	4.0
1	B	159	HIS	3.9
1	E	127	ASP	3.9
1	E	305	HIS	3.9
1	F	116	GLY	3.8
1	D	14	ILE	3.7
1	C	164	GLY	3.7
1	C	185	ASN	3.6
1	B	243	ARG	3.6

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Mol	Chain	Res	Type	RSRZ
1	H	234	LYS	3.6
1	F	159	HIS	3.5
1	H	297	THR	3.5
1	F	304	HIS	3.5
1	C	165	ASN	3.5
1	B	20	VAL	3.5
1	H	304	HIS	3.5
1	F	114	ALA	3.4
1	E	304	HIS	3.4
1	C	188	LEU	3.4
1	B	11	THR	3.4
1	G	234	LYS	3.4
1	D	18	HIS	3.4
1	F	198	SER	3.3
1	C	305	HIS	3.3
1	F	305	HIS	3.3
1	B	23	ASN	3.3
1	G	235	ASN	3.3
1	D	306	HIS	3.2
1	B	303	ALA	3.2
1	C	267	ALA	3.2
1	H	23	ASN	3.2
1	F	306	HIS	3.2
1	C	83	ALA	3.1
1	A	138	GLY	3.1
1	F	134	ASN	3.1
1	D	23	ASN	3.0
1	D	164	GLY	3.0
1	C	252	GLU	3.0
1	C	299	THR	3.0
1	D	13	ILE	3.0
1	C	306	HIS	3.0
1	D	270	VAL	2.9
1	B	217	ILE	2.9
1	C	117	ASP	2.9
1	A	20	VAL	2.9
1	C	221	GLU	2.9
1	G	302	LYS	2.9
1	E	235	ASN	2.8
1	E	164	GLY	2.8
1	B	218	SER	2.8
1	E	138	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	304	HIS	2.8
1	H	115	ILE	2.8
1	B	305	HIS	2.8
1	B	306	HIS	2.8
1	C	175	ASN	2.8
1	D	305	HIS	2.8
1	C	146	SER	2.8
1	C	300	ALA	2.7
1	B	63	PHE	2.7
1	D	285	GLU	2.7
1	E	163	GLU	2.7
1	D	238	ARG	2.7
1	C	81	GLU	2.7
1	H	303	ALA	2.7
1	C	172	PHE	2.6
1	E	162	ARG	2.6
1	H	260	GLY	2.6
1	H	15	SER	2.6
1	A	305	HIS	2.6
1	C	302	LYS	2.6
1	C	203	GLU	2.6
1	D	59	LEU	2.6
1	B	302	LYS	2.6
1	D	256	GLY	2.6
1	A	142	GLU	2.6
1	C	122	GLY	2.6
1	G	250	GLU	2.6
1	A	306	HIS	2.5
1	G	305	HIS	2.5
1	G	164	GLY	2.5
1	C	281	HIS	2.5
1	G	299	THR	2.5
1	C	304	HIS	2.5
1	C	268	LEU	2.5
1	C	181	GLY	2.5
1	G	37	ASN	2.5
1	G	153	ASN	2.5
1	H	236	THR	2.5
1	D	162	ARG	2.5
1	C	293	GLY	2.5
1	B	301	PRO	2.5
1	D	56	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	127	ASP	2.4
1	D	22	PRO	2.4
1	H	305	HIS	2.4
1	C	263	LEU	2.4
1	D	165	ASN	2.4
1	E	134	ASN	2.4
1	E	64	ASP	2.4
1	H	191	LYS	2.4
1	C	186	PHE	2.4
1	B	17	HIS	2.3
1	C	37	ASN	2.3
1	D	202	ALA	2.3
1	C	104	MET	2.3
1	G	285	GLU	2.3
1	C	13	ILE	2.3
1	H	165	ASN	2.3
1	D	250	GLU	2.3
1	C	46	ASP	2.3
1	D	183	GLN	2.3
1	C	131	ALA	2.3
1	C	225	LEU	2.3
1	C	240	VAL	2.3
1	C	270	VAL	2.2
1	E	35	ASN	2.2
1	B	150	GLU	2.2
1	C	245	VAL	2.2
1	H	14	ILE	2.2
1	B	138	GLY	2.2
1	C	301	PRO	2.2
1	D	52	ILE	2.2
1	E	121	GLU	2.2
1	H	160	PRO	2.2
1	G	158	LEU	2.2
1	B	252	GLU	2.2
1	B	273	ALA	2.2
1	D	159	HIS	2.2
1	D	302	LYS	2.1
1	B	300	ALA	2.1
1	B	35	ASN	2.1
1	E	20	VAL	2.1
1	C	11	THR	2.1
1	C	168	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	121	GLU	2.1
1	D	16	PRO	2.1
1	G	237	GLY	2.1
1	G	304	HIS	2.1
1	A	25	THR	2.1
1	G	230	MET	2.1
1	C	99	ALA	2.1
1	C	57	GLU	2.1
1	B	165	ASN	2.1
1	E	243	ARG	2.1
1	H	162	ARG	2.1
1	G	287	LEU	2.1
1	B	65	THR	2.1
1	D	209	PRO	2.1
1	E	165	ASN	2.0
1	E	242	ASP	2.0
1	F	242	ASP	2.0
1	H	168	THR	2.0
1	G	203	GLU	2.0
1	B	204	ASN	2.0
1	C	210	MET	2.0
1	H	11	THR	2.0
1	F	113	PHE	2.0
1	G	124	GLN	2.0
1	B	61	GLU	2.0
1	C	162	ARG	2.0
1	C	14	ILE	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
2	SO4	H	310[A]	5/5	0.64	0.19	59,59,60,60	5
2	SO4	H	310[B]	5/5	0.64	0.19	48,49,49,49	5
2	SO4	F	310[A]	5/5	0.83	0.18	54,54,55,55	5
2	SO4	F	310[B]	5/5	0.83	0.18	45,46,47,47	5
2	SO4	D	310[A]	5/5	0.83	0.22	63,63,63,64	5
2	SO4	D	310[B]	5/5	0.83	0.22	29,30,31,31	5
2	SO4	C	310[A]	5/5	0.86	0.17	63,64,64,64	5
2	SO4	C	310[B]	5/5	0.86	0.17	36,37,37,37	5
2	SO4	B	310[A]	5/5	0.90	0.25	54,54,54,54	5
2	SO4	B	310[B]	5/5	0.90	0.25	22,23,23,24	5
2	SO4	F	311	5/5	0.91	0.20	78,78,78,78	0
2	SO4	E	310[A]	5/5	0.91	0.21	57,58,58,58	5
2	SO4	E	310[B]	5/5	0.91	0.21	23,23,24,24	5
2	SO4	B	311	5/5	0.92	0.21	66,67,67,67	0
2	SO4	G	310[A]	5/5	0.93	0.22	41,42,43,43	5
2	SO4	G	310[B]	5/5	0.93	0.22	27,28,29,29	5
2	SO4	A	310[A]	5/5	0.95	0.25	31,32,33,33	5
2	SO4	A	310[B]	5/5	0.95	0.25	50,50,51,51	5

6.5 Other polymers

There are no such residues in this entry.