



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:40 AM UTC

PDB ID : 3O4F / pdb_00003o4f
Title : Crystal Structure of Spermidine Synthase from E. coli
Authors : Zhou, X.; Tkaczuk, K.L.; Chruszcz, M.; Chua, T.K.; Minor, W.; Sivaraman, J.
Deposited on : 2010-07-27
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:

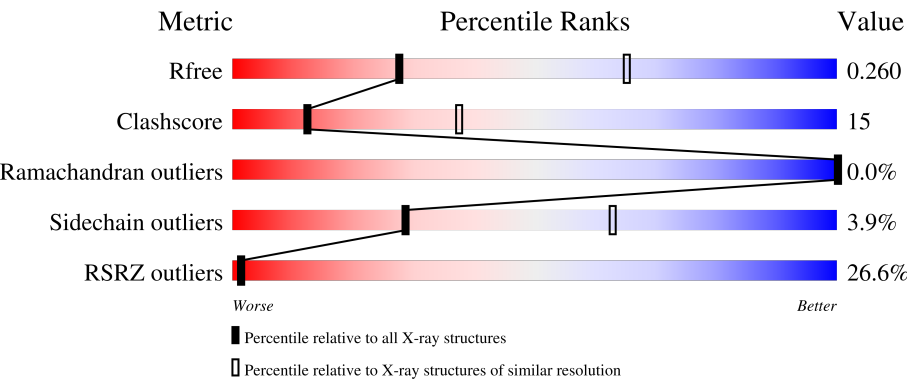
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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	294	28% 70% 23% ..
1	B	294	10% 64% 24% .. 8%
1	C	294	26% 66% 27% ..
1	D	294	6% 69% 21% . 6%
1	E	294	37% 68% 22% 5% ..

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Mol	Chain	Length	Quality of chain
1	F	294	
1	G	294	
1	H	294	

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	A	292	-	-	X	-
2	SO4	C	291	-	-	X	-
2	SO4	E	290	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17519 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 Spermidine synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	282	Total	C	N	O	S	0	0	0
			2212	1409	376	415	12			
1	B	270	Total	C	N	O	S	0	0	0
			2135	1359	366	398	12			
1	C	284	Total	C	N	O	S	0	0	0
			2228	1417	379	420	12			
1	D	276	Total	C	N	O	S	0	0	0
			2176	1385	371	408	12			
1	E	283	Total	C	N	O	S	0	0	0
			2208	1406	372	418	12			
1	F	269	Total	C	N	O	S	0	0	0
			2116	1347	361	396	12			
1	G	279	Total	C	N	O	S	0	0	0
			2189	1396	371	410	12			
1	H	264	Total	C	N	O	S	0	0	0
			2087	1330	356	389	12			

There are 48 discrepancies between the modelled and reference sequences:

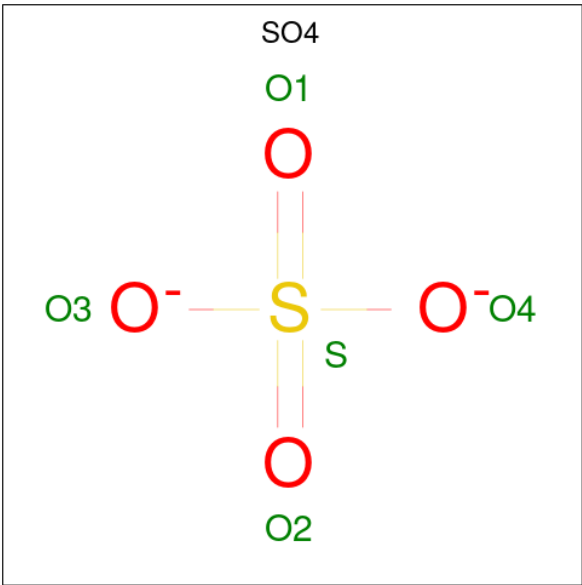
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	expression tag	UNP P09158
A	-4	HIS	-	expression tag	UNP P09158
A	-3	HIS	-	expression tag	UNP P09158
A	-2	HIS	-	expression tag	UNP P09158
A	-1	HIS	-	expression tag	UNP P09158
A	0	HIS	-	expression tag	UNP P09158
B	-5	HIS	-	expression tag	UNP P09158
B	-4	HIS	-	expression tag	UNP P09158
B	-3	HIS	-	expression tag	UNP P09158
B	-2	HIS	-	expression tag	UNP P09158
B	-1	HIS	-	expression tag	UNP P09158
B	0	HIS	-	expression tag	UNP P09158
C	-5	HIS	-	expression tag	UNP P09158

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	HIS	-	expression tag	UNP P09158
C	-3	HIS	-	expression tag	UNP P09158
C	-2	HIS	-	expression tag	UNP P09158
C	-1	HIS	-	expression tag	UNP P09158
C	0	HIS	-	expression tag	UNP P09158
D	-5	HIS	-	expression tag	UNP P09158
D	-4	HIS	-	expression tag	UNP P09158
D	-3	HIS	-	expression tag	UNP P09158
D	-2	HIS	-	expression tag	UNP P09158
D	-1	HIS	-	expression tag	UNP P09158
D	0	HIS	-	expression tag	UNP P09158
E	-5	HIS	-	expression tag	UNP P09158
E	-4	HIS	-	expression tag	UNP P09158
E	-3	HIS	-	expression tag	UNP P09158
E	-2	HIS	-	expression tag	UNP P09158
E	-1	HIS	-	expression tag	UNP P09158
E	0	HIS	-	expression tag	UNP P09158
F	-5	HIS	-	expression tag	UNP P09158
F	-4	HIS	-	expression tag	UNP P09158
F	-3	HIS	-	expression tag	UNP P09158
F	-2	HIS	-	expression tag	UNP P09158
F	-1	HIS	-	expression tag	UNP P09158
F	0	HIS	-	expression tag	UNP P09158
G	-5	HIS	-	expression tag	UNP P09158
G	-4	HIS	-	expression tag	UNP P09158
G	-3	HIS	-	expression tag	UNP P09158
G	-2	HIS	-	expression tag	UNP P09158
G	-1	HIS	-	expression tag	UNP P09158
G	0	HIS	-	expression tag	UNP P09158
H	-5	HIS	-	expression tag	UNP P09158
H	-4	HIS	-	expression tag	UNP P09158
H	-3	HIS	-	expression tag	UNP P09158
H	-2	HIS	-	expression tag	UNP P09158
H	-1	HIS	-	expression tag	UNP P09158
H	0	HIS	-	expression tag	UNP P09158

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



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

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	O	0	0
			2	2		
3	B	1	Total	O	0	0
			1	1		

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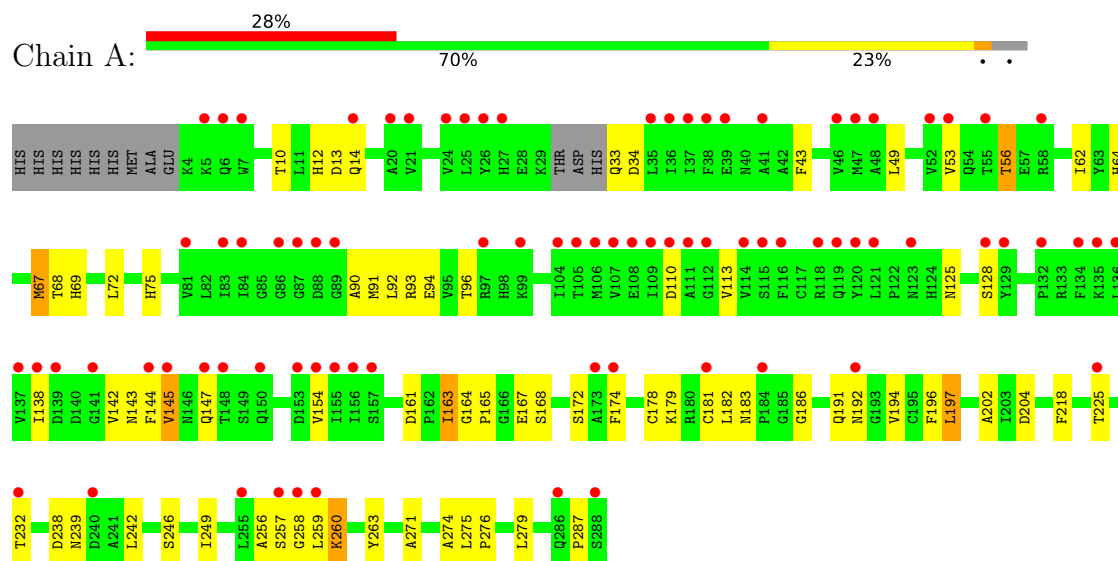
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	3	Total 3	O 3	0	0
3	D	1	Total 1	O 1	0	0
3	E	3	Total 3	O 3	0	0
3	F	1	Total 1	O 1	0	0
3	G	1	Total 1	O 1	0	0
3	H	1	Total 1	O 1	0	0

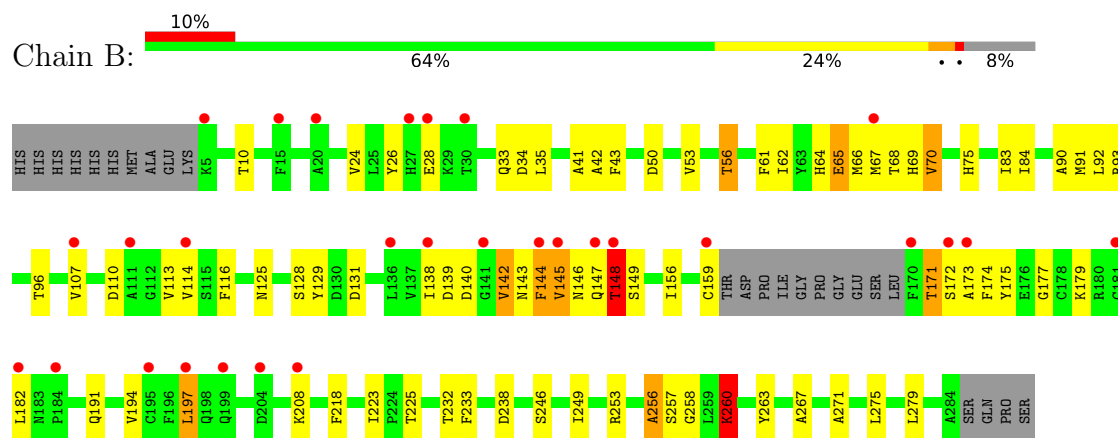
3 Residue-property plots [i](#)

