



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:33 PM GMT

PDB ID : 1FZW  
Title : THE STRUCTURAL BASIS OF THE CATALYTIC MECHANISM AND  
REGULATION OF GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE (RMLA). APO ENZYME.  
Authors : Blankenfeldt, W.; Asuncion, M.; Lam, J.S.; Naismith, J.H.  
Deposited on : 2000-10-04  
Resolution : 1.90 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

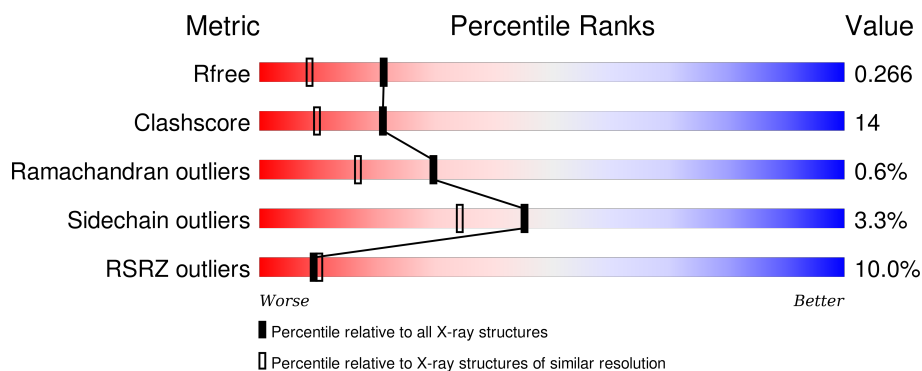
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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))
$R_{free}$	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	293	<div> <div>12%</div> <div>71%</div> <div>24%</div> <div>.</div> </div>
1	B	293	<div> <div>12%</div> <div>69%</div> <div>26%</div> <div>5%</div> </div>
1	C	293	<div> <div>9%</div> <div>72%</div> <div>24%</div> <div>.</div> </div>
1	D	293	<div> <div>11%</div> <div>73%</div> <div>24%</div> <div>.</div> </div>
1	E	293	<div> <div>9%</div> <div>70%</div> <div>25%</div> <div>5%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	293	
1	G	293	
1	H	293	

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	C	5000	-	-	X	-
2	SO4	D	3601	-	X	-	-
2	SO4	H	6101	-	-	X	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 21094 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 GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	292	Total	C	N	O	S	0	2	0
			2302	1472	388	437	5			
1	B	292	Total	C	N	O	S	0	5	0
			2322	1484	391	442	5			
1	C	293	Total	C	N	O	S	0	6	0
			2340	1494	394	446	6			
1	D	292	Total	C	N	O	S	0	1	0
			2294	1467	387	436	4			
1	E	292	Total	C	N	O	S	0	7	0
			2339	1491	396	447	5			
1	F	293	Total	C	N	O	S	0	3	0
			2316	1480	389	441	6			
1	G	292	Total	C	N	O	S	0	4	0
			2318	1480	392	441	5			
1	H	292	Total	C	N	O	S	0	0	0
			2285	1462	385	434	4			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

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

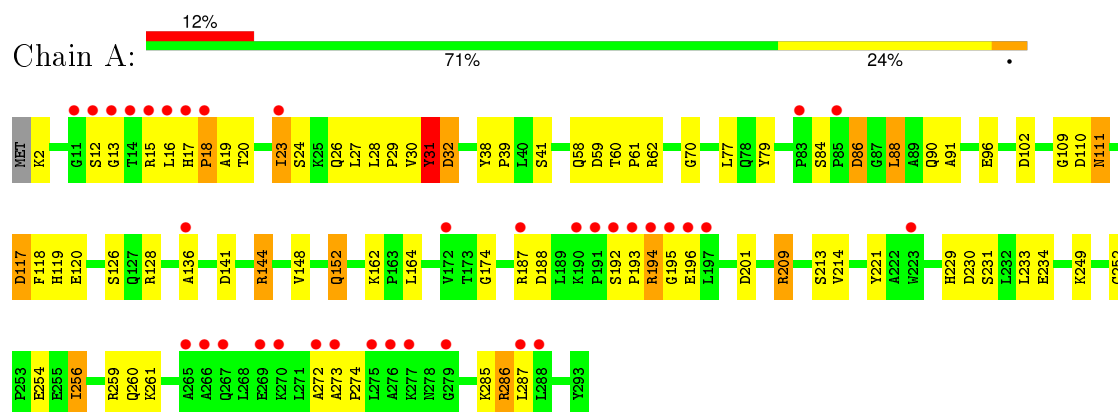
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	325	Total	O	0	0
			325	325		
3	B	335	Total	O	0	0
			335	335		
3	C	286	Total	O	0	0
			286	286		
3	D	259	Total	O	0	0
			259	259		
3	E	282	Total	O	0	0
			282	282		
3	F	321	Total	O	0	0
			321	321		
3	G	367	Total	O	0	0
			367	367		
3	H	303	Total	O	0	0
			303	303		

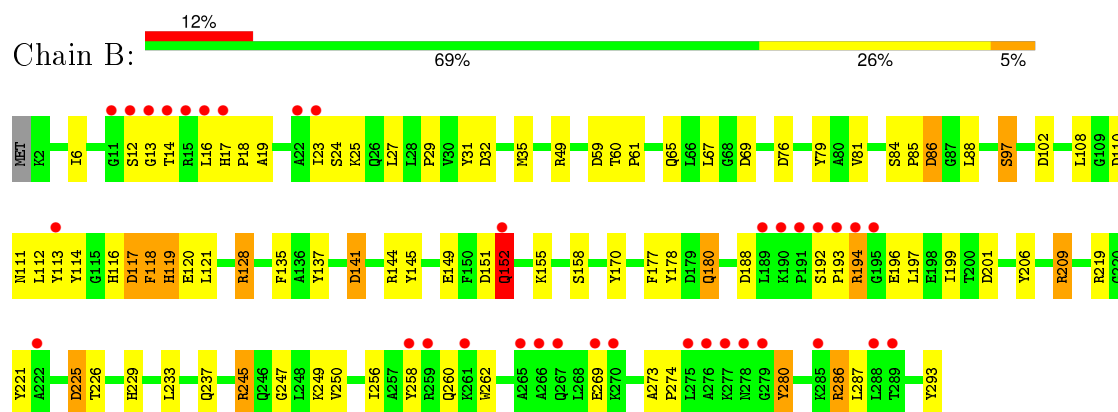
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

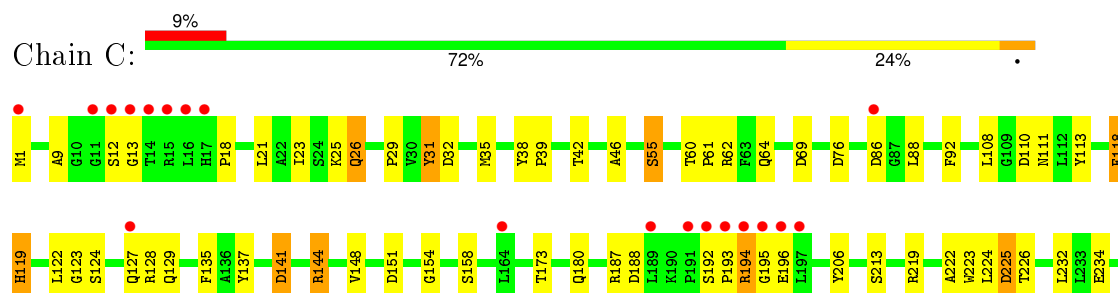
#### • Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLTRANSFERASE

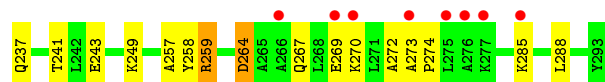


#### • Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLTRANSFERASE

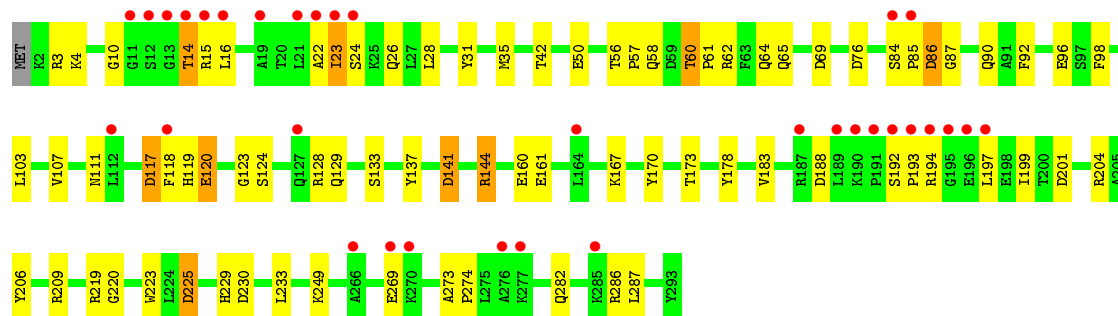
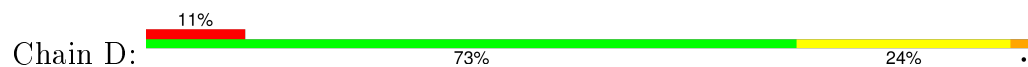


#### • Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLTRANSFERASE

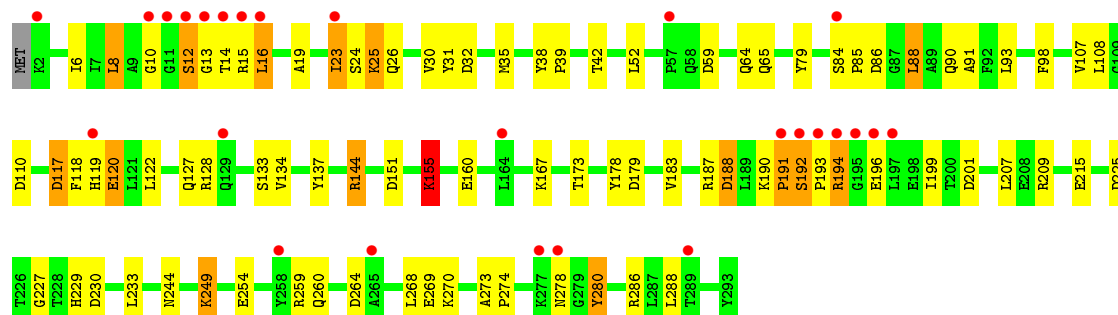




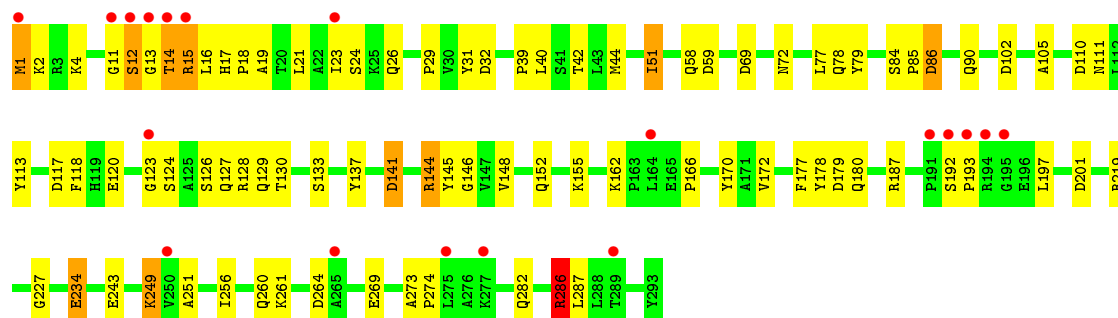
• Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLTRANSFERASE



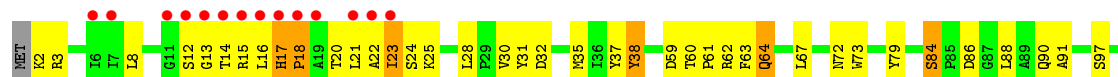
• Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLTRANSFERASE



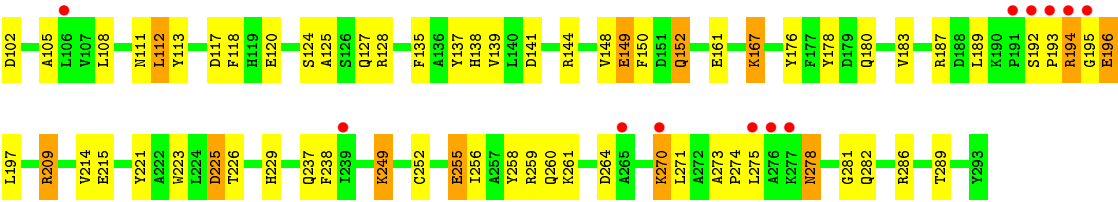
• Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLTRANSFERASE



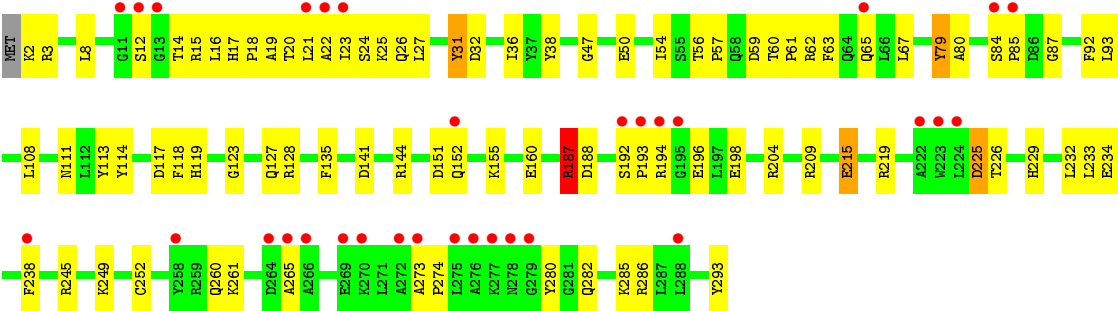
• Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLTRANSFERASE







● Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.66 Å   73.66 Å   134.47 Å 89.98°   80.91°   80.91°	Depositor
Resolution (Å)	73.00 – 1.90 40.41 – 1.90	Depositor EDS
% Data completeness (in resolution range)	95.8 (73.00-1.90) 94.7 (40.41-1.90)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.94 (at 1.89 Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, $R_{free}$	0.176   ,   0.251 0.195   ,   0.266	Depositor DCC
$R_{free}$ test set	10144 reflections (5.05%)	DCC
Wilson B-factor (Å <sup>2</sup> )	21.7	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 62.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 200900 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	21094	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.49% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	1.63	21/2352 (0.9%)	1.28	15/3190 (0.5%)
1	B	1.59	22/2372 (0.9%)	1.35	25/3217 (0.8%)
1	C	1.55	17/2390 (0.7%)	1.30	20/3239 (0.6%)
1	D	1.56	18/2344 (0.8%)	1.28	13/3180 (0.4%)
1	E	1.47	10/2389 (0.4%)	1.27	17/3240 (0.5%)
1	F	1.64	25/2366 (1.1%)	1.33	17/3208 (0.5%)
1	G	1.80	41/2368 (1.7%)	1.35	19/3212 (0.6%)
1	H	1.58	18/2335 (0.8%)	1.31	17/3168 (0.5%)
All	All	1.60	172/18916 (0.9%)	1.31	143/25654 (0.6%)

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	C	0	1
1	G	0	2
1	H	0	1
All	All	0	4

All (172) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	128	ARG	CZ-NH2	-10.10	1.20	1.33
1	D	35	MET	CG-SD	-9.53	1.56	1.81
1	G	255	GLU	CD-OE2	-8.60	1.16	1.25
1	E	249	LYS	CD-CE	8.24	1.71	1.51
1	F	251	ALA	CA-CB	7.93	1.69	1.52
1	F	137	TYR	CG-CD2	-7.90	1.28	1.39
1	G	249	LYS	CD-CE	7.76	1.70	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	249	LYS	CD-CE	7.68	1.70	1.51
1	G	148	VAL	CB-CG1	-7.65	1.36	1.52
1	C	206	TYR	CG-CD1	-7.46	1.29	1.39
1	G	118	PHE	CG-CD1	-7.41	1.27	1.38
1	G	124	SER	CB-OG	7.34	1.51	1.42
1	B	114	TYR	CD2-CE2	-7.27	1.28	1.39
1	F	79	TYR	CE1-CZ	7.26	1.48	1.38
1	C	92	PHE	CE1-CZ	-7.26	1.23	1.37
1	H	293	TYR	CE2-CZ	-7.14	1.29	1.38
1	D	120	GLU	CD-OE1	7.13	1.33	1.25
1	D	137	TYR	CD2-CE2	7.13	1.50	1.39
1	H	79	TYR	CD1-CE1	7.02	1.49	1.39
1	E	280	TYR	CD1-CE1	6.95	1.49	1.39
1	H	293	TYR	CG-CD1	-6.92	1.30	1.39
1	G	223	TRP	CB-CG	6.92	1.62	1.50
1	G	105	ALA	CA-CB	-6.91	1.38	1.52
1	E	137	TYR	CD2-CE2	6.84	1.49	1.39
1	D	120	GLU	CD-OE2	6.83	1.33	1.25
1	B	35[A]	MET	CG-SD	-6.77	1.63	1.81
1	B	35[B]	MET	CG-SD	-6.77	1.63	1.81
1	B	135	PHE	CE2-CZ	-6.75	1.24	1.37
1	B	180	GLN	CG-CD	6.75	1.66	1.51
1	G	282	GLN	CB-CG	6.73	1.70	1.52
1	B	245	ARG	CG-CD	-6.69	1.35	1.51
1	E	120	GLU	CD-OE1	6.69	1.33	1.25
1	A	249	LYS	CE-NZ	6.65	1.65	1.49
1	A	213	SER	CB-OG	6.64	1.50	1.42
1	F	286	ARG	CG-CD	6.63	1.68	1.51
1	G	214	VAL	CB-CG2	-6.57	1.39	1.52
1	A	38	TYR	CE1-CZ	6.55	1.47	1.38
1	B	178	TYR	CD1-CE1	6.53	1.49	1.39
1	C	257	ALA	CA-CB	-6.48	1.38	1.52
1	F	172	VAL	CB-CG1	6.48	1.66	1.52
1	B	145	TYR	CE1-CZ	-6.48	1.30	1.38
1	G	261	LYS	CE-NZ	6.46	1.65	1.49
1	F	124	SER	CB-OG	6.42	1.50	1.42
1	H	238	PHE	CE1-CZ	-6.39	1.25	1.37
1	H	38	TYR	CD2-CE2	6.35	1.48	1.39
1	D	206	TYR	CD2-CE2	-6.32	1.29	1.39
1	C	137	TYR	CE2-CZ	-6.30	1.30	1.38
1	F	51	ILE	N-CA	-6.25	1.33	1.46
1	G	149	GLU	CD-OE2	-6.23	1.18	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	92	PHE	CB-CG	-6.23	1.40	1.51
1	G	178	TYR	CE2-CZ	6.21	1.46	1.38
1	E	38	TYR	CG-CD1	6.19	1.47	1.39
1	G	120	GLU	CD-OE1	6.19	1.32	1.25
1	F	144	ARG	CG-CD	6.16	1.67	1.51
1	G	118	PHE	CE2-CZ	6.15	1.49	1.37
1	G	128	ARG	CB-CG	-6.15	1.35	1.52
1	C	222	ALA	CA-CB	-6.14	1.39	1.52
1	G	118	PHE	CE1-CZ	-6.13	1.25	1.37
1	A	221	TYR	CD2-CE2	6.12	1.48	1.39
1	H	114	TYR	CD2-CE2	-6.11	1.30	1.39
1	F	249	LYS	CD-CE	6.10	1.66	1.51
1	A	148	VAL	CB-CG1	-6.08	1.40	1.52
1	G	252	CYS	CB-SG	-6.08	1.72	1.82
1	H	92	PHE	CB-CG	-6.06	1.41	1.51
1	A	136	ALA	CA-CB	-6.00	1.39	1.52
1	A	30	VAL	CB-CG1	-5.99	1.40	1.52
1	F	148	VAL	CB-CG1	-5.97	1.40	1.52
1	G	37	TYR	CE1-CZ	-5.95	1.30	1.38
1	D	206	TYR	CD1-CE1	-5.94	1.30	1.39
1	G	258	TYR	CG-CD2	-5.90	1.31	1.39
1	C	113	TYR	CE2-CZ	-5.90	1.30	1.38
1	B	206	TYR	CD2-CE2	-5.89	1.30	1.39
1	G	238	PHE	CE1-CZ	-5.87	1.26	1.37
1	B	152	GLN	CG-CD	5.87	1.64	1.51
1	A	254	GLU	CD-OE1	5.86	1.32	1.25
1	B	81	VAL	CB-CG1	-5.85	1.40	1.52
1	C	249	LYS	CD-CE	5.85	1.65	1.51
1	B	221	TYR	CE2-CZ	-5.81	1.30	1.38
1	F	234	GLU	CG-CD	5.78	1.60	1.51
1	F	177	PHE	CE2-CZ	-5.76	1.26	1.37
1	D	167	LYS	CD-CE	5.75	1.65	1.51
1	G	139	VAL	CB-CG2	5.74	1.64	1.52
1	B	293	TYR	CE2-CZ	-5.73	1.31	1.38
1	B	280	TYR	CE2-CZ	-5.72	1.31	1.38
1	G	64	GLN	CB-CG	-5.70	1.37	1.52
1	B	6	ILE	C-O	5.69	1.34	1.23
1	E	155	LYS	CE-NZ	5.68	1.63	1.49
1	C	92	PHE	CG-CD1	-5.66	1.30	1.38
1	G	125	ALA	CA-CB	-5.63	1.40	1.52
1	E	249	LYS	CE-NZ	5.63	1.63	1.49
1	A	256	ILE	C-O	5.61	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	214	VAL	CB-CG2	-5.60	1.41	1.52
1	B	118	PHE	CE2-CZ	5.60	1.48	1.37
1	B	158	SER	CB-OG	-5.60	1.34	1.42
1	G	137	TYR	CE2-CZ	5.60	1.45	1.38
1	C	35[A]	MET	CG-SD	-5.58	1.66	1.81
1	C	35[B]	MET	CG-SD	-5.58	1.66	1.81
1	G	128	ARG	NE-CZ	-5.58	1.25	1.33
1	C	148	VAL	CB-CG1	-5.58	1.41	1.52
1	G	118	PHE	CB-CG	-5.57	1.41	1.51
1	D	170	TYR	CE1-CZ	5.56	1.45	1.38
1	H	219	ARG	CG-CD	5.56	1.65	1.51
1	G	73	TRP	CB-CG	5.54	1.60	1.50
1	G	180	GLN	CG-CD	5.51	1.63	1.51
1	H	198	GLU	CD-OE1	5.51	1.31	1.25
1	C	158	SER	CA-CB	5.51	1.61	1.52
1	B	177	PHE	CG-CD2	-5.50	1.30	1.38
1	G	38	TYR	CD1-CE1	5.49	1.47	1.39
1	F	249	LYS	CA-CB	5.48	1.66	1.53
1	C	137	TYR	CD1-CE1	-5.47	1.31	1.39
1	A	31	TYR	CB-CG	5.46	1.59	1.51
1	G	2	LYS	N-CA	5.44	1.57	1.46
1	C	135	PHE	CG-CD2	-5.44	1.30	1.38
1	D	178	TYR	CD2-CE2	-5.44	1.31	1.39
1	G	167	LYS	CD-CE	5.43	1.64	1.51
1	D	65	GLN	CG-CD	5.42	1.63	1.51
1	H	245	ARG	CZ-NH1	-5.42	1.26	1.33
1	D	220	GLY	N-CA	5.41	1.54	1.46
1	C	29	PRO	CG-CD	-5.39	1.32	1.50
1	C	258	TYR	CB-CG	5.39	1.59	1.51
1	H	113	TYR	CE2-CZ	5.39	1.45	1.38
1	G	221	TYR	CE2-CZ	-5.38	1.31	1.38
1	G	113	TYR	CE2-CZ	5.37	1.45	1.38
1	G	63	PHE	CG-CD1	-5.36	1.30	1.38
1	F	130	THR	CB-CG2	5.36	1.70	1.52
1	B	247	GLY	C-O	-5.35	1.15	1.23
1	D	107	VAL	CB-CG2	-5.33	1.41	1.52
1	F	26	GLN	C-O	5.33	1.33	1.23
1	E	134	VAL	CB-CG2	5.33	1.64	1.52
1	B	258	TYR	CD2-CE2	5.32	1.47	1.39
1	G	120	GLU	CD-OE2	5.31	1.31	1.25
1	F	105	ALA	CA-CB	-5.31	1.41	1.52
1	H	31	TYR	CG-CD1	-5.29	1.32	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	118	PHE	CB-CG	-5.29	1.42	1.51
1	D	219	ARG	CA-CB	-5.28	1.42	1.53
1	G	37	TYR	CG-CD2	-5.27	1.32	1.39
1	A	91	ALA	CA-CB	5.26	1.63	1.52
1	B	97	SER	CB-OG	5.26	1.49	1.42
1	A	286	ARG	CB-CG	-5.25	1.38	1.52
1	A	252	CYS	CB-SG	-5.25	1.73	1.81
1	C	31	TYR	CD2-CE2	5.24	1.47	1.39
1	A	152	GLN	CG-CD	5.23	1.63	1.51
1	A	128	ARG	CB-CG	-5.22	1.38	1.52
1	G	249	LYS	CE-NZ	5.22	1.62	1.49
1	G	221	TYR	CB-CG	-5.22	1.43	1.51
1	H	215	GLU	CD-OE2	5.21	1.31	1.25
1	D	133	SER	CB-OG	-5.19	1.35	1.42
1	A	41	SER	CB-OG	-5.16	1.35	1.42
1	F	146	GLY	C-O	-5.12	1.15	1.23
1	D	144	ARG	NE-CZ	5.12	1.39	1.33
1	F	170	TYR	CE1-CZ	5.12	1.45	1.38
1	F	120	GLU	CD-OE1	5.11	1.31	1.25
1	A	118	PHE	CE2-CZ	5.09	1.47	1.37
1	F	243	GLU	CD-OE2	-5.09	1.20	1.25
1	F	166	PRO	CA-C	-5.08	1.42	1.52
1	G	128	ARG	CZ-NH2	-5.08	1.26	1.33
1	G	30	VAL	CB-CG1	-5.08	1.42	1.52
1	H	252	CYS	CB-SG	-5.06	1.73	1.81
1	B	170	TYR	CE1-CZ	5.06	1.45	1.38
1	F	177	PHE	CD2-CE2	5.06	1.49	1.39
1	H	65	GLN	CG-CD	5.06	1.62	1.51
1	A	79	TYR	CD2-CE2	-5.04	1.31	1.39
1	F	178	TYR	CD2-CE2	-5.04	1.31	1.39
1	F	133	SER	CB-OG	-5.04	1.35	1.42
1	D	128	ARG	CB-CG	-5.02	1.39	1.52
1	A	110	ASP	C-O	-5.02	1.13	1.23
1	D	249	LYS	CD-CE	5.02	1.63	1.51
1	E	25	LYS	CD-CE	5.01	1.63	1.51
1	H	234	GLU	CD-OE1	5.01	1.31	1.25
1	F	113	TYR	CG-CD2	-5.01	1.32	1.39
1	E	167	LYS	CD-CE	5.01	1.63	1.51
1	G	152	GLN	CG-CD	5.01	1.62	1.51