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

• Molecule 1: Spermidine synthase

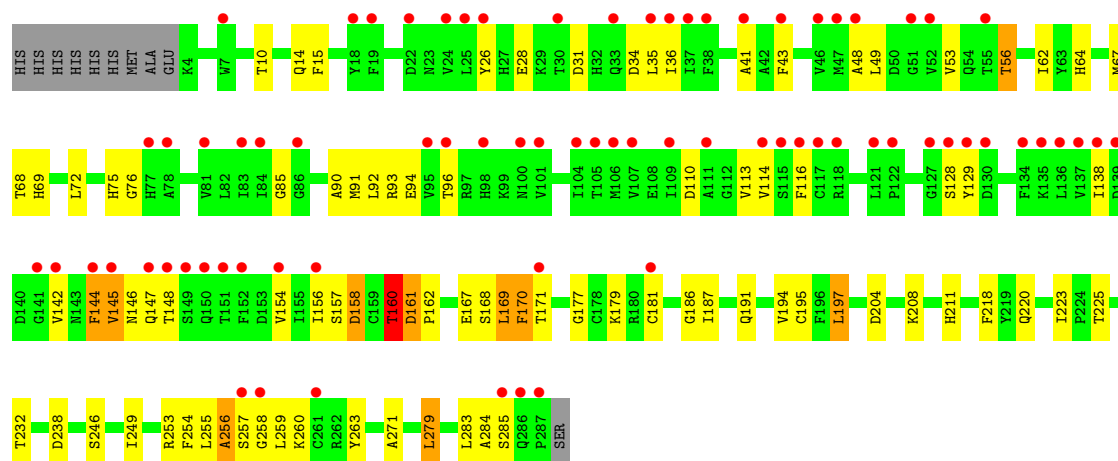


• Molecule 1: Spermidine synthase

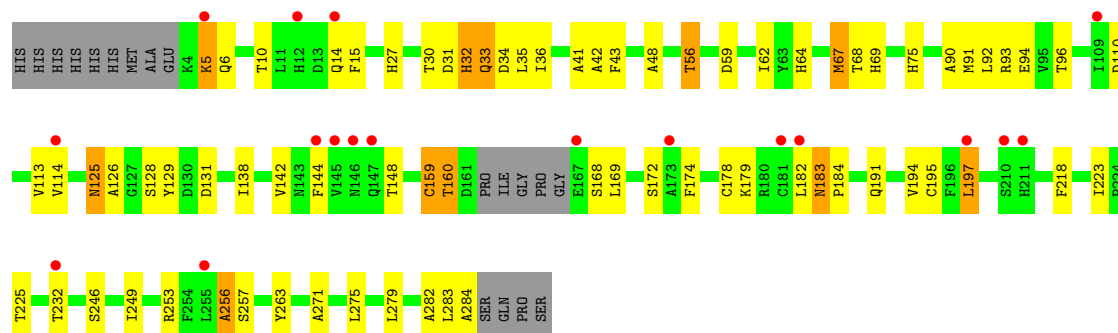


• Molecule 1: Spermidine synthase

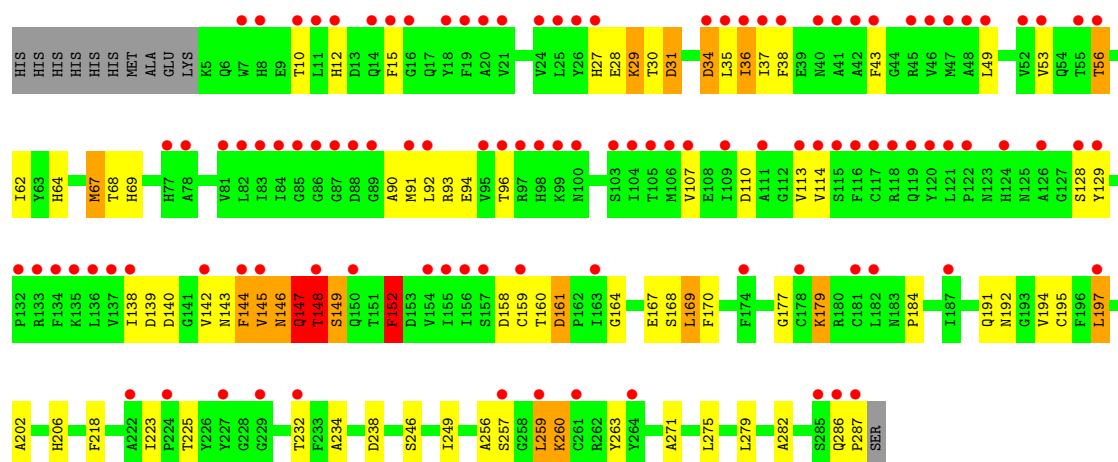




• Molecule 1: Spermidine synthase

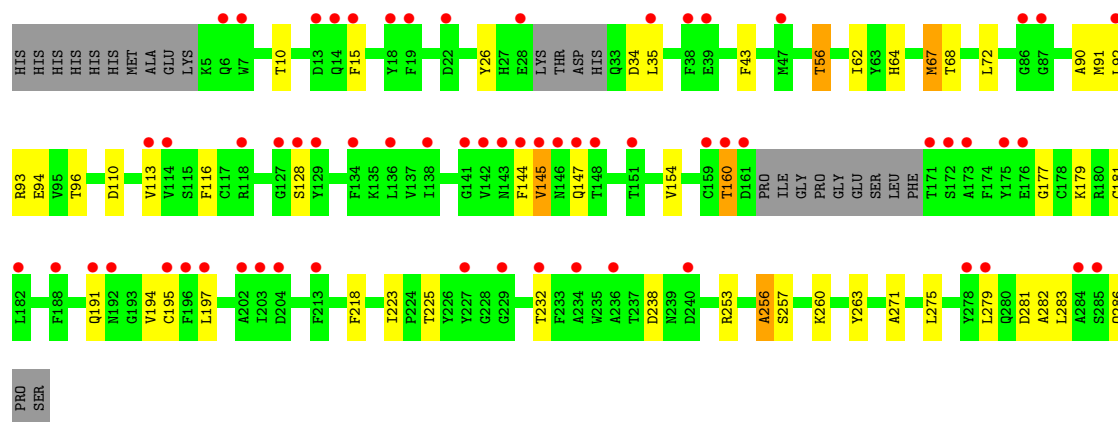


• Molecule 1: Spermidine synthase

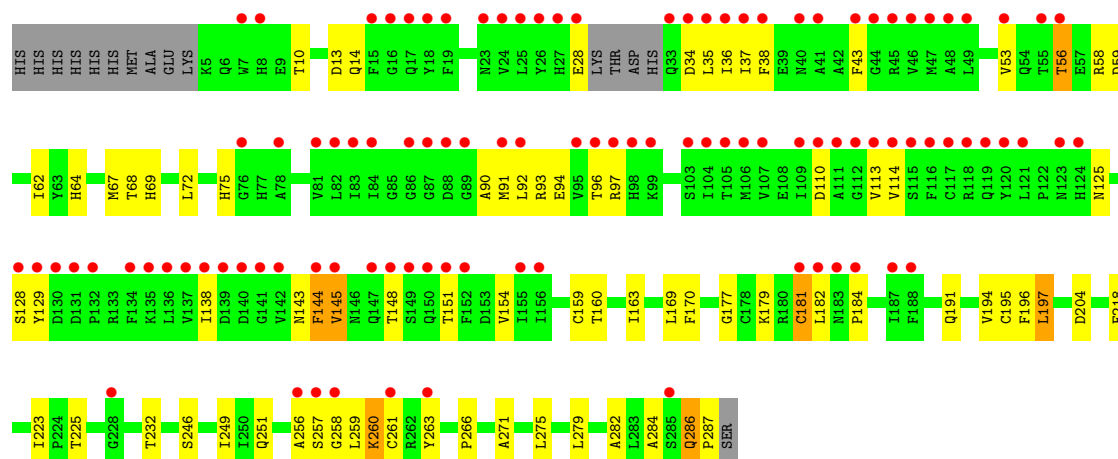


• Molecule 1: Spermidine synthase

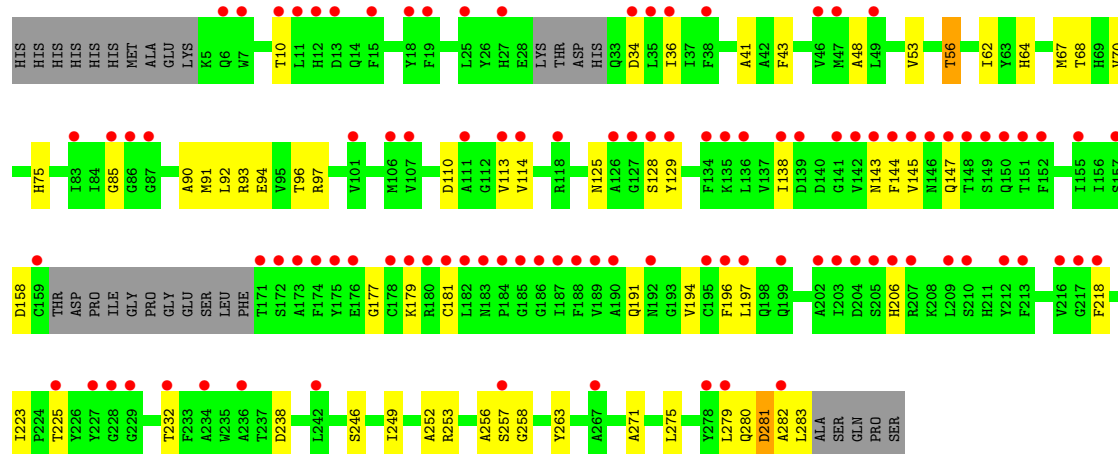




• Molecule 1: Spermidine synthase



• Molecule 1: Spermidine synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	123.11Å 123.11Å 210.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.29 – 2.90 48.29 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.9 (48.29-2.90) 98.9 (48.29-2.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.6.0070	Depositor
R, R_{free}	0.208 , 0.241 0.247 , 0.260	Depositor DCC
R_{free} test set	3486 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	62.7	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 97.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.108 for h,-k,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	17519	wwPDB-VP
Average B, all atoms (Å ²)	110.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.02	1/2269 (0.0%)	1.02	5/3083 (0.2%)
1	B	1.15	7/2189 (0.3%)	1.06	10/2971 (0.3%)
1	C	1.15	4/2287 (0.2%)	1.12	16/3111 (0.5%)
1	D	1.11	4/2231 (0.2%)	1.05	8/3030 (0.3%)
1	E	1.03	3/2266 (0.1%)	1.07	13/3084 (0.4%)
1	F	0.90	2/2168 (0.1%)	0.96	2/2943 (0.1%)
1	G	1.08	5/2246 (0.2%)	1.02	6/3052 (0.2%)
1	H	0.94	3/2139 (0.1%)	0.96	2/2903 (0.1%)
All	All	1.05	29/17795 (0.2%)	1.03	62/24177 (0.3%)

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	256	ALA	CA-C	-7.16	1.43	1.52
1	C	156	ILE	CA-CB	-6.68	1.46	1.54
1	B	256	ALA	CA-CB	-6.48	1.43	1.53
1	H	70	VAL	CA-CB	-6.46	1.50	1.54
1	D	126	ALA	CA-CB	-6.42	1.43	1.53
1	D	256	ALA	CA-CB	-5.95	1.43	1.53
1	H	143	ASN	CG-ND2	5.89	1.45	1.33
1	G	282	ALA	CA-CB	-5.87	1.44	1.53
1	B	256	ALA	CA-C	-5.82	1.45	1.52
1	E	282	ALA	CA-CB	-5.72	1.44	1.53
1	G	261	CYS	CA-C	-5.70	1.45	1.52
1	B	267	ALA	CA-CB	-5.64	1.44	1.53
1	C	144	PHE	CA-C	5.55	1.61	1.52
1	G	144	PHE	CA-C	5.55	1.61	1.52
1	C	256	ALA	CA-CB	-5.48	1.44	1.53
1	G	284	ALA	CA-CB	-5.40	1.44	1.53
1	G	148	THR	N-CA	5.33	1.52	1.46
1	F	256	ALA	CA-CB	-5.33	1.43	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	279	LEU	C-O	-5.31	1.18	1.24
1	F	256	ALA	CA-C	-5.31	1.46	1.52
1	A	274	ALA	CA-CB	5.27	1.60	1.53
1	B	65	GLU	C-O	-5.25	1.18	1.24
1	B	24	VAL	CA-CB	-5.23	1.47	1.54
1	B	171	THR	CA-CB	5.14	1.61	1.53
1	B	142	VAL	CA-CB	-5.09	1.47	1.54
1	H	252	ALA	CA-CB	-5.09	1.45	1.53
1	E	147	GLN	CA-C	-5.06	1.46	1.52
1	E	234	ALA	CA-CB	-5.06	1.45	1.53
1	D	282	ALA	CA-CB	-5.05	1.45	1.53