All (143) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	209	ARG	NE-CZ-NH2	-13.72	113.44	120.30
1	A	128	ARG	NE-CZ-NH2	-13.27	113.67	120.30
1	G	209	ARG	NE-CZ-NH2	-11.89	114.36	120.30
1	B	188	ASP	CB-CG-OD2	9.89	127.20	118.30
1	D	141	ASP	CB-CG-OD1	9.71	127.04	118.30
1	G	128	ARG	NE-CZ-NH1	-9.70	115.45	120.30
1	A	117	ASP	CB-CG-OD2	9.65	126.99	118.30
1	G	209	ARG	NE-CZ-NH1	9.39	124.99	120.30
1	B	102	ASP	CB-CG-OD2	9.34	126.71	118.30
1	A	209	ARG	NE-CZ-NH2	-9.28	115.66	120.30
1	B	209	ARG	NE-CZ-NH1	8.90	124.75	120.30
1	E	88	LEU	CA-CB-CG	8.86	135.68	115.30
1	G	286	ARG	NE-CZ-NH2	-8.56	116.02	120.30
1	H	194	ARG	NE-CZ-NH1	8.52	124.56	120.30
1	C	141	ASP	CB-CG-OD1	8.49	125.94	118.30
1	D	69	ASP	CB-CG-OD1	8.37	125.83	118.30
1	H	204	ARG	NE-CZ-NH2	-8.36	116.12	120.30
1	A	128	ARG	NE-CZ-NH1	8.29	124.44	120.30
1	C	264	ASP	CB-CG-OD2	8.23	125.71	118.30
1	B	151	ASP	CB-CG-OD1	8.07	125.56	118.30
1	D	76	ASP	CB-CG-OD2	8.00	125.50	118.30
1	B	201	ASP	CB-CG-OD1	7.99	125.49	118.30
1	H	209	ARG	NE-CZ-NH1	7.96	124.28	120.30
1	H	194	ARG	NE-CZ-NH2	-7.88	116.36	120.30
1	H	209	ARG	NE-CZ-NH2	-7.86	116.37	120.30
1	C	232	LEU	CB-CG-CD1	7.81	124.27	111.00
1	C	151	ASP	CB-CG-OD1	7.68	125.21	118.30
1	H	117	ASP	CB-CG-OD2	7.51	125.06	118.30
1	E	151	ASP	CB-CG-OD1	7.51	125.06	118.30
1	E	144	ARG	NE-CZ-NH1	7.47	124.03	120.30
1	F	141	ASP	CB-CG-OD1	7.46	125.02	118.30
1	F	69	ASP	CB-CG-OD1	7.45	125.00	118.30
1	B	286	ARG	NE-CZ-NH2	-7.32	116.64	120.30
1	C	69	ASP	CB-CG-OD1	7.22	124.80	118.30
1	F	187	ARG	NE-CZ-NH1	7.20	123.90	120.30
1	B	86	ASP	CB-CG-OD1	7.18	124.77	118.30
1	B	76	ASP	CB-CG-OD1	7.17	124.75	118.30
1	B	245	ARG	NE-CZ-NH2	-7.16	116.72	120.30
1	E	144	ARG	NE-CZ-NH2	-7.15	116.72	120.30
1	B	121	LEU	CB-CG-CD1	-7.14	98.87	111.00
1	A	286	ARG	NE-CZ-NH2	-7.11	116.75	120.30
1	D	86	ASP	CB-CG-OD2	7.10	124.69	118.30
1	G	3	ARG	NE-CZ-NH2	-7.07	116.77	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	102	ASP	CB-CG-OD2	7.06	124.65	118.30
1	B	117	ASP	CB-CG-OD2	7.06	124.65	118.30
1	H	286	ARG	NE-CZ-NH2	-6.95	116.83	120.30
1	H	3	ARG	NE-CZ-NH1	6.91	123.75	120.30
1	F	234	GLU	OE1-CD-OE2	-6.88	115.04	123.30
1	D	188	ASP	CB-CG-OD2	6.87	124.48	118.30
1	C	86	ASP	CB-CG-OD2	6.87	124.48	118.30
1	F	86	ASP	CB-CG-OD2	6.85	124.47	118.30
1	B	69	ASP	CB-CG-OD1	6.78	124.40	118.30
1	E	88	LEU	CB-CG-CD2	6.75	122.47	111.00
1	C	144	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	B	219	ARG	NE-CZ-NH2	-6.69	116.95	120.30
1	A	201	ASP	CB-CG-OD1	6.61	124.25	118.30
1	C	144	ARG	NE-CZ-NH2	-6.58	117.01	120.30
1	B	35[A]	MET	CG-SD-CE	6.58	110.73	100.20
1	B	35[B]	MET	CG-SD-CE	6.58	110.73	100.20
1	C	118	PHE	CB-CA-C	6.46	123.31	110.40
1	C	226	THR	OG1-CB-CG2	-6.46	95.15	110.00
1	F	201	ASP	CB-CG-OD1	6.45	124.11	118.30
1	H	226	THR	OG1-CB-CG2	-6.45	95.16	110.00
1	F	59	ASP	CB-CG-OD1	6.45	124.10	118.30
1	H	204	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	H	187	ARG	NE-CZ-NH1	-6.37	117.12	120.30
1	C	154	GLY	N-CA-C	6.31	128.87	113.10
1	E	188	ASP	CB-CG-OD2	6.29	123.96	118.30
1	C	259	ARG	NE-CZ-NH1	-6.29	117.16	120.30
1	G	226	THR	OG1-CB-CG2	-6.17	95.81	110.00
1	H	3	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	G	112	LEU	CA-CB-CG	6.10	129.34	115.30
1	G	102	ASP	CB-CG-OD2	6.08	123.77	118.30
1	C	259	ARG	NE-CZ-NH2	6.07	123.33	120.30
1	G	286	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	B	137	TYR	CA-CB-CG	5.99	124.79	113.40
1	H	128	ARG	NE-CZ-NH1	-5.96	117.32	120.30
1	A	230	ASP	CB-CG-OD1	5.95	123.66	118.30
1	C	141	ASP	OD1-CG-OD2	-5.95	112.00	123.30
1	F	179	ASP	CB-CG-OD1	5.90	123.61	118.30
1	C	76	ASP	CB-CG-OD1	5.89	123.60	118.30
1	G	150	PHE	CB-CG-CD2	5.87	124.91	120.80
1	F	110	ASP	CB-CG-OD1	5.85	123.56	118.30
1	H	8	LEU	CB-CG-CD2	-5.84	101.06	111.00
1	A	209	ARG	NE-CZ-NH1	5.84	123.22	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	E	179	ASP	CB-CG-OD1	5.83	123.55	118.30
1	F	219	ARG	NE-CZ-NH1	-5.76	117.42	120.30
1	H	188	ASP	CB-CG-OD2	5.74	123.47	118.30
1	G	3	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	E	264	ASP	CB-CG-OD2	5.72	123.44	118.30
1	A	32	ASP	CB-CG-OD2	5.71	123.44	118.30
1	E	110	ASP	CB-CG-OD1	5.71	123.44	118.30
1	E	230	ASP	CB-CG-OD2	5.71	123.44	118.30
1	C	124	SER	N-CA-CB	-5.70	101.95	110.50
1	D	230	ASP	CB-CG-OD1	5.68	123.42	118.30
1	D	173	THR	OG1-CB-CG2	-5.64	97.04	110.00
1	H	118	PHE	CB-CG-CD2	-5.60	116.88	120.80
1	E	207	LEU	CB-CG-CD1	5.60	120.53	111.00
1	F	264	ASP	CB-CG-OD2	5.60	123.34	118.30
1	F	249	LYS	CB-CG-CD	5.59	126.14	111.60
1	C	219	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	D	201	ASP	CB-CG-OD1	5.54	123.28	118.30
1	G	271	LEU	CB-CG-CD2	-5.52	101.61	111.00
1	G	117	ASP	CB-CG-OD2	5.52	123.27	118.30
1	C	173	THR	OG1-CB-CG2	-5.51	97.33	110.00
1	B	144	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	E	201	ASP	CB-CG-OD2	5.46	123.22	118.30
1	A	188	ASP	CB-CG-OD2	5.46	123.21	118.30
1	E	188	ASP	OD1-CG-OD2	-5.46	112.93	123.30
1	A	144	ARG	NE-CZ-NH1	5.45	123.02	120.30
1	C	188	ASP	CB-CG-OD2	5.45	123.20	118.30
1	F	227	GLY	CA-C-O	-5.45	110.80	120.60
1	E	254	GLU	OE1-CD-OE2	-5.41	116.81	123.30
1	C	225	ASP	N-CA-CB	5.40	120.33	110.60
1	B	226	THR	OG1-CB-CG2	-5.39	97.61	110.00
1	H	286	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	G	264	ASP	CB-CG-OD2	5.35	123.11	118.30
1	A	286	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	G	67	LEU	CB-CG-CD2	-5.33	101.93	111.00
1	B	121	LEU	CB-CG-CD2	5.33	120.06	111.00
1	E	188	ASP	CB-CG-OD1	5.33	123.09	118.30
1	B	108	LEU	CB-CG-CD1	-5.32	101.95	111.00
1	G	249	LYS	CD-CE-NZ	5.31	123.91	111.70
1	B	128	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	D	223	TRP	N-CA-CB	5.27	120.08	110.60
1	G	189	LEU	CB-CG-CD1	-5.27	102.04	111.00
1	A	86	ASP	CB-CG-OD2	5.25	123.03	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	D	225	ASP	CB-CG-OD1	5.25	123.03	118.30
1	F	179	ASP	CB-CG-OD2	-5.23	113.60	118.30
1	D	219	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	E	173	THR	OG1-CB-CG2	-5.22	98.00	110.00
1	D	144	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	A	194	ARG	CB-CA-C	-5.19	100.02	110.40
1	G	225	ASP	N-CA-CB	5.19	119.93	110.60
1	E	110	ASP	CB-CG-OD2	-5.18	113.64	118.30
1	F	117	ASP	CB-CG-OD2	5.17	122.96	118.30
1	D	3	ARG	NE-CZ-NH2	5.13	122.86	120.30
1	B	141	ASP	CB-CG-OD1	5.13	122.92	118.30
1	F	187	ARG	NE-CZ-NH2	-5.11	117.74	120.30
1	B	250	VAL	CG1-CB-CG2	5.07	119.01	110.90
1	F	69	ASP	CB-CG-OD2	-5.06	113.75	118.30
1	G	176	TYR	CB-CG-CD2	5.04	124.03	121.00
1	B	225	ASP	CB-CA-C	5.01	120.43	110.40

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	119	HIS	Sidechain
1	G	138	HIS	Sidechain
1	G	17	HIS	Sidechain
1	H	17	HIS	Sidechain

## 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	2302	0	2287	89	0
1	B	2322	0	2305	89	0
1	C	2340	0	2324	66	0
1	D	2294	0	2279	64	0
1	E	2339	0	2316	87	0
1	F	2316	0	2301	66	0
1	G	2318	0	2300	58	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	2285	0	2272	58	0
2	A	10	0	0	0	0
2	B	10	0	0	1	0
2	C	15	0	0	2	0
2	D	15	0	0	0	0
2	E	15	0	0	0	0
2	F	10	0	0	0	0
2	G	15	0	0	1	0
2	H	10	0	0	2	0
3	A	325	0	0	35	1
3	B	335	0	0	25	0
3	C	286	0	0	14	0
3	D	259	0	0	17	0
3	E	282	0	0	31	0
3	F	321	0	0	22	4
3	G	367	0	0	23	3
3	H	303	0	0	15	1
All	All	21094	0	18384	530	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 14.

All (530) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:ILE:HG23	1:A:28:LEU:HD21	1.33	1.09
1:E:23:ILE:HG21	1:F:23:ILE:HG12	1.22	1.09
1:C:23:ILE:HG12	1:D:23:ILE:HG21	1.14	1.07
1:A:23:ILE:HB	1:B:23:ILE:HD12	1.11	1.06
1:A:23:ILE:CB	1:B:23:ILE:HD12	1.86	1.06
1:G:14:THR:HA	3:G:4997:HOH:O	1.56	1.04
1:E:23:ILE:HD13	1:F:23:ILE:HD13	1.04	1.04
1:B:23:ILE:HG13	3:B:4009:HOH:O	1.55	1.03
1:F:273:ALA:HB3	1:F:274:PRO:HD3	1.37	1.02
1:C:119:HIS:CD2	3:C:5244:HOH:O	2.13	1.01
1:B:192:SER:HB2	1:B:193:PRO:HD2	1.41	0.99
1:G:141[A]:ASP:OD2	1:G:144:ARG:HD3	1.59	0.99
1:G:141[B]:ASP:OD2	1:G:144:ARG:HD3	1.59	0.99
1:A:23:ILE:CG2	1:A:28:LEU:HD21	1.93	0.99
1:A:23:ILE:HG23	1:A:28:LEU:CD2	1.93	0.98
1:A:23:ILE:HD13	1:B:23:ILE:HB	1.43	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:LYS:NZ	1:A:194:ARG:HH21	1.61	0.97
1:C:23:ILE:CG1	1:D:23:ILE:HG21	1.95	0.96
1:E:23:ILE:CD1	1:F:23:ILE:HD13	1.96	0.95
1:A:162:LYS:HZ3	1:A:194:ARG:HH21	1.11	0.94
1:F:17:HIS:NE2	1:F:21:LEU:HD23	1.83	0.94
1:A:23:ILE:HB	1:B:23:ILE:CD1	1.98	0.93
1:C:119:HIS:HB2	3:C:5275:HOH:O	1.71	0.91
1:E:23:ILE:HD13	1:F:23:ILE:CD1	1.98	0.91
1:B:192:SER:HB2	1:B:193:PRO:CD	2.01	0.91
1:A:23:ILE:CG2	1:A:28:LEU:CD2	2.49	0.90
1:C:23:ILE:HG21	1:D:23:ILE:HG12	1.52	0.90
1:C:192:SER:HB2	1:C:193:PRO:HD2	1.54	0.89
1:G:90:GLN:HG2	1:G:197:LEU:HD12	1.55	0.88
1:E:273:ALA:HB3	1:E:274:PRO:HD3	1.57	0.87
1:C:13:GLY:O	3:C:5196:HOH:O	1.92	0.87
1:E:227:GLY:N	3:E:6150:HOH:O	2.04	0.84
1:H:2:LYS:N	3:H:6268:HOH:O	2.09	0.84
1:D:23:ILE:HD13	1:D:28:LEU:HD21	1.59	0.84
1:F:123:GLY:O	1:F:127:GLN:HG3	1.78	0.84
1:H:60:THR:HG23	3:H:6390:HOH:O	1.78	0.84
1:H:60:THR:HB	1:H:61:PRO:HD3	1.60	0.83
1:F:141:ASP:OD2	1:F:144:ARG:NH2	2.12	0.83
1:F:15:ARG:NH2	3:F:4951:HOH:O	2.12	0.83
1:A:162:LYS:NZ	1:A:194:ARG:NH2	2.25	0.83
1:E:23:ILE:CD1	1:F:23:ILE:HG21	2.08	0.82
1:H:25:LYS:HE3	1:H:26:GLN:HE22	1.45	0.82
1:D:160:GLU:HG2	3:D:3996:HOH:O	1.80	0.82
1:F:269:GLU:OE2	3:F:4984:HOH:O	1.97	0.81
1:E:190:LYS:HD2	1:E:190:LYS:C	2.02	0.79
1:E:128:ARG:NH2	1:E:215:GLU:OE2	2.15	0.79
1:G:209:ARG:HD3	3:G:5132:HOH:O	1.80	0.79
1:A:31:TYR:CD1	1:B:233[B]:LEU:HD11	2.18	0.79
1:E:128:ARG:NH1	1:E:133:SER:OG	2.16	0.79
1:G:270:LYS:HG2	3:G:5175:HOH:O	1.80	0.79
1:B:141:ASP:HB2	3:B:3773:HOH:O	1.83	0.79
1:E:190:LYS:HD2	1:E:191:PRO:N	1.97	0.79
1:G:16:LEU:HD12	1:G:25:LYS:HB2	1.65	0.78
1:H:273:ALA:HB3	1:H:274:PRO:HD3	1.65	0.78
1:F:23:ILE:HA	3:F:4846:HOH:O	1.84	0.78
1:F:287:LEU:HD23	3:F:5016:HOH:O	1.83	0.78
1:A:31:TYR:HD1	1:B:233[B]:LEU:HD11	1.49	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:152:GLN:HB2	3:F:4947:HOH:O	1.84	0.77
1:H:260:GLN:NE2	3:H:6392:HOH:O	2.17	0.77
1:A:12:SER:HB3	3:A:3800:HOH:O	1.83	0.77
1:D:161:GLU:HG3	1:D:194:ARG:HH21	1.49	0.76
1:B:16:LEU:HA	1:B:229:HIS:CE1	2.20	0.76
1:A:194:ARG:HB2	1:A:196:GLU:HG3	1.66	0.76
1:D:161:GLU:HG3	1:D:194:ARG:NH2	2.00	0.76
1:H:260:GLN:CD	3:H:6392:HOH:O	2.24	0.76
1:A:119:HIS:HB3	3:A:3841:HOH:O	1.85	0.76
1:E:119:HIS:HE1	3:E:6270:HOH:O	1.67	0.75
1:D:161:GLU:CG	1:D:194:ARG:HH21	1.99	0.75
1:E:23:ILE:HG21	1:F:23:ILE:CG1	2.12	0.75
1:F:32:ASP:OD2	1:F:249:LYS:HE3	1.87	0.75
1:A:162:LYS:HZ3	1:A:194:ARG:NH2	1.81	0.75
1:A:31:TYR:CD1	1:B:233[A]:LEU:HD11	2.22	0.74
1:E:119:HIS:CE1	3:E:6270:HOH:O	2.40	0.74
1:B:155:LYS:HD3	3:B:3982:HOH:O	1.86	0.74
1:B:192:SER:CB	1:B:193:PRO:CD	2.62	0.74
1:E:26:GLN:NE2	3:E:6286:HOH:O	2.09	0.74
1:B:23:ILE:HD11	1:B:27:LEU:HB3	1.69	0.74
1:E:86:ASP:HB2	3:E:6335:HOH:O	1.86	0.73
1:B:141:ASP:OD1	3:B:3954:HOH:O	2.07	0.73
1:B:84:SER:OG	1:B:85:PRO:HD2	1.89	0.73
1:B:273:ALA:HB3	1:B:274:PRO:HD3	1.69	0.73
1:G:273:ALA:HB3	1:G:274:PRO:HD3	1.71	0.73
1:G:60:THR:HG23	3:G:4915:HOH:O	1.87	0.73
1:D:64:GLN:NE2	3:D:3933:HOH:O	2.22	0.73
1:B:17:HIS:NE2	3:B:3873:HOH:O	2.14	0.72
1:A:259:ARG:HD2	3:A:3728:HOH:O	1.89	0.72
1:E:188:ASP:HB2	3:E:6209:HOH:O	1.87	0.72
1:B:86:ASP:HB3	3:B:3977:HOH:O	1.90	0.72
3:A:3921:HOH:O	1:C:241:THR:HG23	1.90	0.71
1:G:127:GLN:OE1	3:G:5199:HOH:O	2.09	0.71
1:A:31:TYR:HD1	1:B:233[A]:LEU:HD11	1.53	0.71
1:F:234:GLU:CD	3:F:4818:HOH:O	2.29	0.71
1:F:234:GLU:CG	3:F:4818:HOH:O	2.39	0.71
1:F:273:ALA:HB3	1:F:274:PRO:CD	2.18	0.71
1:A:96:GLU:OE1	1:A:187:ARG:NH1	2.24	0.71
1:F:273:ALA:CB	1:F:274:PRO:HD3	2.19	0.70
1:F:141:ASP:OD2	1:F:144:ARG:NE	2.24	0.70
1:B:192:SER:CB	1:B:193:PRO:HD2	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:273:ALA:HB3	1:D:274:PRO:CD	2.20	0.70
1:F:123:GLY:O	1:F:126:SER:HB3	1.92	0.70
1:E:98:PHE:N	3:E:6239:HOH:O	2.02	0.70
1:E:23:ILE:HD13	1:F:23:ILE:HG21	1.74	0.70
1:G:152:GLN:OE1	3:G:5042:HOH:O	2.09	0.70
1:H:282:GLN:HG2	3:H:6351:HOH:O	1.91	0.70
1:E:190:LYS:HD3	3:E:6294:HOH:O	1.92	0.69
1:B:119:HIS:C	1:B:119:HIS:CD2	2.65	0.69
1:A:194:ARG:CB	1:A:196:GLU:HG3	2.22	0.69
1:F:282:GLN:O	1:F:286:ARG:HG3	1.92	0.69
1:F:16:LEU:HD22	3:F:4861:HOH:O	1.91	0.69
1:C:234:GLU:OE2	3:C:5256:HOH:O	2.11	0.68
1:B:149:GLU:OE2	3:B:3960:HOH:O	2.09	0.68
1:A:234:GLU:CG	3:A:3904:HOH:O	2.41	0.68
1:A:194:ARG:CD	1:A:196:GLU:HG3	2.24	0.68
1:G:16:LEU:HA	1:G:229:HIS:CE1	2.29	0.68
1:B:12:SER:HB2	3:B:3895:HOH:O	1.95	0.67
1:A:209:ARG:HD3	3:A:3863:HOH:O	1.95	0.67
1:A:141:ASP:OD1	3:A:3913:HOH:O	2.12	0.67
1:H:141:ASP:OD2	1:H:144:ARG:NH1	2.23	0.67