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	148	THR	N-CA-C	-12.01	98.15	112.92
1	E	148	THR	N-CA-C	-11.95	98.69	113.02
1	H	281	ASP	N-CA-C	-10.36	99.99	111.28
1	D	183	ASN	N-CA-C	-8.92	97.07	110.01
1	C	186	GLY	N-CA-C	8.50	121.71	111.93
1	E	161	ASP	N-CA-C	-7.91	98.09	109.48
1	E	145	VAL	N-CA-C	-7.51	103.98	113.22
1	E	260	LYS	N-CA-C	-7.49	96.69	108.90
1	A	260	LYS	N-CA-C	-7.35	96.43	108.41
1	A	145	VAL	N-CA-C	-7.34	102.23	113.16
1	G	260	LYS	N-CA-C	-7.10	96.84	108.41
1	G	145	VAL	N-CA-C	-7.10	105.80	112.83
1	C	260	LYS	N-CA-C	-6.80	97.33	108.41
1	E	29	LYS	N-CA-C	6.72	122.97	114.31
1	C	161	ASP	CA-C-N	6.70	126.61	119.85
1	C	161	ASP	C-N-CA	6.70	126.61	119.85
1	E	142	VAL	N-CA-C	-6.61	103.88	110.62
1	D	256	ALA	N-CA-C	-6.58	97.49	108.75
1	C	259	LEU	N-CA-C	-6.53	99.11	109.23
1	B	145	VAL	N-CA-C	-6.48	102.56	111.89
1	B	75	HIS	N-CA-C	-6.40	101.65	110.35
1	D	75	HIS	N-CA-C	-6.23	101.88	110.35
1	E	28	GLU	N-CA-C	-6.19	98.30	108.76
1	A	197	LEU	N-CA-C	5.99	117.89	111.36
1	C	145	VAL	N-CA-C	-5.98	105.92	112.80
1	E	147	GLN	N-CA-C	-5.94	98.16	110.80
1	C	162	PRO	N-CA-C	5.88	120.73	111.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	148	THR	N-CA-C	-5.88	104.25	112.25
1	C	197	LEU	N-CA-C	5.85	117.73	111.36
1	F	282	ALA	N-CA-C	-5.74	106.12	113.01
1	F	145	VAL	N-CA-C	-5.60	106.36	112.80
1	E	31	ASP	N-CA-C	-5.59	102.75	110.35
1	C	148	THR	N-CA-C	-5.57	104.67	112.25
1	C	75	HIS	N-CA-C	-5.57	102.16	110.23
1	C	169	LEU	N-CA-C	5.53	117.39	111.36
1	E	152	PHE	N-CA-C	5.49	117.75	109.41
1	D	148	THR	N-CA-C	-5.48	104.79	112.25
1	B	260	LYS	N-CA-C	-5.46	98.30	108.02
1	H	75	HIS	N-CA-C	-5.46	102.31	110.23
1	G	261	CYS	N-CA-C	-5.45	101.07	109.52
1	D	32	HIS	N-CA-C	5.44	117.29	111.36
1	A	75	HIS	N-CA-C	-5.42	102.38	110.23
1	D	197	LEU	N-CA-C	5.39	117.16	111.28
1	B	175	TYR	N-CA-C	5.38	116.95	111.14
1	D	131	ASP	CA-C-N	5.36	125.69	119.47
1	D	131	ASP	C-N-CA	5.36	125.69	119.47
1	A	287	PRO	N-CA-C	5.34	121.84	112.01
1	C	187	ILE	CB-CA-C	-5.34	102.67	110.62
1	B	68	THR	CB-CA-C	-5.33	101.34	110.24
1	G	148	THR	N-CA-CB	5.32	118.66	110.79
1	G	75	HIS	N-CA-C	-5.30	102.54	110.23
1	B	131	ASP	CA-C-N	5.29	125.10	119.28
1	B	131	ASP	C-N-CA	5.29	125.10	119.28
1	E	169	LEU	N-CA-C	5.25	117.08	111.36
1	B	70	VAL	N-CA-CB	5.17	113.99	110.52
1	B	197	LEU	N-CA-C	5.17	116.91	111.28
1	C	220	GLN	N-CA-C	5.16	116.91	109.07
1	C	157	SER	N-CA-C	5.15	117.29	108.90
1	E	197	LEU	N-CA-C	5.14	117.78	111.82
1	C	160	THR	N-CA-C	-5.11	101.53	109.24
1	C	31	ASP	N-CA-C	-5.08	105.74	111.28
1	E	146	ASN	N-CA-C	-5.08	105.92	111.82

There are no chirality outliers.

There are no planarity outliers.

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	2212	0	2078	66	0
1	B	2135	0	2012	76	0
1	C	2228	0	2084	63	0
1	D	2176	0	2039	57	0
1	E	2208	0	2060	108	0
1	F	2116	0	1985	44	0
1	G	2189	0	2060	72	0
1	H	2087	0	1962	50	0
2	A	20	0	0	5	0
2	B	10	0	0	0	0
2	C	30	0	0	5	0
2	D	20	0	0	0	0
2	E	20	0	0	4	0
2	F	20	0	0	0	0
2	G	25	0	0	0	0
2	H	10	0	0	0	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
3	C	3	0	0	0	0
3	D	1	0	0	0	0
3	E	3	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
All	All	17519	0	16280	521	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 15.

All (521) 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:G:258:GLY:O	1:G:259:LEU:HD12	1.38	1.20
1:E:145:VAL:HG23	1:E:177:GLY:CA	1.80	1.12
1:B:171:THR:HG22	1:B:173:ALA:H	1.11	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:258:GLY:C	1:G:259:LEU:HD12	1.78	1.09
1:E:145:VAL:HG23	1:E:177:GLY:HA2	1.39	1.01
1:G:256:ALA:HA	1:G:257:SER:C	1.83	1.00
1:G:93:ARG:HG2	1:G:97:ARG:NH2	1.75	1.00
1:A:256:ALA:HA	1:A:257:SER:C	1.87	1.00
1:E:259:LEU:N	1:E:259:LEU:HD23	1.76	0.97
1:G:93:ARG:HG2	1:G:97:ARG:HH22	1.28	0.97
1:E:146:ASN:O	1:E:147:GLN:HB2	1.63	0.96
1:E:271:ALA:HB1	1:F:271:ALA:HB1	1.48	0.94
1:A:271:ALA:HB1	1:B:271:ALA:HB1	1.51	0.92
1:H:279:LEU:O	1:H:282:ALA:HB3	1.68	0.91
1:G:258:GLY:C	1:G:259:LEU:CD1	2.46	0.89
1:E:145:VAL:CG2	1:E:177:GLY:HA2	2.03	0.89
1:B:145:VAL:HG22	1:B:177:GLY:HA3	1.56	0.88
1:E:145:VAL:HG23	1:E:177:GLY:HA3	1.53	0.88
1:H:68:THR:HB	1:H:91:MET:CE	2.04	0.88
1:C:76:GLY:HA2	1:C:253:ARG:NH1	1.90	0.87
1:G:93:ARG:CG	1:G:97:ARG:HH22	1.87	0.87
1:B:148:THR:HG22	1:B:148:THR:O	1.75	0.87
1:E:145:VAL:CG2	1:E:177:GLY:CA	2.52	0.87
1:C:271:ALA:HB1	1:D:271:ALA:HB1	1.57	0.87
1:D:68:THR:HB	1:D:91:MET:CE	2.07	0.85
1:E:144:PHE:CD1	1:E:144:PHE:O	2.30	0.85
1:G:286:GLN:HG3	1:G:287:PRO:HD2	1.58	0.85
1:F:68:THR:HB	1:F:91:MET:CE	2.08	0.84
1:G:271:ALA:HB1	1:H:271:ALA:HB1	1.58	0.84
1:B:171:THR:HG22	1:B:173:ALA:N	1.93	0.83
1:C:168:SER:HB3	2:C:291:SO4:S	2.17	0.83
1:B:143:ASN:O	1:B:146:ASN:HB2	1.79	0.83
1:A:182:LEU:HD23	1:A:183:ASN:O	1.79	0.82
1:A:182:LEU:HD21	1:A:186:GLY:CA	2.09	0.81
1:C:68:THR:HB	1:C:91:MET:CE	2.10	0.81
1:B:140:ASP:HB3	1:B:143:ASN:HB2	1.62	0.80
1:H:68:THR:HB	1:H:91:MET:HE2	1.63	0.80
1:E:68:THR:HB	1:E:91:MET:CE	2.11	0.80
1:D:33:GLN:HG3	1:D:34:ASP:N	1.98	0.79
1:C:256:ALA:HA	1:C:257:SER:C	2.05	0.79
1:E:35:LEU:O	1:E:36:ILE:HG22	1.83	0.79
1:E:30:THR:HG22	1:E:31:ASP:N	1.98	0.78
1:E:107:VAL:HG21	1:E:144:PHE:CD2	2.19	0.77
1:C:168:SER:HB3	2:C:291:SO4:O1	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:275:LEU:HD13	1:H:279:LEU:HD23	1.65	0.77
1:A:182:LEU:HD21	1:A:186:GLY:HA3	1.65	0.76
1:B:148:THR:O	1:B:149:SER:HB2	1.85	0.75
1:D:283:LEU:O	1:D:284:ALA:C	2.30	0.74
1:E:34:ASP:OD2	1:E:34:ASP:C	2.29	0.74
1:G:256:ALA:HA	1:G:258:GLY:N	2.00	0.74
1:E:67:MET:HE1	1:E:191:GLN:N	2.02	0.74
1:B:84:ILE:HD13	1:B:174:PHE:CE1	2.23	0.74
1:E:147:GLN:HB3	1:E:149:SER:H	1.52	0.74
1:G:286:GLN:CG	1:G:287:PRO:HD2	2.18	0.74
1:D:34:ASP:OD2	1:D:34:ASP:C	2.30	0.73
1:E:145:VAL:CG2	1:E:177:GLY:HA3	2.17	0.73
1:A:68:THR:HB	1:A:91:MET:CE	2.18	0.73
1:E:30:THR:HG22	1:E:31:ASP:H	1.53	0.73
1:G:275:LEU:HB3	1:G:279:LEU:HD23	1.70	0.73
1:G:67:MET:HE1	1:G:191:GLN:N	2.04	0.72
1:D:68:THR:HB	1:D:91:MET:HE2	1.71	0.72
1:C:67:MET:HE1	1:C:191:GLN:N	2.07	0.70
1:E:148:THR:HG22	1:E:148:THR:O	1.90	0.70
1:A:164:GLY:HA3	1:A:167:GLU:CG	2.22	0.70
1:B:139:ASP:OD1	1:B:143:ASN:ND2	2.21	0.70
1:B:139:ASP:OD2	1:B:143:ASN:HB3	1.92	0.70
1:E:68:THR:HB	1:E:91:MET:HE2	1.73	0.69
1:H:67:MET:HE1	1:H:191:GLN:N	2.07	0.69
1:C:68:THR:HB	1:C:91:MET:HE2	1.74	0.69
1:A:182:LEU:CD2	1:A:186:GLY:HA3	2.22	0.69
1:B:256:ALA:HA	1:B:257:SER:C	2.16	0.69
1:C:34:ASP:OD2	1:C:34:ASP:C	2.33	0.69
1:F:10:THR:HG22	1:F:10:THR:O	1.93	0.69
1:G:68:THR:HB	1:G:91:MET:CE	2.24	0.69
1:D:67:MET:HE1	1:D:191:GLN:N	2.07	0.68
2:A:292:SO4:S	1:E:168:SER:HB2	2.33	0.68
1:D:160:THR:CG2	1:D:160:THR:O	2.41	0.68
1:G:64:HIS:O	1:G:68:THR:HG22	1.93	0.68
1:G:258:GLY:O	1:G:259:LEU:CD1	2.30	0.68
1:B:67:MET:CG	1:B:91:MET:HE1	2.22	0.68
1:H:275:LEU:HD13	1:H:279:LEU:CD2	2.24	0.68
1:G:14:GLN:HG3	1:H:41:ALA:HB3	1.74	0.68
1:E:256:ALA:HA	1:E:257:SER:C	2.19	0.68
1:E:148:THR:O	1:E:148:THR:CG2	2.42	0.68
1:G:68:THR:HB	1:G:91:MET:HE2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:MET:HG2	1:B:91:MET:HE1	1.77	0.67
1:D:160:THR:O	1:D:160:THR:HG22	1.94	0.67
1:B:91:MET:HE3	1:B:156:ILE:HG21	1.75	0.67
1:G:256:ALA:CA	1:G:257:SER:C	2.62	0.67
1:A:67:MET:HE1	1:A:191:GLN:N	2.10	0.67
1:H:256:ALA:HA	1:H:257:SER:C	2.18	0.67
1:B:148:THR:O	1:B:148:THR:CG2	2.42	0.67
1:F:43:PHE:HB3	1:F:56:THR:CG2	2.25	0.66
1:E:35:LEU:C	1:E:36:ILE:HG22	2.20	0.66
1:A:164:GLY:CA	1:A:167:GLU:HG2	2.25	0.66
1:C:64:HIS:O	1:C:68:THR:HG22	1.96	0.66
1:E:35:LEU:C	1:E:36:ILE:CG2	2.69	0.66
1:D:33:GLN:CG	1:D:34:ASP:N	2.58	0.66
1:A:256:ALA:CA	1:A:257:SER:C	2.66	0.66
1:C:167:GLU:OE1	1:C:167:GLU:N	2.29	0.66
1:A:256:ALA:HA	1:A:258:GLY:N	2.11	0.65
1:E:140:ASP:O	1:E:143:ASN:HB3	1.96	0.65
1:E:144:PHE:CD1	1:E:144:PHE:C	2.73	0.65
1:F:68:THR:HG21	1:F:94:GLU:HB3	1.79	0.65
1:B:84:ILE:HD13	1:B:174:PHE:HE1	1.59	0.65
1:A:164:GLY:HA3	1:A:167:GLU:HG2	1.77	0.65
1:E:139:ASP:OD1	1:E:140:ASP:N	2.29	0.65
1:H:196:PHE:HD2	1:H:197:LEU:HD12	1.62	0.65
1:A:164:GLY:C	1:A:167:GLU:HG2	2.22	0.64
1:B:172:SER:HB2	1:B:208:LYS:NZ	2.11	0.64
1:A:68:THR:HB	1:A:91:MET:HE2	1.80	0.64
1:F:68:THR:HB	1:F:91:MET:HE2	1.80	0.64
1:F:67:MET:HE1	1:F:191:GLN:N	2.12	0.64
1:E:27:HIS:CE1	1:E:36:ILE:HG21	2.32	0.64
1:E:64:HIS:O	1:E:68:THR:HG22	1.99	0.63
1:B:43:PHE:HB3	1:B:56:THR:CG2	2.29	0.63
1:C:170:PHE:N	1:C:170:PHE:CD1	2.65	0.63
1:H:64:HIS:O	1:H:68:THR:HG22	1.98	0.63
1:B:179:LYS:HZ1	1:B:238:ASP:CG	2.06	0.63
1:E:143:ASN:O	1:E:145:VAL:N	2.30	0.63
1:G:68:THR:HG21	1:G:94:GLU:HB3	1.81	0.63
1:A:68:THR:HG21	1:A:94:GLU:HB3	1.81	0.62
1:E:143:ASN:C	1:E:145:VAL:H	2.06	0.62
1:E:34:ASP:OD2	1:E:35:LEU:N	2.33	0.62
1:E:147:GLN:C	1:E:149:SER:H	2.08	0.62
1:E:36:ILE:HD11	1:E:38:PHE:HD1	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:10:THR:HG22	1:G:10:THR:O	1.99	0.62
1:A:165:PRO:HD2	1:A:167:GLU:OE2	2.00	0.61
1:C:34:ASP:OD2	1:C:35:LEU:N	2.33	0.61
1:G:34:ASP:O	1:G:34:ASP:CG	2.42	0.61
1:H:68:THR:HG21	1:H:94:GLU:HB3	1.83	0.61
1:G:259:LEU:CD1	1:G:259:LEU:N	2.61	0.61
1:D:10:THR:HG22	1:D:10:THR:O	2.01	0.61
1:E:30:THR:CG2	1:E:31:ASP:H	2.13	0.61
1:E:107:VAL:HG21	1:E:144:PHE:HD2	1.64	0.61
1:D:68:THR:HG21	1:D:94:GLU:HB3	1.83	0.60
1:F:179:LYS:HZ1	1:F:238:ASP:CG	2.09	0.60
1:B:43:PHE:HB3	1:B:56:THR:HG21	1.83	0.60
1:C:26:TYR:CE2	1:C:28:GLU:HB2	2.36	0.60
1:C:76:GLY:CA	1:C:253:ARG:NH1	2.63	0.60
1:H:10:THR:O	1:H:10:THR:HG22	2.01	0.60
1:C:256:ALA:HA	1:C:258:GLY:N	2.17	0.60
1:E:144:PHE:C	1:E:144:PHE:HD1	2.09	0.60
1:A:64:HIS:O	1:A:68:THR:HG22	2.02	0.60
1:F:145:VAL:HG23	1:F:177:GLY:HA2	1.84	0.60
1:F:43:PHE:HB3	1:F:56:THR:HG21	1.83	0.60
1:C:179:LYS:HZ1	1:C:238:ASP:CG	2.10	0.59
1:C:68:THR:HG21	1:C:94:GLU:HB3	1.85	0.59
1:A:196:PHE:HD2	1:A:197:LEU:HD22	1.66	0.59
1:H:43:PHE:HB3	1:H:56:THR:CG2	2.33	0.59
1:G:286:GLN:CB	1:G:287:PRO:HD2	2.32	0.59
1:E:30:THR:CG2	1:E:31:ASP:N	2.65	0.59
1:B:146:ASN:O	1:B:147:GLN:HB2	2.02	0.59
1:E:68:THR:HG21	1:E:94:GLU:HB3	1.85	0.59
1:A:33:GLN:CG	1:A:49:LEU:HD11	2.33	0.58
2:C:291:SO4:O4	1:G:13:ASP:N	2.23	0.58
1:A:275:LEU:HD13	1:A:279:LEU:HD23	1.85	0.58
1:B:91:MET:HE3	1:B:156:ILE:CG2	2.33	0.58
1:F:286:GLN:O	1:F:286:GLN:HG3	2.02	0.58
1:H:196:PHE:CD2	1:H:197:LEU:HD12	2.38	0.58
1:D:183:ASN:HB3	1:D:184:PRO:CD	2.33	0.58
1:B:159:CYS:C	1:B:191:GLN:NE2	2.62	0.58
1:D:275:LEU:HD13	1:D:279:LEU:HD23	1.85	0.58
1:E:35:LEU:HD23	1:E:36:ILE:N	2.18	0.58
1:C:26:TYR:CZ	1:C:28:GLU:HB2	2.38	0.58
2:A:292:SO4:O2	1:E:168:SER:HB2	2.03	0.58
1:F:68:THR:HG21	1:F:94:GLU:CB	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:MET:CE	1:B:156:ILE:HG21	2.33	0.58
1:C:10:THR:O	1:C:10:THR:HG22	2.04	0.57
1:E:275:LEU:HD13	1:E:279:LEU:HD23	1.87	0.57
1:F:67:MET:HB3	1:F:91:MET:HE1	1.87	0.57
1:C:160:THR:CG2	1:C:161:ASP:N	2.64	0.57
1:F:64:HIS:O	1:F:68:THR:HG22	2.03	0.57
1:E:10:THR:HG22	1:E:10:THR:O	2.04	0.57
1:H:43:PHE:HB3	1:H:56:THR:HG21	1.85	0.57
1:D:43:PHE:HB3	1:D:56:THR:CG2	2.35	0.57
1:D:249:ILE:O	1:D:253:ARG:HG3	2.05	0.57
1:G:114:VAL:HG13	1:G:129:TYR:OH	2.05	0.57
1:B:148:THR:O	1:B:149:SER:CB	2.53	0.56
1:E:43:PHE:HB3	1:E:56:THR:CG2	2.34	0.56
1:E:114:VAL:HG13	1:E:129:TYR:OH	2.04	0.56
1:E:152:PHE:N	1:E:152:PHE:CD2	2.71	0.56
1:G:72:LEU:HD12	1:G:154:VAL:HG21	1.87	0.56
1:F:15:PHE:HZ	1:F:197:LEU:HD11	1.69	0.56
1:F:64:HIS:NE2	1:F:90:ALA:HB3	2.20	0.56
1:A:182:LEU:HD21	1:A:186:GLY:C	2.31	0.56
1:C:171:THR:HB	2:C:291:SO4:O1	2.05	0.56
1:E:148:THR:O	1:E:149:SER:CB	2.53	0.56
1:G:36:ILE:O	1:G:37:ILE:HG12	2.05	0.56
1:A:179:LYS:HZ1	1:A:238:ASP:CG	2.14	0.56
1:B:10:THR:HG22	1:B:10:THR:O	2.06	0.56
1:C:160:THR:HG23	1:C:161:ASP:N	2.19	0.56
1:E:144:PHE:O	1:E:144:PHE:HD1	1.87	0.56
1:E:179:LYS:HZ1	1:E:238:ASP:CG	2.13	0.55
1:G:43:PHE:HB3	1:G:56:THR:CG2	2.36	0.55
1:D:64:HIS:O	1:D:68:THR:HG22	2.06	0.55
1:E:27:HIS:CE1	1:E:36:ILE:CG2	2.89	0.55
1:B:197:LEU:HD22	1:B:197:LEU:H	1.73	0.55
1:H:43:PHE:O	1:H:56:THR:HG23	2.06	0.55
1:B:275:LEU:HD13	1:B:279:LEU:HD23	1.89	0.54
1:E:246:SER:O	1:E:249:ILE:HG22	2.07	0.54
1:G:68:THR:HG21	1:G:94:GLU:CB	2.36	0.54
1:A:163:ILE:HG23	1:A:163:ILE:O	2.07	0.54
1:E:15:PHE:CZ	1:E:197:LEU:HD11	2.41	0.54
1:F:15:PHE:CZ	1:F:197:LEU:HD11	2.42	0.54
1:G:246:SER:O	1:G:249:ILE:HG22	2.07	0.54
1:G:34:ASP:C	1:G:34:ASP:OD2	2.51	0.54
1:E:34:ASP:O	1:E:49:LEU:HD12	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:ASN:C	1:A:145:VAL:H	2.15	0.54
1:C:283:LEU:O	1:C:284:ALA:C	2.49	0.54
1:E:145:VAL:O	1:E:147:GLN:NE2	2.41	0.54
1:E:36:ILE:HD11	1:E:38:PHE:CD1	2.43	0.54
1:G:225:THR:HG22	1:G:225:THR:O	2.06	0.54
1:A:68:THR:HG21	1:A:94:GLU:CB	2.38	0.54
1:A:72:LEU:HD12	1:A:154:VAL:HG21	1.91	0.53
1:E:259:LEU:HD23	1:E:259:LEU:H	1.67	0.53
1:A:10:THR:O	1:A:10:THR:HG22	2.07	0.53
1:C:147:GLN:HG2	1:C:181:CYS:HB3	1.91	0.53
1:G:275:LEU:HD13	1:G:279:LEU:CD2	2.38	0.53
1:B:249:ILE:O	1:B:253:ARG:HG3	2.09	0.53
1:B:42:ALA:HA	1:E:170:PHE:CZ	2.44	0.53
1:H:147:GLN:HG2	1:H:181:CYS:HB3	1.91	0.53
1:A:161:ASP:OD2	1:A:172:SER:HB2	2.09	0.53
1:B:92:LEU:HG	1:B:128:SER:OG	2.09	0.53
1:G:35:LEU:C	1:G:36:ILE:HG23	2.33	0.53
1:C:246:SER:O	1:C:249:ILE:HG22	2.09	0.52
1:D:34:ASP:OD2	1:D:35:LEU:N	2.42	0.52
1:A:33:GLN:HG3	1:A:49:LEU:HD11	1.91	0.52
1:F:223:ILE:HD12	1:F:223:ILE:N	2.24	0.52
1:F:43:PHE:O	1:F:56:THR:HG23	2.09	0.52
1:F:275:LEU:HD13	1:F:279:LEU:HD23	1.91	0.52
1:D:43:PHE:HB3	1:D:56:THR:HG23	1.91	0.52
1:E:27:HIS:ND1	1:E:36:ILE:HG22	2.24	0.52
1:H:68:THR:HG21	1:H:94:GLU:CB	2.39	0.52
1:C:43:PHE:HB3	1:C:56:THR:CG2	2.39	0.52
1:E:43:PHE:HB3	1:E:56:THR:HG23	1.91	0.52
1:B:83:ILE:HD13	1:B:91:MET:HG3	1.91	0.52
1:H:179:LYS:HZ1	1:H:238:ASP:CG	2.17	0.52
1:E:31:ASP:OD1	1:E:31:ASP:C	2.53	0.52
1:E:143:ASN:C	1:E:145:VAL:N	2.67	0.52
1:E:145:VAL:O	1:E:145:VAL:HG22	2.09	0.52
1:F:43:PHE:HB3	1:F:56:THR:HG23	1.91	0.52
1:F:253:ARG:O	1:F:256:ALA:O	2.28	0.52
1:B:146:ASN:O	1:B:147:GLN:CB	2.58	0.52
1:A:147:GLN:HG2	1:A:181:CYS:HB3	1.92	0.51
1:D:159:CYS:SG	1:D:169:LEU:HD12	2.50	0.51
1:E:27:HIS:ND1	1:E:36:ILE:CG2	2.73	0.51
1:F:64:HIS:CE1	1:F:90:ALA:HB3	2.44	0.51
1:C:85:GLY:HA3	1:C:158:ASP:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:160:THR:H	1:D:191:GLN:NE2	2.09	0.51
1:A:110:ASP:O	1:A:113:VAL:HG12	2.11	0.51
1:A:259:LEU:HD12	1:A:259:LEU:H	1.75	0.51
1:C:110:ASP:O	1:C:113:VAL:HG12	2.11	0.51
1:G:43:PHE:HB3	1:G:56:THR:HG23	1.92	0.51
1:D:93:ARG:O	1:D:96:THR:HB	2.10	0.51
1:F:256:ALA:HA	1:F:257:SER:C	2.35	0.51
1:F:68:THR:HB	1:F:91:MET:HE3	1.90	0.51
1:D:142:VAL:HG21	1:D:168:SER:OG	2.10	0.51
1:B:28:GLU:HA	1:D:27:HIS:O	2.11	0.50
1:B:83:ILE:HD13	1:B:91:MET:CG	2.41	0.50
1:B:159:CYS:C	1:B:191:GLN:HE21	2.20	0.50
1:D:182:LEU:C	1:D:183:ASN:O	2.46	0.50
1:F:92:LEU:HG	1:F:128:SER:OG	2.11	0.50
1:H:253:ARG:O	1:H:256:ALA:O	2.30	0.50
1:C:68:THR:HG23	1:C:69:HIS:N	2.25	0.50
1:G:53:VAL:HG11	1:G:225:THR:CG2	2.41	0.50