1:C:55:SER:OG	3:C:5263:HOH:O	2.00	0.67
1:B:245:ARG:HG2	3:D:3974:HOH:O	1.93	0.67
1:E:260[A]:GLN:NE2	3:E:6211:HOH:O	2.16	0.67
1:F:4:LYS:HE2	3:F:4786:HOH:O	1.93	0.67
1:G:16:LEU:HD22	3:G:4952:HOH:O	1.94	0.67
1:E:26:GLN:O	3:E:6299:HOH:O	2.11	0.67
1:G:24:SER:HB2	1:G:59:ASP:OD2	1.95	0.67
1:A:194:ARG:HD3	1:A:196:GLU:HG3	1.77	0.66
1:E:260[B]:GLN:NE2	3:E:6211:HOH:O	2.15	0.66
1:B:23:ILE:HD11	1:B:27:LEU:CB	2.24	0.66
1:E:144:ARG:NH2	1:E:225:ASP:OD2	2.29	0.66
1:H:225:ASP:OD1	1:H:225:ASP:C	2.33	0.66
1:G:18:PRO:HD3	1:H:280:TYR:CD1	2.31	0.66
1:G:16:LEU:HD11	3:G:4989:HOH:O	1.96	0.65
1:D:124:SER:HB2	3:D:3948:HOH:O	1.96	0.65
1:C:23:ILE:HG12	1:D:23:ILE:CG2	2.09	0.65
1:H:23:ILE:HD11	1:H:27:LEU:HD12	1.79	0.65
1:D:60:THR:HG22	1:D:61:PRO:HD3	1.79	0.65
1:C:23:ILE:CG2	1:D:23:ILE:HG12	2.24	0.65
1:C:119:HIS:CD2	1:C:119:HIS:C	2.69	0.65
1:E:244:ASN:HB3	3:E:6338:HOH:O	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:199:ILE:HG22	3:D:3978:HOH:O	1.96	0.65
1:H:23:ILE:HD12	1:H:62:ARG:HH11	1.62	0.64
1:D:10:GLY:O	1:D:26:GLN:NE2	2.28	0.64
1:B:16:LEU:HD22	3:B:3752:HOH:O	1.96	0.64
1:F:12:SER:HB2	3:F:4976:HOH:O	1.97	0.64
1:E:42:THR:HG23	1:E:118:PHE:CE2	2.32	0.64
1:B:273:ALA:HB3	1:B:274:PRO:CD	2.27	0.64
1:B:194:ARG:HD2	3:B:3798:HOH:O	1.98	0.64
1:H:141:ASP:OD2	1:H:144:ARG:HD3	1.98	0.64
1:A:152:GLN:HG3	3:A:3846:HOH:O	1.96	0.64
1:E:10:GLY:HA3	3:E:6180:HOH:O	1.98	0.64
1:H:232:LEU:HD22	3:H:6319:HOH:O	1.98	0.64
1:A:164:LEU:HD22	3:A:4009:HOH:O	1.97	0.63
1:B:16:LEU:O	1:B:19:ALA:HB3	1.98	0.63
1:A:90:GLN:OE1	3:A:3877:HOH:O	2.15	0.63
1:G:88:LEU:HG	3:G:4993:HOH:O	1.98	0.63
1:F:17:HIS:CD2	1:F:21:LEU:HD23	2.33	0.63
1:G:195:GLY:C	1:G:196:GLU:HG2	2.18	0.63
1:G:72:ASN:ND2	3:G:5085:HOH:O	2.31	0.63
1:C:234:GLU:HA	1:C:237[B]:GLN:HE21	1.64	0.62
1:E:178:TYR:OH	1:E:199:ILE:HD11	1.99	0.62
1:C:123:GLY:O	1:C:127:GLN:HG2	1.99	0.62
1:A:26:GLN:HB3	3:A:3866:HOH:O	1.98	0.62
1:A:23:ILE:HD13	1:B:23:ILE:CB	2.22	0.62
1:A:162:LYS:HZ2	1:A:194:ARG:NH2	1.97	0.62
1:E:190:LYS:HA	3:E:6240:HOH:O	1.99	0.62
1:E:30:VAL:HG21	1:E:35[B]:MET:SD	2.40	0.62
1:A:18:PRO:HD3	1:B:280:TYR:CD1	2.35	0.62
1:D:117:ASP:CG	1:D:120:GLU:OE1	2.39	0.61
3:A:3745:HOH:O	1:B:233[B]:LEU:HD23	1.99	0.61
1:E:155:LYS:NZ	3:E:6237:HOH:O	2.33	0.61
1:C:223:TRP:O	1:C:224:LEU:HD23	2.00	0.61
1:B:16:LEU:O	1:B:229:HIS:HE1	1.83	0.61
1:A:16:LEU:HA	1:A:229:HIS:CE1	2.34	0.61
1:G:152:GLN:CD	3:G:5235:HOH:O	2.39	0.60
1:E:23:ILE:HD11	1:F:23:ILE:HG21	1.84	0.60
1:G:149:GLU:OE2	3:G:5106:HOH:O	2.17	0.60
1:A:285:LYS:HE2	3:A:3865:HOH:O	2.01	0.60
1:C:273:ALA:HB3	1:C:274:PRO:CD	2.32	0.60
1:E:15:ARG:HB3	3:E:6280:HOH:O	2.02	0.60
1:B:209:ARG:HD3	3:B:3830:HOH:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:286:ARG:HG3	3:E:6382:HOH:O	2.01	0.60
1:H:25:LYS:HE3	1:H:26:GLN:NE2	2.17	0.59
1:H:160:GLU:CD	3:H:6286:HOH:O	2.40	0.59
1:B:65:GLN:HB2	3:B:4022:HOH:O	2.01	0.59
1:H:87:GLY:N	1:H:196:GLU:OE1	2.35	0.59
1:E:30:VAL:HG21	1:E:35[A]:MET:SD	2.42	0.59
3:A:3745:HOH:O	1:B:233[A]:LEU:HD23	2.02	0.59
1:F:144:ARG:NH1	1:F:145:TYR:OH	2.36	0.59
1:A:23:ILE:CG2	1:A:28:LEU:HD23	2.30	0.59
1:E:12:SER:OG	1:E:13:GLY:N	2.35	0.59
1:D:60:THR:HG22	1:D:61:PRO:CD	2.32	0.58
1:D:192:SER:HB2	1:D:193:PRO:HD2	1.85	0.58
1:D:50:GLU:HB2	3:D:4038:HOH:O	2.02	0.58
1:E:191:PRO:HD2	3:E:6240:HOH:O	2.04	0.58
1:E:183:VAL:O	1:E:187:ARG:HG3	2.03	0.58
1:B:155:LYS:HE3	3:B:3950:HOH:O	2.03	0.58
1:A:109:GLY:O	3:A:3866:HOH:O	2.17	0.58
1:C:234:GLU:HA	1:C:237[A]:GLN:HE21	1.67	0.58
1:G:18:PRO:HD2	1:H:32:ASP:O	2.02	0.58
1:A:273:ALA:HB3	1:A:274:PRO:HD3	1.85	0.58
1:B:88:LEU:HD12	1:B:199:ILE:HG21	1.85	0.58
1:F:152:GLN:CB	3:F:4947:HOH:O	2.48	0.58
1:F:58:GLN:HG3	3:F:4922:HOH:O	2.04	0.58
1:C:237[A]:GLN:HG3	1:D:233:LEU:HD11	1.85	0.57
1:C:237[B]:GLN:HG3	1:D:233:LEU:HD11	1.86	0.57
1:G:23:ILE:HG12	1:G:28:LEU:HD23	1.87	0.57
1:F:21:LEU:O	3:F:5001:HOH:O	2.18	0.57
1:H:232:LEU:HB2	3:H:6319:HOH:O	2.04	0.57
1:F:234:GLU:HG3	3:F:4818:HOH:O	2.03	0.57
1:C:1:MET:N	1:C:129:GLN:NE2	2.52	0.57
1:G:60:THR:HG22	1:G:64:GLN:HE21	1.70	0.57
1:F:16:LEU:O	1:F:19:ALA:HB3	2.04	0.57
1:D:60:THR:HG22	1:D:61:PRO:N	2.20	0.57
1:B:194:ARG:HH11	1:B:194:ARG:HB2	1.69	0.57
1:D:282:GLN:HG3	3:D:3970:HOH:O	2.03	0.57
1:B:60:THR:HB	1:B:61:PRO:HD3	1.87	0.56
1:F:141:ASP:OD2	1:F:144:ARG:CZ	2.54	0.56
1:E:42:THR:HG23	1:E:118:PHE:HE2	1.67	0.56
1:C:23:ILE:HD13	1:D:23:ILE:HG12	1.87	0.56
1:F:13:GLY:O	1:F:16:LEU:N	2.38	0.56
1:E:88:LEU:HD12	1:E:199:ILE:CG2	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:128:ARG:NE	3:C:5286:HOH:O	2.38	0.56
1:D:96:GLU:HG3	1:D:183:VAL:HG11	1.88	0.56
1:G:183:VAL:O	1:G:187:ARG:HG3	2.06	0.56
1:F:128:ARG:NE	3:F:5021:HOH:O	2.30	0.56
1:G:195:GLY:O	1:G:196:GLU:HG2	2.06	0.55
1:E:65:GLN:HB2	3:E:6217:HOH:O	2.05	0.55
1:A:32:ASP:O	1:B:18:PRO:HD2	2.05	0.55
1:G:13:GLY:O	1:G:16:LEU:N	2.37	0.55
1:B:197:LEU:HD11	3:B:3801:HOH:O	2.07	0.55
1:C:119:HIS:CB	3:C:5275:HOH:O	2.40	0.55
1:A:192:SER:HB2	1:A:193:PRO:HD2	1.88	0.55
1:H:285:LYS:NZ	3:H:6347:HOH:O	2.39	0.55
1:C:264:ASP:N	1:C:267:GLN:OE1	2.37	0.55
1:E:118:PHE:CZ	1:E:122:LEU:HD21	2.41	0.55
1:A:287:LEU:HD22	3:A:3750:HOH:O	2.08	0.54
1:E:273:ALA:CB	1:E:274:PRO:HD3	2.34	0.54
1:E:25:LYS:NZ	3:E:6374:HOH:O	2.39	0.54
1:G:256:ILE:O	1:G:260:GLN:HG2	2.08	0.54
1:E:84:SER:OG	1:E:85:PRO:HD2	2.07	0.54
1:A:194:ARG:HD3	1:A:196:GLU:CG	2.37	0.54
3:A:3987:HOH:O	1:B:29:PRO:HG3	2.07	0.54
1:D:90:GLN:HG2	1:D:197:LEU:HD12	1.90	0.53
1:E:274:PRO:HD2	3:E:6255:HOH:O	2.07	0.53
1:E:30:VAL:CG2	1:E:35[B]:MET:SD	2.96	0.53
1:H:12:SER:OG	2:H:6101:SO4:O2	2.27	0.53
1:A:23:ILE:HG21	1:A:28:LEU:CD2	2.36	0.53
1:A:194:ARG:HD3	1:A:196:GLU:CD	2.29	0.53
1:G:144:ARG:NH2	3:G:5144:HOH:O	2.41	0.53
1:G:278:ASN:HB3	3:G:5127:HOH:O	2.07	0.53
1:D:42:THR:HG23	1:D:118:PHE:CE2	2.44	0.52
1:F:1:MET:CE	1:F:180:GLN:HE22	2.21	0.52
1:E:8:LEU:HD22	1:E:91:ALA:HB2	1.92	0.52
1:D:23:ILE:HD12	1:D:23:ILE:H	1.73	0.52
1:E:269:GLU:HG3	3:E:6254:HOH:O	2.07	0.52
1:G:24:SER:HB2	1:G:59:ASP:CG	2.30	0.52
1:C:1:MET:CE	1:C:180:GLN:HE22	2.22	0.52