1:G:92:LEU:HG	1:G:128:SER:OG	2.12	0.50
1:B:43:PHE:O	1:B:56:THR:HG23	2.11	0.50
1:F:147:GLN:HG2	1:F:181:CYS:HB3	1.92	0.50
1:B:197:LEU:HD22	1:B:197:LEU:N	2.27	0.50
1:E:148:THR:O	1:E:149:SER:OG	2.30	0.50
1:F:93:ARG:O	1:F:96:THR:HB	2.12	0.50
1:H:64:HIS:NE2	1:H:90:ALA:HB3	2.27	0.50
1:C:92:LEU:HG	1:C:128:SER:OG	2.12	0.50
1:D:68:THR:HG21	1:D:94:GLU:CB	2.42	0.50
1:E:92:LEU:HG	1:E:128:SER:OG	2.12	0.50
1:H:145:VAL:HG23	1:H:177:GLY:HA2	1.94	0.50
1:H:93:ARG:O	1:H:96:THR:HB	2.11	0.49
1:F:110:ASP:O	1:F:113:VAL:HG12	2.11	0.49
1:D:225:THR:O	1:D:225:THR:HG22	2.11	0.49
1:E:147:GLN:CB	1:E:149:SER:H	2.22	0.49
1:C:35:LEU:HD21	1:C:116:PHE:CZ	2.48	0.49
1:C:62:ILE:HG12	1:C:263:TYR:CD1	2.47	0.49
1:C:41:ALA:HB3	1:D:14:GLN:HG3	1.94	0.49
1:E:62:ILE:HG12	1:E:263:TYR:CD1	2.48	0.49
1:A:218:PHE:CD1	1:A:232:THR:HG22	2.47	0.49
1:C:145:VAL:HG23	1:C:177:GLY:HA2	1.94	0.49
1:F:218:PHE:CD1	1:F:232:THR:HG22	2.47	0.49
1:G:34:ASP:O	1:G:34:ASP:OD2	2.30	0.49
1:H:197:LEU:HD12	1:H:197:LEU:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:14:GLN:HG3	1:D:41:ALA:HB3	1.94	0.49
1:G:275:LEU:HD13	1:G:279:LEU:HD21	1.93	0.49
1:B:64:HIS:CE1	1:B:90:ALA:HB3	2.48	0.49
1:C:283:LEU:O	1:C:285:SER:N	2.45	0.49
1:F:160:THR:O	1:F:160:THR:OG1	2.30	0.49
1:A:192:ASN:HD21	1:A:202:ALA:HA	1.77	0.49
1:D:62:ILE:HG12	1:D:263:TYR:CD1	2.48	0.49
1:E:161:ASP:C	1:E:161:ASP:OD2	2.53	0.49
2:A:292:SO4:O1	1:E:168:SER:HB2	2.14	0.48
1:B:64:HIS:NE2	1:B:90:ALA:HB3	2.28	0.48
1:D:5:LYS:CG	1:D:6:GLN:N	2.76	0.48
1:D:43:PHE:O	1:D:56:THR:HG23	2.13	0.48
1:G:151:THR:HA	1:G:181:CYS:O	2.13	0.48
1:A:67:MET:HB3	1:A:91:MET:HE1	1.94	0.48
1:A:161:ASP:OD2	1:A:172:SER:CB	2.61	0.48
1:A:163:ILE:HD12	1:A:204:ASP:HB2	1.95	0.48
1:H:218:PHE:CD1	1:H:232:THR:HG22	2.48	0.48
1:E:29:LYS:O	1:E:29:LYS:HG2	2.13	0.48
1:E:223:ILE:N	1:E:223:ILE:HD12	2.27	0.48
1:A:14:GLN:HG3	1:B:41:ALA:HB3	1.94	0.48
1:E:147:GLN:HB3	1:E:149:SER:N	2.25	0.48
1:D:110:ASP:O	1:D:113:VAL:HG12	2.13	0.48
1:E:110:ASP:O	1:E:113:VAL:HG12	2.14	0.48
1:D:30:THR:O	1:D:31:ASP:C	2.55	0.48
1:E:184:PRO:O	2:E:292:SO4:O1	2.32	0.48
1:F:64:HIS:CD2	1:F:90:ALA:HB3	2.49	0.48
1:C:76:GLY:HA2	1:C:253:ARG:HH11	1.75	0.48
1:D:256:ALA:HA	1:D:257:SER:C	2.38	0.48
1:A:92:LEU:HG	1:A:128:SER:OG	2.14	0.48
1:A:246:SER:O	1:A:249:ILE:HG22	2.14	0.48
1:B:62:ILE:HG12	1:B:263:TYR:CD1	2.49	0.48
1:B:107:VAL:HG21	1:B:144:PHE:CD2	2.49	0.48
1:C:114:VAL:HG13	1:C:129:TYR:OH	2.13	0.48
1:F:145:VAL:HG23	1:F:177:GLY:CA	2.43	0.48
1:B:53:VAL:HG11	1:B:225:THR:CG2	2.43	0.48
1:C:68:THR:HG21	1:C:94:GLU:CB	2.43	0.48
1:H:36:ILE:CG2	1:H:48:ALA:HB3	2.43	0.47
1:A:168:SER:HB3	2:E:290:SO4:O2	2.14	0.47
1:G:258:GLY:C	1:G:259:LEU:HD13	2.35	0.47
1:B:172:SER:HB2	1:B:208:LYS:HZ1	1.79	0.47
1:C:34:ASP:O	1:C:49:LEU:HD12	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:67:MET:HB3	1:H:91:MET:HE1	1.97	0.47
1:B:218:PHE:CD1	1:B:232:THR:HG22	2.49	0.47
1:C:171:THR:CB	2:C:291:SO4:O1	2.63	0.47
1:E:31:ASP:OD1	1:E:31:ASP:O	2.32	0.47
1:E:107:VAL:HG21	1:E:144:PHE:CE2	2.49	0.47
1:D:218:PHE:CD1	1:D:232:THR:HG22	2.50	0.47
1:H:64:HIS:CE1	1:H:90:ALA:HB3	2.49	0.47
1:H:206:HIS:CG	1:H:283:LEU:HD21	2.50	0.47
1:A:43:PHE:HB3	1:A:56:THR:CG2	2.44	0.47
1:E:286:GLN:O	1:E:287:PRO:C	2.58	0.47
1:C:43:PHE:HB3	1:C:56:THR:HG23	1.97	0.46
1:D:114:VAL:HG13	1:D:129:TYR:OH	2.15	0.46
1:E:192:ASN:HD21	1:E:202:ALA:HA	1.79	0.46
1:A:62:ILE:HG12	1:A:263:TYR:CD1	2.50	0.46
1:B:225:THR:HG22	1:B:225:THR:O	2.15	0.46
1:C:15:PHE:CZ	1:C:197:LEU:HD11	2.50	0.46
1:D:92:LEU:HG	1:D:128:SER:OG	2.16	0.46
1:E:36:ILE:HG13	1:E:37:ILE:N	2.22	0.46
1:E:206:HIS:ND1	1:E:286:GLN:HG2	2.30	0.46
1:E:68:THR:HG21	1:E:94:GLU:CB	2.43	0.46
1:B:84:ILE:HD13	1:B:174:PHE:CZ	2.49	0.46
1:G:67:MET:HB3	1:G:91:MET:HE1	1.97	0.46
1:H:53:VAL:HG11	1:H:225:THR:CG2	2.46	0.46
1:D:183:ASN:HB3	1:D:184:PRO:HD2	1.96	0.46
1:G:58:ARG:O	1:G:58:ARG:HG3	2.15	0.46
1:G:110:ASP:O	1:G:113:VAL:HG12	2.16	0.46
1:A:174:PHE:CE1	1:A:178:CYS:SG	3.09	0.46
1:B:246:SER:O	1:B:249:ILE:HG22	2.15	0.46
1:E:107:VAL:CG2	1:E:144:PHE:CD2	2.96	0.46
1:E:287:PRO:O	1:E:287:PRO:HG2	2.14	0.46
1:H:68:THR:HB	1:H:91:MET:HE3	1.94	0.46
1:F:62:ILE:HG12	1:F:263:TYR:CD1	2.51	0.46
1:G:163:ILE:HD12	1:G:204:ASP:HB2	1.98	0.46
1:E:195:CYS:SG	1:E:232:THR:OG1	2.59	0.45
1:G:218:PHE:CD1	1:G:232:THR:HG22	2.51	0.45
1:H:62:ILE:HG12	1:H:263:TYR:CD1	2.51	0.45
1:B:93:ARG:O	1:B:96:THR:HB	2.15	0.45
1:D:68:THR:HG23	1:D:69:HIS:N	2.30	0.45
1:E:27:HIS:HD1	1:E:36:ILE:HG22	1.80	0.45
1:F:225:THR:HG22	1:F:225:THR:O	2.15	0.45
1:G:145:VAL:HG23	1:G:177:GLY:CA	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:PHE:HB3	1:B:56:THR:HG23	1.97	0.45
1:B:114:VAL:HG13	1:B:129:TYR:OH	2.17	0.45
1:E:67:MET:HB3	1:E:91:MET:HE1	1.98	0.45
1:G:28:GLU:O	1:G:34:ASP:OD2	2.34	0.45
1:A:142:VAL:O	1:A:145:VAL:HB	2.17	0.45
1:B:256:ALA:HA	1:B:258:GLY:N	2.30	0.45
1:B:146:ASN:C	1:B:147:GLN:HG3	2.41	0.45
1:G:225:THR:O	1:G:225:THR:CG2	2.64	0.45
1:B:142:VAL:O	1:B:145:VAL:HG23	2.17	0.45
1:A:163:ILE:O	1:A:163:ILE:CG2	2.65	0.45
1:B:33:GLN:HA	1:B:50:ASP:OD1	2.17	0.45
1:C:218:PHE:CD1	1:C:232:THR:HG22	2.52	0.45
1:G:196:PHE:CD2	1:G:197:LEU:HD13	2.52	0.45
1:H:114:VAL:HG13	1:H:129:TYR:OH	2.17	0.45
1:E:68:THR:HG23	1:E:69:HIS:N	2.31	0.45
1:F:26:TYR:CE2	1:F:35:LEU:HD23	2.51	0.45
1:H:92:LEU:HG	1:H:128:SER:OG	2.17	0.45
1:D:174:PHE:CZ	1:D:178:CYS:SG	3.10	0.45
1:B:144:PHE:C	1:B:146:ASN:N	2.73	0.45
1:A:43:PHE:O	1:A:56:THR:HG23	2.16	0.44
1:E:146:ASN:C	1:E:147:GLN:O	2.58	0.44
1:H:280:GLN:O	1:H:281:ASP:C	2.56	0.44
1:A:197:LEU:HB3	1:E:169:LEU:HD13	1.99	0.44
1:E:43:PHE:HB3	1:E:56:THR:HG21	1.99	0.44
1:H:246:SER:O	1:H:249:ILE:HG22	2.16	0.44
1:A:93:ARG:O	1:A:96:THR:HB	2.16	0.44
1:B:69:HIS:O	1:B:70:VAL:C	2.60	0.44
1:B:223:ILE:N	1:B:223:ILE:HD12	2.33	0.44
1:F:281:ASP:C	1:F:283:LEU:N	2.75	0.44
1:D:246:SER:O	1:D:249:ILE:HG22	2.17	0.44
1:E:160:THR:O	1:E:161:ASP:C	2.56	0.44
1:C:211:HIS:NE2	1:H:41:ALA:HB2	2.33	0.44
1:E:218:PHE:CD1	1:E:232:THR:HG22	2.52	0.44
1:E:15:PHE:CZ	1:E:197:LEU:CD1	3.01	0.44
1:A:53:VAL:HG11	1:A:225:THR:CG2	2.48	0.44
1:A:225:THR:HG22	1:A:225:THR:O	2.17	0.44
1:C:53:VAL:HG11	1:C:225:THR:CG2	2.48	0.44
1:C:204:ASP:OD2	1:C:208:LYS:NZ	2.49	0.44
1:F:64:HIS:CE1	1:F:90:ALA:CB	3.01	0.44
1:G:35:LEU:HD23	1:G:36:ILE:N	2.31	0.44
1:A:68:THR:HG23	1:A:69:HIS:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:142:VAL:O	1:C:145:VAL:HG12	2.18	0.44
1:G:159:CYS:C	1:G:160:THR:HG23	2.43	0.44
1:H:110:ASP:O	1:H:113:VAL:HG12	2.17	0.44
1:H:223:ILE:N	1:H:223:ILE:HD12	2.33	0.44
1:D:56:THR:HB	1:D:59:ASP:OD2	2.18	0.44
1:E:64:HIS:NE2	1:E:90:ALA:HB3	2.32	0.44
1:B:26:TYR:CE2	1:B:35:LEU:HD23	2.53	0.43
1:B:145:VAL:O	1:B:147:GLN:HG3	2.18	0.43
1:E:12:HIS:HB3	2:E:290:SO4:O1	2.17	0.43
1:G:37:ILE:HG22	1:G:38:PHE:N	2.33	0.43
1:G:110:ASP:HA	1:G:138:ILE:HG23	2.00	0.43
1:H:34:ASP:OD2	1:H:34:ASP:C	2.60	0.43
1:A:43:PHE:HB3	1:A:56:THR:HG23	2.00	0.43
1:D:160:THR:H	1:D:191:GLN:HE21	1.64	0.43
1:E:256:ALA:CA	1:E:257:SER:C	2.90	0.43
1:G:35:LEU:C	1:G:35:LEU:HD23	2.43	0.43
1:C:169:LEU:HB2	1:C:170:PHE:CE1	2.53	0.43
1:D:64:HIS:NE2	1:D:90:ALA:HB3	2.34	0.43
1:B:182:LEU:HD23	1:B:182:LEU:HA	1.78	0.43
1:F:35:LEU:HD21	1:F:116:PHE:CZ	2.53	0.43
1:H:279:LEU:O	1:H:282:ALA:CB	2.53	0.43
1:E:53:VAL:HG11	1:E:225:THR:CG2	2.48	0.43
1:F:15:PHE:HZ	1:F:197:LEU:CD1	2.31	0.43
1:G:62:ILE:HG12	1:G:263:TYR:CD1	2.54	0.43
1:B:110:ASP:O	1:B:113:VAL:HG12	2.18	0.43
1:D:15:PHE:HZ	1:D:197:LEU:HD11	1.83	0.43
1:D:67:MET:HB3	1:D:91:MET:HE1	2.01	0.43
1:C:36:ILE:CG2	1:C:48:ALA:HB3	2.48	0.43
1:G:56:THR:HB	1:G:59:ASP:OD2	2.19	0.43
1:B:260:LYS:HD2	1:B:260:LYS:HA	1.73	0.43
1:E:29:LYS:O	1:E:29:LYS:CG	2.66	0.43
1:B:67:MET:HE2	1:B:233:PHE:CE1	2.52	0.43
1:D:64:HIS:CE1	1:D:90:ALA:HB3	2.54	0.43
1:A:34:ASP:OD2	1:A:34:ASP:C	2.62	0.42
1:C:72:LEU:HD12	1:C:154:VAL:HG21	2.01	0.42
1:F:34:ASP:OD2	1:F:34:ASP:C	2.62	0.42
1:G:68:THR:HG23	1:G:69:HIS:N	2.34	0.42
1:A:182:LEU:C	1:A:183:ASN:O	2.62	0.42
1:C:146:ASN:C	1:C:147:GLN:O	2.60	0.42
1:E:93:ARG:O	1:E:96:THR:HB	2.19	0.42
1:F:72:LEU:HD12	1:F:154:VAL:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:195:CYS:SG	1:G:232:THR:OG1	2.63	0.42
1:H:275:LEU:HB3	1:H:279:LEU:HD23	2.01	0.42
1:A:110:ASP:HA	1:A:138:ILE:HG23	2.01	0.42
1:B:34:ASP:C	1:B:34:ASP:OD2	2.62	0.42
1:B:67:MET:HG3	1:B:91:MET:HE1	2.01	0.42
1:C:26:TYR:OH	1:C:28:GLU:HB2	2.20	0.42
1:D:5:LYS:HG3	1:D:6:GLN:H	1.84	0.42
1:G:223:ILE:N	1:G:223:ILE:HD12	2.34	0.42
1:A:12:HIS:HB3	2:A:292:SO4:O3	2.20	0.42
1:A:64:HIS:CE1	1:A:90:ALA:HB3	2.54	0.42
1:B:35:LEU:HD21	1:B:116:PHE:CZ	2.54	0.42
1:E:164:GLY:HA3	1:E:167:GLU:HG3	2.01	0.42
1:A:168:SER:CB	2:E:290:SO4:O4	2.68	0.42
1:C:43:PHE:O	1:C:56:THR:HG23	2.20	0.42
1:D:43:PHE:HB3	1:D:56:THR:HG21	2.00	0.42
1:E:15:PHE:HZ	1:E:197:LEU:CD1	2.32	0.42
1:G:64:HIS:NE2	1:G:90:ALA:HB3	2.35	0.42
1:G:36:ILE:C	1:G:36:ILE:HD12	2.45	0.42
1:H:225:THR:HG22	1:H:225:THR:O	2.20	0.42
1:A:239:ASN:ND2	1:A:242:LEU:HG	2.34	0.42
1:E:35:LEU:C	1:E:35:LEU:HD23	2.45	0.42
1:G:43:PHE:HB3	1:G:56:THR:HG21	2.01	0.42
1:G:93:ARG:HG2	1:G:97:ARG:HH21	1.76	0.42
1:A:13:ASP:HB2	2:A:292:SO4:O1	2.20	0.41
1:D:182:LEU:O	1:D:183:ASN:C	2.62	0.41
1:D:223:ILE:HD12	1:D:223:ILE:N	2.35	0.41
1:G:35:LEU:C	1:G:36:ILE:CG2	2.93	0.41
1:H:85:GLY:HA3	1:H:158:ASP:O	2.20	0.41
1:F:283:LEU:HA	1:F:283:LEU:HD23	1.63	0.41
1:G:251:GLN:OE1	1:G:266:PRO:HG2	2.20	0.41
1:B:110:ASP:HA	1:B:138:ILE:HG23	2.02	0.41
1:B:172:SER:HB2	1:B:208:LYS:HZ2	1.84	0.41
1:H:256:ALA:HA	1:H:258:GLY:N	2.34	0.41
1:B:225:THR:CG2	1:B:225:THR:O	2.68	0.41
1:C:254:PHE:O	1:C:255:LEU:C	2.62	0.41
1:C:64:HIS:CE1	1:C:90:ALA:HB3	2.55	0.41
1:E:110:ASP:HA	1:E:138:ILE:HG23	2.02	0.41
1:H:196:PHE:HD2	1:H:197:LEU:CD1	2.30	0.41
1:C:223:ILE:N	1:C:223:ILE:HD12	2.35	0.41
1:D:42:ALA:HA	1:G:170:PHE:CZ	2.55	0.41
1:G:93:ARG:O	1:G:96:THR:HB	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:144:PHE:O	1:E:144:PHE:CG	2.70	0.41
1:E:147:GLN:C	1:E:149:SER:N	2.74	0.41
1:B:61:PHE:O	1:B:65:GLU:HB2	2.21	0.41
1:C:26:TYR:CE2	1:C:35:LEU:HD23	2.56	0.41
1:C:26:TYR:CE2	1:C:28:GLU:CB	3.03	0.41
1:C:110:ASP:HA	1:C:138:ILE:HG23	2.03	0.41
1:D:225:THR:O	1:D:225:THR:CG2	2.68	0.41
1:G:143:ASN:C	1:G:145:VAL:H	2.29	0.41
1:A:164:GLY:CA	1:A:167:GLU:CG	2.91	0.41
1:D:36:ILE:CG2	1:D:48:ALA:HB3	2.51	0.41
1:G:93:ARG:CD	1:G:97:ARG:HH22	2.31	0.41
1:H:110:ASP:HA	1:H:138:ILE:HG23	2.03	0.41
1:B:147:GLN:C	1:B:149:SER:H	2.25	0.40
1:C:64:HIS:NE2	1:C:90:ALA:HB3	2.36	0.40
1:H:94:GLU:HA	1:H:97:ARG:HD3	2.03	0.40
1:A:276:PRO:HB3	1:B:263:TYR:CE1	2.56	0.40
1:D:110:ASP:HA	1:D:138:ILE:HG23	2.03	0.40
1:E:43:PHE:O	1:E:56:THR:HG23	2.22	0.40
1:B:83:ILE:CD1	1:B:91:MET:HG3	2.51	0.40
1:C:93:ARG:O	1:C:96:THR:HB	2.21	0.40
1:D:125:ASN:O	1:D:128:SER:CB	2.70	0.40
1:A:196:PHE:CD2	1:A:197:LEU:HD22	2.50	0.40
1:A:218:PHE:HD1	1:A:232:THR:HG22	1.85	0.40
1:E:271:ALA:HB1	1:F:271:ALA:CB	2.34	0.40
1:G:169:LEU:HD23	1:G:169:LEU:HA	1.88	0.40
1:H:64:HIS:CD2	1:H:90:ALA:HB3	2.56	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	278/294 (95%)	269 (97%)	9 (3%)	0	100	100
1	B	266/294 (90%)	255 (96%)	11 (4%)	0	100	100
1	C	282/294 (96%)	272 (96%)	10 (4%)	0	100	100
1	D	272/294 (92%)	263 (97%)	9 (3%)	0	100	100
1	E	281/294 (96%)	272 (97%)	8 (3%)	1 (0%)	30	59
1	F	263/294 (90%)	254 (97%)	9 (3%)	0	100	100
1	G	275/294 (94%)	264 (96%)	11 (4%)	0	100	100
1	H	258/294 (88%)	248 (96%)	10 (4%)	0	100	100
All	All	2175/2352 (92%)	2097 (96%)	77 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	149	SER

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	230/247 (93%)	223 (97%)	7 (3%)	36	70
1	B	222/247 (90%)	215 (97%)	7 (3%)	34	68
1	C	232/247 (94%)	224 (97%)	8 (3%)	32	66
1	D	226/247 (92%)	213 (94%)	13 (6%)	18	49
1	E	229/247 (93%)	215 (94%)	14 (6%)	17	46
1	F	219/247 (89%)	212 (97%)	7 (3%)	34	68
1	G	228/247 (92%)	217 (95%)	11 (5%)	23	55
1	H	217/247 (88%)	213 (98%)	4 (2%)	51	80
All	All	1803/1976 (91%)	1732 (96%)	71 (4%)	28	63

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	THR
1	A	67	MET
1	A	125	ASN
1	A	144	PHE
1	A	163	ILE
1	A	194	VAL
1	A	260	LYS
1	B	56	THR
1	B	66	MET
1	B	125	ASN
1	B	144	PHE
1	B	148	THR
1	B	194	VAL
1	B	260	LYS
1	C	56	THR
1	C	144	PHE
1	C	158	ASP
1	C	160	THR
1	C	170	PHE
1	C	194	VAL
1	C	195	CYS
1	C	279	LEU
1	D	5	LYS
1	D	32	HIS
1	D	33	GLN
1	D	56	THR
1	D	67	MET
1	D	125	ASN
1	D	144	PHE
1	D	159	CYS
1	D	160	THR
1	D	172	SER
1	D	179	LYS
1	D	194	VAL
1	D	195	CYS
1	E	34	ASP
1	E	36	ILE
1	E	56	THR
1	E	67	MET
1	E	144	PHE
1	E	147	GLN
1	E	148	THR
1	E	152	PHE

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Mol	Chain	Res	Type
1	E	158	ASP
1	E	159	CYS
1	E	179	LYS
1	E	194	VAL
1	E	259	LEU
1	E	260	LYS
1	F	56	THR
1	F	67	MET
1	F	144	PHE
1	F	160	THR
1	F	194	VAL
1	F	195	CYS
1	F	260	LYS
1	G	56	THR
1	G	125	ASN
1	G	144	PHE
1	G	179	LYS
1	G	181	CYS
1	G	182	LEU
1	G	184	PRO
1	G	194	VAL
1	G	197	LEU
1	G	260	LYS
1	G	286	GLN
1	H	56	THR
1	H	125	ASN
1	H	144	PHE
1	H	194	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	33	GLN
1	A	192	ASN
1	B	6	GLN
1	B	14	GLN
1	B	54	GLN
1	B	125	ASN
1	C	14	GLN
1	C	54	GLN
1	D	125	ASN

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Mol	Chain	Res	Type
1	D	191	GLN
1	E	14	GLN
1	E	54	GLN
1	E	147	GLN
1	E	183	ASN
1	F	14	GLN
1	G	54	GLN
1	H	14	GLN
1	H	54	GLN

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](#)