1:D:103:LEU:HD11	1:D:129:GLN:HG2	1.91	0.52
1:D:90:GLN:NE2	3:D:3989:HOH:O	2.41	0.52
1:A:286:ARG:HG3	3:A:3812:HOH:O	2.08	0.52
1:B:119:HIS:CE1	3:B:3794:HOH:O	2.63	0.52
1:E:118:PHE:O	1:E:119:HIS:C	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:162:LYS:HE3	3:F:4895:HOH:O	2.10	0.52
1:D:23:ILE:HD13	1:D:28:LEU:CD2	2.37	0.52
1:C:128:ARG:CD	3:C:5286:HOH:O	2.58	0.52
1:C:60:THR:HG22	1:C:64:GLN:HE21	1.75	0.52
1:H:15:ARG:HG3	1:H:15:ARG:HH11	1.75	0.51
1:E:30:VAL:CG2	1:E:35[A]:MET:SD	2.98	0.51
1:A:174:GLY:O	3:A:3902:HOH:O	2.19	0.51
1:B:119:HIS:C	1:B:119:HIS:HD2	2.10	0.51
1:H:23:ILE:HG13	1:H:24:SER:N	2.25	0.51
1:G:23:ILE:HG12	1:G:28:LEU:CD2	2.40	0.51
1:A:58:GLN:NE2	3:A:3963:HOH:O	2.29	0.51
1:D:273:ALA:HB3	1:D:274:PRO:HD2	1.91	0.51
1:C:60:THR:N	1:C:61:PRO:CD	2.73	0.51
1:H:108:LEU:HD22	3:H:6398:HOH:O	2.09	0.51
1:F:11:GLY:HA2	1:F:85:PRO:HB3	1.93	0.51
1:G:249:LYS:NZ	3:G:5022:HOH:O	2.42	0.51
1:C:119:HIS:CD2	1:C:119:HIS:O	2.63	0.51
1:B:16:LEU:CD1	1:B:25:LYS:HD3	2.41	0.51
1:F:261:LYS:HE2	3:F:4971:HOH:O	2.10	0.51
1:F:141:ASP:CG	1:F:144:ARG:HH21	2.13	0.51
1:F:4:LYS:NZ	1:F:102:ASP:OD2	2.44	0.51
1:B:88:LEU:HG	3:B:3959:HOH:O	2.11	0.50
1:H:16:LEU:HA	1:H:229:HIS:CE1	2.46	0.50
1:E:227:GLY:CA	3:E:6150:HOH:O	2.52	0.50
1:C:60:THR:HB	1:C:61:PRO:HD3	1.93	0.50
1:A:152:GLN:HG2	3:A:3725:HOH:O	2.11	0.50
1:C:119:HIS:NE2	3:C:5244:HOH:O	2.35	0.50
1:G:152:GLN:NE2	3:G:5054:HOH:O	2.44	0.50
1:E:16:LEU:HD13	1:E:229:HIS:CD2	2.46	0.50
1:B:119:HIS:ND1	3:B:3937:HOH:O	2.34	0.50
3:B:3997:HOH:O	1:E:155:LYS:HE2	2.12	0.50
1:G:15:ARG:NH2	3:G:5168:HOH:O	2.44	0.50
1:C:194:ARG:HD2	1:C:196:GLU:HG3	1.94	0.50
1:C:270:LYS:HE2	3:C:5169:HOH:O	2.10	0.50
1:A:234:GLU:HG3	3:A:3904:HOH:O	2.07	0.49
1:C:119:HIS:CD2	3:C:5250:HOH:O	2.65	0.49
1:D:42:THR:HG23	1:D:118:PHE:CZ	2.47	0.49
1:C:26:GLN:NE2	1:C:26:GLN:H	2.10	0.49
2:C:5000:SO4:O4	1:D:62:ARG:NH2	2.26	0.49
1:A:234:GLU:CD	3:A:3904:HOH:O	2.51	0.49
1:C:1:MET:SD	1:C:180:GLN:NE2	2.86	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:32:ASP:OD2	1:C:243:GLU:OE1	2.30	0.49
1:D:269:GLU:HG3	3:D:3871:HOH:O	2.12	0.49
1:G:88:LEU:HD13	1:G:108:LEU:HD21	1.95	0.49
1:D:22:ALA:HA	3:D:3920:HOH:O	2.11	0.49
1:G:60:THR:HB	1:G:61:PRO:HD3	1.95	0.49
1:D:56:THR:HB	1:D:58:GLN:NE2	2.28	0.49
1:D:86:ASP:HB2	1:D:90:GLN:NE2	2.28	0.48
1:G:8:LEU:HD22	1:G:91:ALA:HB2	1.94	0.48
1:H:260:GLN:O	1:H:261:LYS:HB2	2.13	0.48
1:B:60:THR:HG23	3:B:3717:HOH:O	2.13	0.48
1:A:15:ARG:HH11	1:A:15:ARG:HG3	1.78	0.48
1:B:286:ARG:HG3	3:B:3875:HOH:O	2.13	0.48
1:C:60:THR:N	1:C:61:PRO:HD2	2.29	0.48
1:B:117:ASP:HA	1:B:120:GLU:OE1	2.13	0.48
1:H:60:THR:CB	1:H:61:PRO:HD3	2.39	0.48
1:B:256:ILE:O	1:B:260:GLN:HG2	2.14	0.48
1:B:49:ARG:HD2	1:B:262:TRP:CE2	2.49	0.48
1:B:128:ARG:NH2	2:B:3701:SO4:O4	2.47	0.48
1:B:97:SER:OG	3:B:3956:HOH:O	2.19	0.48
1:H:2:LYS:NZ	1:H:50:GLU:OE1	2.42	0.48
1:G:167:LYS:NZ	3:G:5153:HOH:O	2.46	0.48
1:C:141:ASP:OD2	1:C:144:ARG:HD3	2.14	0.48
1:C:193:PRO:C	1:C:195:GLY:H	2.17	0.47
1:D:56:THR:HB	1:D:58:GLN:HE21	1.79	0.47
1:H:123:GLY:O	1:H:127:GLN:HB2	2.14	0.47
1:A:233:LEU:HD21	1:B:237[B]:GLN:HA	1.96	0.47
1:F:273:ALA:CB	1:F:274:PRO:CD	2.83	0.47
1:C:234:GLU:CD	3:C:5256:HOH:O	2.52	0.47
1:E:155:LYS:CE	3:E:6237:HOH:O	2.61	0.47
1:G:255:GLU:O	1:G:259:ARG:HG3	2.14	0.47
1:C:18:PRO:HA	1:C:21:LEU:HG	1.96	0.47
1:A:88:LEU:HG	3:A:3758:HOH:O	2.14	0.47
1:G:161:GLU:O	1:G:194[A]:ARG:NH2	2.47	0.47
1:E:32:ASP:OD2	1:E:249:LYS:HE3	2.14	0.47
1:B:152:GLN:NE2	1:B:152:GLN:HA	2.29	0.47
1:F:141:ASP:OD1	3:F:4873:HOH:O	2.20	0.47
1:D:60:THR:O	1:D:64:GLN:HG3	2.14	0.47
1:A:23:ILE:CB	1:B:23:ILE:CD1	2.74	0.47
1:A:60:THR:HB	1:A:61:PRO:HD3	1.96	0.47
3:A:3911:HOH:O	1:B:14:THR:HA	2.15	0.47
1:B:88:LEU:HD12	1:B:199:ILE:CG2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:192:SER:HB2	1:H:193:PRO:HD2	1.97	0.47
1:H:84:SER:OG	1:H:85:PRO:HD2	2.15	0.47
1:E:193:PRO:O	1:E:194:ARG:C	2.53	0.47
1:C:1:MET:H2	1:C:129:GLN:NE2	2.13	0.47
1:C:187:ARG:NH1	1:C:187:ARG:HG2	2.30	0.47
1:A:23:ILE:HG23	1:A:28:LEU:HD23	1.85	0.47
1:A:23:ILE:CD1	1:B:23:ILE:HB	2.30	0.47
1:A:231:SER:HA	3:A:3904:HOH:O	2.15	0.47
1:D:60:THR:N	1:D:61:PRO:HD2	2.30	0.47
1:A:23:ILE:CG2	1:B:23:ILE:CD1	2.93	0.46
1:B:23:ILE:CD1	1:B:27:LEU:HB2	2.46	0.46
1:E:15:ARG:HG2	1:E:16:LEU:HD23	1.96	0.46
1:A:233:LEU:HD21	1:B:237[A]:GLN:HA	1.96	0.46
1:H:19:ALA:O	3:H:6271:HOH:O	2.20	0.46
1:B:269:GLU:CD	3:B:3940:HOH:O	2.54	0.46
1:C:25:LYS:HE3	1:C:110:ASP:HB3	1.97	0.46
1:E:268:LEU:HD23	1:E:288:LEU:CD2	2.44	0.46
1:E:191:PRO:CD	3:E:6240:HOH:O	2.60	0.46
1:E:160:GLU:HG2	3:E:6247:HOH:O	2.15	0.46
1:B:25:LYS:NZ	1:B:110:ASP:OD2	2.43	0.46
1:G:270:LYS:HE3	3:G:5175:HOH:O	2.15	0.46
1:G:192:SER:HB2	1:G:193:PRO:HD2	1.98	0.46
1:H:36:ILE:HD12	1:H:63:PHE:CE2	2.51	0.46
1:D:4:LYS:HB3	1:D:98:PHE:CE2	2.51	0.46
1:C:42:THR:HG23	1:C:118:PHE:CE2	2.51	0.46
1:E:23:ILE:HG12	1:F:23:ILE:HG23	1.97	0.46
1:C:237[A]:GLN:CG	1:D:233:LEU:HD11	2.46	0.46
1:C:237[A]:GLN:HA	1:D:233:LEU:HD21	1.97	0.46
1:H:151:ASP:OD2	1:H:155:LYS:HB3	2.16	0.46
1:E:23:ILE:CG2	1:F:23:ILE:HG12	2.16	0.46
1:E:191:PRO:O	1:E:192:SER:O	2.33	0.46
1:C:237[B]:GLN:HA	1:D:233:LEU:HD21	1.97	0.46
1:A:19:ALA:HB1	1:B:29:PRO:HB3	1.96	0.46
1:D:16:LEU:HD22	1:D:229:HIS:CE1	2.51	0.46
1:D:14:THR:O	1:D:15:ARG:C	2.54	0.46
1:G:237:GLN:HA	1:H:233:LEU:HD21	1.97	0.46
1:C:1:MET:H3	1:C:129:GLN:NE2	2.14	0.45
1:E:268:LEU:HD23	1:E:288:LEU:HD21	1.98	0.45
1:E:90:GLN:O	1:E:93:LEU:N	2.42	0.45
1:B:23:ILE:O	1:B:23:ILE:HG23	2.16	0.45
1:H:93:LEU:CD2	1:H:187:ARG:HG2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:190:LYS:HD2	1:E:191:PRO:CD	2.46	0.45
1:G:275:LEU:O	1:G:281:GLY:HA3	2.16	0.45
1:E:209:ARG:CZ	3:E:6168:HOH:O	2.65	0.45
1:E:190:LYS:C	1:E:190:LYS:CD	2.75	0.45
1:A:164:LEU:HB3	3:A:4009:HOH:O	2.16	0.45
1:H:56:THR:HB	1:H:57:PRO:HD2	1.97	0.45
1:B:13:GLY:O	1:B:14:THR:C	2.55	0.45
1:C:273:ALA:HB3	1:C:274:PRO:HD3	1.98	0.45
1:A:13:GLY:HA2	3:A:3851:HOH:O	2.15	0.45
1:E:64:GLN:HA	1:E:79:TYR:CZ	2.52	0.45
1:F:86:ASP:HB2	1:F:90:GLN:NE2	2.32	0.45
1:A:193:PRO:C	1:A:195:GLY:N	2.68	0.45
1:C:194:ARG:CD	1:C:196:GLU:HG3	2.47	0.45
1:D:225:ASP:HB3	3:D:3975:HOH:O	2.16	0.45
1:B:16:LEU:CD2	3:B:3980:HOH:O	2.65	0.45
1:A:23:ILE:HG21	1:A:28:LEU:HD23	1.98	0.45
1:H:18:PRO:O	1:H:21:LEU:HB2	2.17	0.45
1:F:78:GLN:NE2	3:F:4781:HOH:O	2.39	0.45
1:D:273:ALA:HB3	1:D:274:PRO:HD3	1.98	0.45
1:H:16:LEU:HB3	1:H:20:THR:HG23	1.99	0.45
1:G:35[B]:MET:HE3	1:G:38:TYR:HB2	1.99	0.45
1:F:51:ILE:HB	1:F:77:LEU:HD23	1.99	0.45
1:E:278:ASN:HB3	3:E:6363:HOH:O	2.16	0.45
1:B:24:SER:HB3	1:B:27:LEU:HD12	1.97	0.44
1:A:111:ASN:HB2	3:A:3902:HOH:O	2.16	0.44
1:C:88:LEU:HD13	1:C:108:LEU:HD21	1.99	0.44
1:C:23:ILE:CD1	1:D:23:ILE:HG21	2.47	0.44
1:D:123:GLY:HA3	3:D:3912:HOH:O	2.16	0.44
1:F:192:SER:HB2	1:F:193:PRO:CD	2.47	0.44
1:F:192:SER:HB2	1:F:193:PRO:HD2	1.99	0.44
1:H:23:ILE:HG23	1:H:23:ILE:O	2.17	0.44
1:H:135:PHE:HA	1:H:215:GLU:O	2.18	0.44
1:G:141[B]:ASP:OD1	3:G:5077:HOH:O	2.21	0.44
1:F:21:LEU:HA	1:F:21:LEU:HD23	1.85	0.44
1:A:234:GLU:HB2	3:A:3904:HOH:O	2.18	0.44
1:H:24:SER:HB2	1:H:59:ASP:OD2	2.17	0.44
1:A:59:ASP:HA	1:A:62:ARG:HD2	1.99	0.44
1:D:87:GLY:HA2	3:D:3990:HOH:O	2.17	0.44
1:G:289:THR:OG1	3:G:5111:HOH:O	2.21	0.44
1:H:119:HIS:CD2	3:H:6299:HOH:O	2.69	0.44
1:E:88:LEU:HD12	1:E:199:ILE:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:60:THR:HB	1:H:61:PRO:CD	2.38	0.44
1:E:191:PRO:HA	1:E:196:GLU:O	2.18	0.44
1:G:278:ASN:CG	3:G:5127:HOH:O	2.56	0.44
1:D:118:PHE:HB2	3:D:3916:HOH:O	2.18	0.43
1:F:256:ILE:O	1:F:260:GLN:HG2	2.18	0.43
1:D:119:HIS:HE1	3:D:4030:HOH:O	2.01	0.43
1:G:20:THR:O	1:G:21:LEU:C	2.57	0.43
1:A:39:PRO:HA	3:A:3791:HOH:O	2.17	0.43
1:G:86:ASP:HB2	1:G:90:GLN:NE2	2.33	0.43
1:H:25:LYS:CE	1:H:26:GLN:HE22	2.25	0.43
1:A:272:ALA:HB1	1:A:285:LYS:HG3	2.00	0.43
1:E:23:ILE:CD1	1:F:23:ILE:CG2	2.89	0.43
1:G:62:ARG:NE	2:G:4900:SO4:O3	2.51	0.43
1:H:265:ALA:HB3	3:H:6161:HOH:O	2.17	0.43
1:C:269:GLU:HG2	3:C:5162:HOH:O	2.18	0.43
1:G:135:PHE:HA	1:G:215:GLU:O	2.18	0.43
1:G:84:SER:HA	3:G:5000:HOH:O	2.18	0.43
1:F:42:THR:HG23	1:F:118:PHE:CE2	2.54	0.43
1:D:273:ALA:CB	1:D:274:PRO:CD	2.88	0.43
1:B:13:GLY:O	1:B:16:LEU:N	2.49	0.43
1:G:32:ASP:O	1:H:18:PRO:HD2	2.18	0.43
1:E:117:ASP:CG	1:E:120:GLU:OE1	2.57	0.43
1:F:17:HIS:HB3	1:F:18:PRO:HA	2.00	0.43
1:G:64:GLN:HG2	1:G:79:TYR:CD1	2.54	0.43
1:G:22:ALA:HB1	1:H:27:LEU:HD22	2.00	0.43
1:B:23:ILE:HD11	1:B:27:LEU:HB2	2.00	0.43
1:B:273:ALA:CB	1:B:274:PRO:CD	2.92	0.43
1:H:27:LEU:HD23	1:H:27:LEU:HA	1.71	0.43
1:A:16:LEU:HB3	1:A:20:THR:HG23	2.01	0.43
1:E:16:LEU:O	1:E:19:ALA:HB3	2.19	0.43
1:C:128:ARG:NH1	1:C:213[B]:SER:OG	2.51	0.43
1:B:16:LEU:C	1:B:229:HIS:CE1	2.92	0.43
1:C:259:ARG:NH2	3:C:5019:HOH:O	2.51	0.43
1:A:84:SER:O	1:A:86:ASP:N	2.52	0.43
1:A:117:ASP:HA	1:A:120:GLU:OE1	2.19	0.42
1:F:40:LEU:O	1:F:44:MET:HG3	2.19	0.42
1:A:29:PRO:HD2	3:A:3898:HOH:O	2.19	0.42
1:A:24:SER:HB2	1:A:59:ASP:OD2	2.19	0.42
1:A:119:HIS:CE1	3:A:3875:HOH:O	2.72	0.42
1:A:141:ASP:OD2	1:A:144:ARG:NH1	2.38	0.42
1:A:16:LEU:HD22	3:A:3909:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:16:LEU:HD23	1:H:229:HIS:ND1	2.34	0.42
1:D:56:THR:HB	1:D:57:PRO:HD2	2.01	0.42
1:E:35[B]:MET:O	1:E:39:PRO:HD2	2.19	0.42
1:H:15:ARG:HG3	2:H:6101:SO4:O1	2.19	0.42
1:B:88:LEU:HB2	1:B:199:ILE:HB	2.01	0.42
1:E:107:VAL:HG22	1:E:108:LEU:N	2.35	0.42
1:A:59:ASP:O	1:A:60:THR:C	2.58	0.42
1:A:23:ILE:CG2	1:B:23:ILE:HD12	2.43	0.42
1:F:2:LYS:HD3	1:F:4:LYS:HE3	2.01	0.42
1:C:128:ARG:NH1	1:C:213[A]:SER:OG	2.51	0.42
1:B:67:LEU:HB2	1:B:79:TYR:OH	2.19	0.42
1:H:273:ALA:HB3	1:H:274:PRO:CD	2.45	0.42
1:B:16:LEU:CA	1:B:229:HIS:CE1	2.98	0.42
1:E:259[A]:ARG:NH2	3:E:6119:HOH:O	2.52	0.42
1:E:259[B]:ARG:NH2	3:E:6119:HOH:O	2.52	0.42
1:D:204:ARG:HH11	1:D:204:ARG:HD2	1.59	0.42
1:B:23:ILE:HG12	1:B:27:LEU:HB2	2.01	0.42
1:C:9:ALA:O	1:C:55:SER:OG	2.38	0.42
1:A:18:PRO:HD2	1:B:32:ASP:O	2.19	0.42
1:E:278:ASN:OD1	1:E:280:TYR:N	2.51	0.42
1:G:192:SER:OG	1:G:194[A]:ARG:HB2	2.19	0.42
1:H:22:ALA:HB3	3:H:6188:HOH:O	2.18	0.42
1:F:72:ASN:OD1	3:F:4813:HOH:O	2.22	0.42
1:D:209:ARG:HH11	1:D:209:ARG:HG2	1.85	0.42
1:C:46:ALA:HB2	1:C:122:LEU:HD13	2.01	0.42
1:A:23:ILE:HG13	1:A:24:SER:N	2.35	0.42
1:A:256:ILE:O	1:A:260:GLN:CG	2.68	0.42
1:B:249:LYS:NZ	3:B:3958:HOH:O	2.47	0.42
1:C:234:GLU:HA	1:C:237[B]:GLN:NE2	2.32	0.41
1:E:6:ILE:HA	1:E:52:LEU:O	2.20	0.41
1:C:272:ALA:HB1	1:C:285:LYS:HG2	2.02	0.41
1:H:67:LEU:HB2	1:H:79:TYR:OH	2.20	0.41
1:H:54:ILE:HA	1:H:80:ALA:O	2.20	0.41
1:E:288:LEU:HA	1:E:288:LEU:HD23	1.85	0.41
1:A:70:GLY:HA3	1:A:77:LEU:HG	2.02	0.41
1:D:84:SER:OG	1:D:85:PRO:HD2	2.21	0.41
1:B:16:LEU:HD11	1:B:25:LYS:HD3	2.03	0.41
1:E:118:PHE:CE2	1:E:122:LEU:HD11	2.56	0.41
1:D:141:ASP:OD2	1:D:144:ARG:HD3	2.21	0.41
1:E:190:LYS:CD	3:E:6294:HOH:O	2.60	0.41
1:D:199:ILE:CG2	3:D:3978:HOH:O	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:HIS:O	1:B:117:ASP:HB2	2.20	0.41
1:F:32:ASP:OD1	1:F:32:ASP:N	2.54	0.41
1:E:24:SER:HB2	1:E:59:ASP:OD2	2.20	0.41
1:C:1:MET:N	1:C:129:GLN:HE22	2.19	0.41
1:A:234:GLU:CD	3:A:3921:HOH:O	2.58	0.40
1:E:35[A]:MET:O	1:E:39:PRO:HD2	2.20	0.40
1:B:180:GLN:NE2	3:B:3887:HOH:O	2.53	0.40
1:C:38:TYR:HB2	1:C:39:PRO:CD	2.52	0.40
1:C:62:ARG:NE	2:C:5000:SO4:O1	2.54	0.40
1:F:129:GLN:NE2	3:F:5005:HOH:O	2.55	0.40
1:B:113:TYR:CB	1:B:118:PHE:CZ	3.04	0.40
1:B:24:SER:HB2	1:B:59:ASP:CG	2.42	0.40
1:D:123:GLY:O	1:D:124:SER:C	2.59	0.40
1:A:15:ARG:NH1	1:A:15:ARG:HG3	2.35	0.40
1:F:84:SER:HB3	1:F:86:ASP:OD2	2.21	0.40
1:H:47:GLY:HA3	3:H:6318:HOH:O	2.21	0.40
1:A:27:LEU:HA	1:A:27:LEU:HD23	1.86	0.40
1:F:17:HIS:CB	1:F:18:PRO:HA	2.52	0.40
1:H:187:ARG:HH11	1:H:187:ARG:HD2	1.64	0.40
1:F:39:PRO:HA	3:F:4943:HOH:O	2.22	0.40
1:D:287:LEU:HD22	3:D:4025:HOH:O	2.20	0.40
1:A:260:GLN:O	1:A:261:LYS:HB2	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:G:84:SER:OG	3:F:4852:HOH:O[1_655]	1.25	0.95
3:A:3776:HOH:O	3:F:4954:HOH:O[1_566]	1.99	0.21
3:F:4955:HOH:O	3:G:5148:HOH:O[1_455]	2.06	0.14
3:G:5209:HOH:O	3:H:6340:HOH:O[1_565]	2.09	0.11
3:F:4950:HOH:O	3:G:4974:HOH:O[1_455]	2.18	0.02