31 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	289	-	4,4,4	0.43	0	6,6,6	0.30	0
2	SO4	G	290	-	4,4,4	0.39	0	6,6,6	0.34	0
2	SO4	C	293	-	4,4,4	0.26	0	6,6,6	0.38	0
2	SO4	E	291	-	4,4,4	0.36	0	6,6,6	0.29	0
2	SO4	C	292	-	4,4,4	0.27	0	6,6,6	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	F	292	-	4,4,4	0.27	0	6,6,6	0.62	0
2	SO4	E	290	-	4,4,4	0.85	0	6,6,6	0.72	0
2	SO4	C	291	-	4,4,4	0.40	0	6,6,6	0.73	0
2	SO4	B	289	-	4,4,4	0.51	0	6,6,6	0.30	0
2	SO4	D	291	-	4,4,4	0.27	0	6,6,6	0.21	0
2	SO4	A	290	-	4,4,4	0.35	0	6,6,6	0.22	0
2	SO4	C	289	-	4,4,4	0.52	0	6,6,6	0.34	0
2	SO4	B	290	-	4,4,4	0.43	0	6,6,6	0.27	0
2	SO4	C	294	-	4,4,4	0.23	0	6,6,6	0.63	0
2	SO4	D	290	-	4,4,4	0.61	0	6,6,6	0.51	0
2	SO4	A	289	-	4,4,4	0.49	0	6,6,6	0.30	0
2	SO4	D	289	-	4,4,4	0.41	0	6,6,6	0.14	0
2	SO4	E	292	-	4,4,4	0.25	0	6,6,6	0.33	0
2	SO4	F	291	-	4,4,4	0.28	0	6,6,6	0.20	0
2	SO4	H	290	-	4,4,4	0.25	0	6,6,6	0.17	0
2	SO4	F	289	-	4,4,4	0.39	0	6,6,6	0.24	0
2	SO4	A	291	-	4,4,4	0.37	0	6,6,6	0.40	0
2	SO4	D	292	-	4,4,4	0.28	0	6,6,6	0.28	0
2	SO4	F	290	-	4,4,4	0.37	0	6,6,6	0.22	0
2	SO4	G	293	-	4,4,4	0.33	0	6,6,6	0.11	0
2	SO4	G	292	-	4,4,4	0.27	0	6,6,6	0.13	0
2	SO4	C	290	-	4,4,4	0.35	0	6,6,6	0.37	0
2	SO4	E	289	-	4,4,4	0.50	0	6,6,6	0.28	0
2	SO4	G	289	-	4,4,4	0.53	0	6,6,6	0.46	0
2	SO4	A	292	-	4,4,4	0.22	0	6,6,6	0.07	0
2	SO4	G	291	-	4,4,4	0.33	0	6,6,6	0.25	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.

4 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	290	SO4	3	0
2	C	291	SO4	5	0
2	E	292	SO4	1	0
2	A	292	SO4	5	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	282/294 (95%)	1.49	83 (29%) 1 1	42, 108, 189, 247	0
1	B	270/294 (91%)	0.87	29 (10%) 11 9	34, 85, 146, 177	0
1	C	284/294 (96%)	1.46	75 (26%) 1 1	36, 104, 186, 242	0
1	D	276/294 (93%)	0.80	18 (6%) 25 20	36, 85, 145, 197	0
1	E	283/294 (96%)	1.76	110 (38%) 1 0	44, 128, 218, 271	0
1	F	269/294 (91%)	1.29	63 (23%) 2 2	35, 107, 186, 241	0
1	G	279/294 (94%)	1.70	105 (37%) 1 0	42, 107, 200, 319	0
1	H	264/294 (89%)	1.70	103 (39%) 1 0	39, 121, 231, 276	0
All	All	2207/2352 (93%)	1.39	586 (26%) 1 1	34, 103, 198, 319	0

All (586) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	111	ALA	7.4
1	A	144	PHE	6.6
1	G	111	ALA	6.5
1	H	218	PHE	6.4
1	B	145	VAL	5.9
1	E	137	VAL	5.8
1	A	41	ALA	5.8
1	E	37	ILE	5.5
1	C	137	VAL	5.3
1	E	47	MET	5.3
1	E	107	VAL	5.3
1	G	115	SER	5.3
1	E	24	VAL	5.2
1	A	136	LEU	5.2
1	C	111	ALA	5.2
1	G	107	VAL	5.1

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Mol	Chain	Res	Type	RSRZ
1	H	144	PHE	5.1
1	G	35	LEU	5.1
1	G	47	MET	5.1
1	H	203	ILE	5.0
1	G	136	LEU	5.0
1	E	106	MET	5.0
1	G	37	ILE	5.0
1	C	144	PHE	4.9
1	F	145	VAL	4.9
1	G	116	PHE	4.9
1	E	136	LEU	4.9
1	C	134	PHE	4.9
1	G	144	PHE	4.8
1	E	26	TYR	4.7
1	G	26	TYR	4.7
1	H	188	PHE	4.7
1	E	104	ILE	4.7
1	F	171	THR	4.6
1	G	137	VAL	4.6
1	A	24	VAL	4.5
1	G	120	TYR	4.5
1	E	35	LEU	4.5
1	E	129	TYR	4.5
1	A	137	VAL	4.4
1	E	83	ILE	4.4
1	E	46	VAL	4.4
1	G	33	GLN	4.4
1	C	37	ILE	4.3
1	F	142	VAL	4.3
1	A	107	VAL	4.3
1	H	145	VAL	4.2
1	F	144	PHE	4.2
1	C	121	LEU	4.2
1	E	105	THR	4.1
1	D	181	CYS	4.1
1	G	46	VAL	4.1
1	F	173	ALA	4.1
1	C	38	PHE	4.1
1	G	25	LEU	4.1
1	A	37	ILE	4.1
1	A	139	ASP	4.1
1	A	35	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
1	G	110	ASP	4.0
1	E	36	ILE	4.0
1	G	48	ALA	4.0
1	A	138	ILE	4.0
1	C	138	ILE	4.0
1	A	25	LEU	4.0
1	G	119	GLN	4.0
1	H	146	ASN	4.0
1	G	49	LEU	4.0
1	C	109	ILE	3.9
1	E	19	PHE	3.9
1	A	115	SER	3.9
1	H	148	THR	3.9
1	G	129	TYR	3.9
1	G	24	VAL	3.9
1	G	106	MET	3.9
1	E	84	ILE	3.9
1	E	96	THR	3.9
1	F	161	ASP	3.9
1	E	43	PHE	3.9
1	E	95	VAL	3.9
1	C	107	VAL	3.9
1	G	89	GLY	3.8
1	E	116	PHE	3.8
1	H	173	ALA	3.8
1	C	136	LEU	3.8
1	H	236	ALA	3.8
1	C	148	THR	3.8
1	E	82	LEU	3.8
1	H	232	THR	3.8
1	D	145	VAL	3.8
1	G	113	VAL	3.8
1	H	192	ASN	3.8
1	H	186	GLY	3.8
1	B	144	PHE	3.8
1	E	144	PHE	3.8
1	D	144	PHE	3.7
1	H	278	TYR	3.7
1	A	112	GLY	3.7
1	F	141	GLY	3.7
1	B	114	VAL	3.7
1	C	287	PRO	3.7

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Mol	Chain	Res	Type	RSRZ
1	F	240	ASP	3.7
1	H	178	CYS	3.7
1	E	142	VAL	3.7
1	D	173	ALA	3.7
1	C	26	TYR	3.6
1	E	114	VAL	3.6
1	G	36	ILE	3.6
1	C	106	MET	3.6
1	G	19	PHE	3.6
1	C	52	VAL	3.6
1	A	7	TRP	3.6
1	A	109	ILE	3.6
1	G	95	VAL	3.6
1	G	151	THR	3.6
1	C	257	SER	3.6
1	G	104	ILE	3.6
1	B	148	THR	3.6
1	E	99	LYS	3.5
1	E	115	SER	3.5
1	G	114	VAL	3.5
1	E	25	LEU	3.5
1	C	171	THR	3.5
1	A	106	MET	3.5
1	C	139	ASP	3.5
1	E	286	GLN	3.5
1	C	83	ILE	3.5
1	H	113	VAL	3.5
1	E	287	PRO	3.5
1	F	192	ASN	3.5
1	A	87	GLY	3.4
1	A	128	SER	3.4
1	A	119	GLN	3.4
1	A	104	ILE	3.4
1	G	38	PHE	3.4
1	H	111	ALA	3.4
1	F	114	VAL	3.4
1	H	229	GLY	3.4
1	E	111	ALA	3.4
1	E	55	THR	3.4
1	G	184	PRO	3.4
1	A	20	ALA	3.4
1	E	156	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	24	VAL	3.3
1	G	81	VAL	3.3
1	H	136	LEU	3.3
1	H	228	GLY	3.3
1	G	28	GLU	3.3
1	A	134	PHE	3.3
1	C	115	SER	3.3
1	E	122	PRO	3.3
1	C	36	ILE	3.3
1	G	84	ILE	3.3
1	A	286	GLN	3.3
1	H	114	VAL	3.3
1	E	128	SER	3.3
1	A	120	TYR	3.3
1	E	27	HIS	3.3
1	E	121	LEU	3.3
1	E	155	ILE	3.2
1	E	86	GLY	3.2
1	E	103	SER	3.2
1	E	78	ALA	3.2
1	H	197	LEU	3.2
1	G	147	GLN	3.2
1	A	148	THR	3.2
1	E	224	PRO	3.2
1	F	278	TYR	3.2
1	G	128	SER	3.2
1	H	172	SER	3.2
1	C	84	ILE	3.2
1	H	134	PHE	3.2
1	C	46	VAL	3.2
1	G	117	CYS	3.2
1	A	83	ILE	3.2
1	H	175	TYR	3.2
1	C	145	VAL	3.2
1	E	81	VAL	3.2
1	H	257	SER	3.1
1	H	216	VAL	3.1
1	E	232	THR	3.1
1	B	204	ASP	3.1
1	G	43	PHE	3.1
1	E	87	GLY	3.1
1	H	171	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	35	LEU	3.1
1	G	256	ALA	3.1
1	C	141	GLY	3.1
1	C	104	ILE	3.1
1	G	118	ARG	3.1
1	A	21	VAL	3.1
1	E	145	VAL	3.1
1	H	147	GLN	3.1
1	F	176	GLU	3.1
1	H	182	LEU	3.1
1	G	105	THR	3.1
1	C	48	ALA	3.0
1	C	116	PHE	3.0
1	H	213	PHE	3.0
1	H	195	CYS	3.0
1	C	25	LEU	3.0
1	E	92	LEU	3.0
1	H	142	VAL	3.0
1	E	98	HIS	3.0
1	G	7	TRP	3.0
1	A	135	LYS	3.0
1	E	85	GLY	3.0
1	F	14	GLN	3.0
1	F	38	PHE	3.0
1	H	15	PHE	3.0
1	H	87	GLY	3.0
1	H	141	GLY	3.0
1	G	103	SER	3.0
1	H	151	THR	3.0
1	A	145	VAL	3.0
1	H	107	VAL	3.0
1	D	182	LEU	2.9
1	H	204	ASP	2.9
1	B	111	ALA	2.9
1	F	134	PHE	2.9
1	G	83	ILE	2.9
1	G	87	GLY	2.9
1	G	257	SER	2.9
1	E	134	PHE	2.9
1	E	135	LYS	2.9
1	F	195	CYS	2.9
1	F	232	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	118	ARG	2.9
1	G	109	ILE	2.9
1	H	209	LEU	2.9
1	C	86	GLY	2.9
1	A	6	GLN	2.9
1	C	150	GLN	2.9
1	G	132	PRO	2.9
1	G	135	LYS	2.9
1	A	36	ILE	2.9
1	G	138	ILE	2.9
1	F	197	LEU	2.9
1	G	150	GLN	2.9
1	E	52	VAL	2.9
1	H	190	ALA	2.9
1	E	118	ARG	2.9
1	E	11	LEU	2.9
1	A	150	GLN	2.8
1	A	88	ASP	2.8
1	A	110	ASP	2.8
1	C	128	SER	2.8
1	G	285	SER	2.8
1	G	148	THR	2.8
1	G	155	ILE	2.8
1	A	47	MET	2.8
1	C	51	GLY	2.8
1	F	147	GLN	2.8
1	G	99	LYS	2.8
1	H	129	TYR	2.8
1	C	135	LYS	2.8
1	H	227	TYR	2.8
1	H	174	PHE	2.8
1	E	8	HIS	2.8
1	D	146	ASN	2.8
1	D	232	THR	2.8
1	A	181	CYS	2.8
1	G	45	ARG	2.8
1	E	120	TYR	2.8
1	H	38	PHE	2.8
1	A	259	LEU	2.8
1	E	138	ILE	2.8
1	F	203	ILE	2.8
1	F	279	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	H	36	ILE	2.8
1	H	155	ILE	2.8
1	C	22	ASP	2.8
1	E	157	SER	2.8
1	E	40	ASN	2.7
1	C	105	THR	2.7
1	E	148	THR	2.7
1	F	151	THR	2.7
1	G	112	GLY	2.7
1	D	197	LEU	2.7
1	G	98	HIS	2.7
1	H	206	HIS	2.7
1	G	183	ASN	2.7
1	C	127	GLY	2.7
1	H	217	GLY	2.7
1	E	257	SER	2.7
1	A	53	VAL	2.7
1	A	99	LYS	2.7
1	D	5	LYS	2.7
1	E	7	TRP	2.7
1	A	26	TYR	2.7
1	C	47	MET	2.7
1	C	151	THR	2.7
1	E	132	PRO	2.7
1	G	149	SER	2.7
1	G	142	VAL	2.7
1	F	138	ILE	2.7
1	G	121	LEU	2.7
1	A	129	TYR	2.7
1	C	117	CYS	2.7
1	E	178	CYS	2.7
1	C	100	ASN	2.7
1	G	55	THR	2.7
1	H	10	THR	2.7
1	G	88	ASP	2.7
1	H	199	GLN	2.7
1	G	53	VAL	2.7
1	H	279	LEU	2.7
1	A	48	ALA	2.6
1	A	174	PHE	2.6
1	H	135	LYS	2.6
1	H	152	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	117	CYS	2.6
1	H	181	CYS	2.6
1	A	89	GLY	2.6
1	A	55	THR	2.6
1	B	30	THR	2.6
1	H	225	THR	2.6
1	D	14	GLN	2.6
1	B	138	ILE	2.6
1	C	19	PHE	2.6
1	E	48	ALA	2.6
1	H	19	PHE	2.6
1	H	47	MET	2.6
1	E	261	CYS	2.6
1	E	16	GLY	2.6
1	E	229	GLY	2.6
1	F	148	THR	2.6
1	A	81	VAL	2.6
1	A	121	LEU	2.6
1	H	11	LEU	2.6
1	A	156	ILE	2.6
1	F	188	PHE	2.6
1	F	87	GLY	2.6
1	G	44	GLY	2.6
1	G	258	GLY	2.6
1	E	159	CYS	2.6
1	F	136	LEU	2.6
1	C	43	PHE	2.6
1	G	139	ASP	2.6
1	F	129	TYR	2.6
1	F	227	TYR	2.6
1	A	84	ILE	2.6
1	C	181	CYS	2.6
1	E	56	THR	2.6
1	B	170	PHE	2.6
1	H	126	ALA	2.6
1	C	77	HIS	2.5
1	A	86	GLY	2.5
1	F	175	TYR	2.5
1	A	46	VAL	2.5
1	D	114	VAL	2.5
1	F	113	VAL	2.5
1	F	19	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	H	196	PHE	2.5
1	H	267	ALA	2.5
1	E	97	ARG	2.5
1	D	12	HIS	2.5
1	G	27	HIS	2.5
1	G	34	ASP	2.5
1	F	285	SER	2.5
1	G	86	GLY	2.5
1	A	114	VAL	2.5
1	E	109	ILE	2.5
1	A	232	THR	2.5
1	G	96	THR	2.5
1	H	6	GLN	2.5
1	F	236	ALA	2.5
1	E	181	CYS	2.5
1	F	159	CYS	2.5
1	F	143	ASN	2.5
1	G	124	HIS	2.5
1	A	153	ASP	2.5
1	A	257	SER	2.5
1	D	255	LEU	2.5
1	F	127	GLY	2.5
1	H	127	GLY	2.5
1	B	173	ALA	2.5
1	C	30	THR	2.5
1	E	119	GLN	2.5
1	F	196	PHE	2.5
1	G	188	PHE	2.5
1	G	182	LEU	2.5
1	H	242	LEU	2.5
1	A	288	SER	2.5
1	G	156	ILE	2.5
1	A	154	VAL	2.5
1	E	113	VAL	2.5
1	G	152	PHE	2.5
1	G	263	TYR	2.5
1	A	147	GLN	2.5
1	E	222	ALA	2.5
1	H	150	GLN	2.5
1	E	12	HIS	2.5
1	F	146	ASN	2.5
1	G	40	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	G	82	LEU	2.4
1	G	187	ILE	2.4
1	H	184	PRO	2.4
1	H	85	GLY	2.4
1	H	189	VAL	2.4
1	H	205	SER	2.4
1	B	20	ALA	2.4
1	C	78	ALA	2.4
1	E	18	TYR	2.4
1	F	160	THR	2.4
1	A	192	ASN	2.4
1	B	67	MET	2.4
1	H	35	LEU	2.4
1	D	109	ILE	2.4
1	E	53	VAL	2.4
1	G	16	GLY	2.4
1	A	118	ARG	2.4
1	F	172	SER	2.4
1	G	134	PHE	2.4
1	E	227	TYR	2.4
1	G	8	HIS	2.4
1	H	179	LYS	2.4
1	E	285	SER	2.4
1	G	78	ALA	2.4
1	B	199	GLN	2.4
1	A	27	HIS	2.4
1	H	25	LEU	2.4
1	G	123	ASN	2.4
1	F	229	GLY	2.4
1	E	133	ARG	2.4
1	E	38	PHE	2.4
1	G	41	ALA	2.4
1	E	150	GLN	2.4
1	G	17	GLN	2.4
1	H	18	TYR	2.4
1	H	12	HIS	2.4
1	A	141	GLY	2.3
1	A	38	PHE	2.3
1	B	159	CYS	2.3
1	E	42	ALA	2.3
1	C	285	SER	2.3
1	H	210	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	18	TYR	2.3
1	E	163	ILE	2.3
1	B	5	LYS	2.3
1	G	145	VAL	2.3
1	E	34	ASP	2.3
1	G	131	ASP	2.3
1	F	284	ALA	2.3
1	G	261	CYS	2.3
1	F	128	SER	2.3
1	H	27	HIS	2.3
1	H	212	TYR	2.3
1	G	141	GLY	2.3
1	H	86	GLY	2.3
1	H	13	ASP	2.3
1	A	255	LEU	2.3
1	E	197	LEU	2.3
1	A	5	LYS	2.3
1	C	7	TRP	2.3
1	C	55	THR	2.3
1	H	207	ARG	2.3
1	E	154	VAL	2.3
1	E	88	ASP	2.3
1	F	22	ASP	2.3
1	F	204	ASP	2.3
1	G	140	ASP	2.3
1	B	195	CYS	2.3
1	C	122	PRO	2.3
1	C	142	VAL	2.3
1	E	21	VAL	2.3
1	C	258	GLY	2.3
1	F	86	GLY	2.3
1	E	100	ASN	2.2
1	F	28	GLU	2.2
1	G	92	LEU	2.2
1	C	147	GLN	2.2
1	H	83	ILE	2.2
1	H	138	ILE	2.2
1	B	27	HIS	2.2
1	H	118	ARG	2.2
1	G	181	CYS	2.2
1	A	105	THR	2.2
1	C	96	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	H	149	SER	2.2
1	G	15	PHE	2.2
1	A	123	ASN	2.2
1	C	156	ILE	2.2
1	F	191	GLN	2.2
1	A	225	THR	2.2
1	F	47	MET	2.2
1	H	202	ALA	2.2
1	A	58	ARG	2.2
1	H	139	ASP	2.2
1	E	91	MET	2.2
1	H	157	SER	2.2
1	B	15	PHE	2.2
1	F	213	PHE	2.2
1	F	92	LEU	2.2
1	A	108	GLU	2.2
1	F	39	GLU	2.2
1	A	97	ARG	2.2
1	C	33	GLN	2.2
1	D	147	GLN	2.2
1	C	98	HIS	2.2
1	E	77	HIS	2.2
1	C	95	VAL	2.2
1	C	114	VAL	2.2
1	E	10	THR	2.2
1	G	56	THR	2.2
1	G	228	GLY	2.2
1	C	149	SER	2.2
1	E	182	LEU	2.2
1	F	35	LEU	2.2
1	H	49	LEU	2.2
1	H	128	SER	2.2
1	H	176	GLU	2.2
1	G	97	ARG	2.1
1	D	211	HIS	2.1
1	H	185	GLY	2.1
1	B	182	LEU	2.1
1	B	172	SER	2.1
1	B	181	CYS	2.1
1	C	41	ALA	2.1
1	F	234	ALA	2.1
1	H	234	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	180	ARG	2.1
1	E	187	ILE	2.1
1	E	14	GLN	2.1
1	H	143	ASN	2.1
1	A	52	VAL	2.1
1	H	34	ASP	2.1
1	B	136	LEU	2.1
1	B	197	LEU	2.1
1	C	129	TYR	2.1
1	D	167	GLU	2.1
1	B	184	PRO	2.1
1	G	23	ASN	2.1
1	A	258	GLY	2.1
1	A	116	PHE	2.1
1	C	130	ASP	2.1
1	E	15	PHE	2.1
1	E	174	PHE	2.1
1	F	7	TRP	2.1
1	H	7	TRP	2.1
1	A	155	ILE	2.1
1	A	173	ALA	2.1
1	E	20	ALA	2.1
1	H	187	ILE	2.1
1	A	157	SER	2.1
1	D	210	SER	2.1
1	B	147	GLN	2.1
1	C	286	GLN	2.1
1	F	6	GLN	2.1
1	H	106	MET	2.1
1	B	107	VAL	2.1
1	C	81	VAL	2.1
1	C	154	VAL	2.1
1	H	101	VAL	2.1
1	E	49	LEU	2.1
1	E	259	LEU	2.1
1	F	182	LEU	2.1
1	C	152	PHE	2.1
1	E	89	GLY	2.1
1	A	240	ASP	2.1
1	E	126	ALA	2.1
1	H	282	ALA	2.1
1	E	264	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	14	GLN	2.0
1	G	91	MET	2.0
1	H	46	VAL	2.0
1	H	183	ASN	2.0
1	B	141	GLY	2.0
1	F	15	PHE	2.0
1	G	76	GLY	2.0
1	E	41	ALA	2.0
1	F	13	ASP	2.0
1	F	202	ALA	2.0
1	G	130	ASP	2.0
1	A	39	GLU	2.0
1	F	18	TYR	2.0
1	C	101	VAL	2.0
1	E	124	HIS	2.0
1	A	132	PRO	2.0
1	A	184	PRO	2.0
1	C	261	CYS	2.0
1	H	159	CYS	2.0
1	E	45	ARG	2.0
1	F	118	ARG	2.0
1	B	28	GLU	2.0
1	B	208	LYS	2.0
1	C	18	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	D	291	5/5	0.50	0.14	115,117,151,165	0
2	SO4	G	293	5/5	0.53	0.11	122,127,140,171	0
2	SO4	C	292	5/5	0.55	0.12	122,128,153,158	0
2	SO4	H	290	5/5	0.55	0.11	101,113,139,153	0
2	SO4	D	292	5/5	0.60	0.09	99,129,147,159	0
2	SO4	G	292	5/5	0.64	0.13	128,131,159,164	0
2	SO4	F	292	5/5	0.67	0.16	96,117,146,154	0
2	SO4	E	292	5/5	0.67	0.12	122,147,162,174	0
2	SO4	A	291	5/5	0.70	0.15	84,119,163,185	0
2	SO4	F	291	5/5	0.71	0.08	109,109,138,141	0
2	SO4	C	293	5/5	0.76	0.12	99,119,140,150	0
2	SO4	A	290	5/5	0.80	0.17	107,109,125,146	0
2	SO4	B	290	5/5	0.82	0.15	85,86,110,114	0
2	SO4	F	289	5/5	0.83	0.15	76,108,119,121	0
2	SO4	G	290	5/5	0.84	0.13	96,108,126,139	0
2	SO4	D	289	5/5	0.84	0.15	88,108,116,119	0
2	SO4	E	291	5/5	0.84	0.13	92,107,125,142	0
2	SO4	C	290	5/5	0.84	0.15	90,90,125,125	0
2	SO4	E	289	5/5	0.86	0.14	74,79,94,102	0
2	SO4	H	289	5/5	0.86	0.18	76,96,100,113	0
2	SO4	G	289	5/5	0.86	0.16	70,77,93,105	0
2	SO4	B	289	5/5	0.88	0.14	78,93,103,115	0
2	SO4	F	290	5/5	0.88	0.18	87,92,101,111	0
2	SO4	A	289	5/5	0.89	0.13	79,87,101,108	0
2	SO4	G	291	5/5	0.89	0.15	99,108,132,153	0
2	SO4	C	291	5/5	0.90	0.15	59,60,82,87	0
2	SO4	C	289	5/5	0.90	0.15	79,87,92,98	0
2	SO4	D	290	5/5	0.91	0.14	58,91,94,98	0
2	SO4	A	292	5/5	0.94	0.12	47,64,68,70	0
2	SO4	E	290	5/5	0.97	0.13	63,65,74,79	0
2	SO4	C	294	5/5	0.98	0.07	56,66,73,74	0

6.5 Other polymers ⓘ

There are no such residues in this entry.