## 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	292/293 (100%)	284 (97%)	7 (2%)	1 (0%)	46	35
1	B	295/293 (101%)	285 (97%)	9 (3%)	1 (0%)	46	35
1	C	297/293 (101%)	290 (98%)	5 (2%)	2 (1%)	26	14
1	D	291/293 (99%)	282 (97%)	7 (2%)	2 (1%)	26	14
1	E	297/293 (101%)	286 (96%)	7 (2%)	4 (1%)	15	4
1	F	294/293 (100%)	285 (97%)	6 (2%)	3 (1%)	19	7
1	G	294/293 (100%)	287 (98%)	6 (2%)	1 (0%)	46	35
1	H	290/293 (99%)	284 (98%)	5 (2%)	1 (0%)	46	35
All	All	2350/2344 (100%)	2283 (97%)	52 (2%)	15 (1%)	30	17

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	14	THR
1	D	14	THR
1	E	31	TYR
1	F	15	ARG
1	F	31	TYR
1	H	31	TYR
1	A	31	TYR
1	B	31	TYR
1	D	31	TYR
1	E	192	SER
1	F	14	THR
1	G	31	TYR
1	C	31	TYR
1	C	194	ARG
1	E	191	PRO

### 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	241/240 (100%)	234 (97%)	7 (3%)	50	40
1	B	244/240 (102%)	236 (97%)	8 (3%)	45	34
1	C	246/240 (102%)	240 (98%)	6 (2%)	57	49
1	D	240/240 (100%)	234 (98%)	6 (2%)	55	47
1	E	246/240 (102%)	236 (96%)	10 (4%)	37	25
1	F	243/240 (101%)	234 (96%)	9 (4%)	41	29
1	G	243/240 (101%)	229 (94%)	14 (6%)	25	13
1	H	239/240 (100%)	234 (98%)	5 (2%)	61	55
All	All	1942/1920 (101%)	1877 (97%)	65 (3%)	45	34

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	17	HIS
1	A	18	PRO
1	A	23	ILE
1	A	88	LEU
1	A	111	ASN
1	A	126	SER
1	B	111	ASN
1	B	112	LEU
1	B	119	HIS
1	B	152	GLN
1	B	194	ARG
1	B	196	GLU
1	B	225	ASP
1	B	287	LEU
1	C	12	SER
1	C	26	GLN
1	C	55	SER
1	C	111	ASN
1	C	225	ASP
1	C	288	LEU
1	D	23	ILE
1	D	24	SER
1	D	60	THR
1	D	111	ASN
1	D	117	ASP
1	D	286	ARG

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Mol	Chain	Res	Type
1	E	8	LEU
1	E	12	SER
1	E	16	LEU
1	E	23	ILE
1	E	117	ASP
1	E	127	GLN
1	E	155	LYS
1	E	194	ARG
1	E	233	LEU
1	E	270	LYS
1	F	1	MET
1	F	12	SER
1	F	14	THR
1	F	24	SER
1	F	29	PRO
1	F	111	ASN
1	F	155	LYS
1	F	197	LEU
1	F	286	ARG
1	G	12	SER
1	G	17	HIS
1	G	18	PRO
1	G	23	ILE
1	G	84	SER
1	G	97	SER
1	G	111	ASN
1	G	112	LEU
1	G	194[A]	ARG
1	G	194[B]	ARG
1	G	196	GLU
1	G	225	ASP
1	G	270	LYS
1	G	278	ASN
1	H	14	THR
1	H	111	ASN
1	H	152	GLN
1	H	187	ARG
1	H	225	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	229	HIS
1	B	82	GLN
1	B	90	GLN
1	B	119	HIS
1	B	152	GLN
1	B	229	HIS
1	C	17	HIS
1	C	26	GLN
1	C	64	GLN
1	C	119	HIS
1	C	129	GLN
1	C	180	GLN
1	C	260	GLN
1	D	58	GLN
1	D	65	GLN
1	D	82	GLN
1	D	90	GLN
1	D	229	HIS
1	E	17	HIS
1	E	229	HIS
1	F	65	GLN
1	F	180	GLN
1	G	64	GLN
1	G	82	GLN
1	G	90	GLN
1	H	26	GLN
1	H	111	ASN
1	H	152	GLN
1	H	229	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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

20 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	A	3602	-	4,4,4	1.56	2 (50%)	6,6,6	0.40	0
2	SO4	A	3700	-	4,4,4	0.51	0	6,6,6	0.57	0
2	SO4	B	3603	-	4,4,4	1.95	2 (50%)	6,6,6	0.91	1 (16%)
2	SO4	B	3701	-	4,4,4	1.16	0	6,6,6	1.21	1 (16%)
2	SO4	C	3600	-	4,4,4	2.28	2 (50%)	6,6,6	0.96	0
2	SO4	C	3702	-	4,4,4	0.16	0	6,6,6	0.51	0
2	SO4	C	5000	-	4,4,4	1.17	1 (25%)	6,6,6	0.91	1 (16%)
2	SO4	D	3601	-	4,4,4	2.32	3 (75%)	6,6,6	1.20	1 (16%)
2	SO4	D	3703	-	4,4,4	0.84	0	6,6,6	0.49	0
2	SO4	D	3800	-	4,4,4	0.39	0	6,6,6	1.80	1 (16%)
2	SO4	E	3607	-	4,4,4	1.71	2 (50%)	6,6,6	0.85	0
2	SO4	E	5001	-	4,4,4	1.02	0	6,6,6	0.98	1 (16%)
2	SO4	E	6100	-	4,4,4	0.98	0	6,6,6	0.50	0
2	SO4	F	3606	-	4,4,4	1.75	1 (25%)	6,6,6	0.66	0
2	SO4	F	4700	-	4,4,4	0.92	0	6,6,6	0.99	1 (16%)
2	SO4	G	3605	-	4,4,4	1.73	1 (25%)	6,6,6	0.66	0
2	SO4	G	3704	-	4,4,4	0.99	0	6,6,6	1.29	1 (16%)
2	SO4	G	4900	-	4,4,4	0.81	0	6,6,6	0.96	1 (16%)
2	SO4	H	3604	-	4,4,4	2.00	3 (75%)	6,6,6	0.51	0
2	SO4	H	6101	-	4,4,4	0.52	0	6,6,6	0.75	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	3602	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	3700	-	-	0/0/0/0	0/0/0/0
2	SO4	B	3603	-	-	0/0/0/0	0/0/0/0
2	SO4	B	3701	-	-	0/0/0/0	0/0/0/0
2	SO4	C	3600	-	-	0/0/0/0	0/0/0/0
2	SO4	C	3702	-	-	0/0/0/0	0/0/0/0
2	SO4	C	5000	-	-	0/0/0/0	0/0/0/0
2	SO4	D	3601	-	-	0/0/0/0	0/0/0/0
2	SO4	D	3703	-	-	0/0/0/0	0/0/0/0
2	SO4	D	3800	-	-	0/0/0/0	0/0/0/0
2	SO4	E	3607	-	-	0/0/0/0	0/0/0/0
2	SO4	E	5001	-	-	0/0/0/0	0/0/0/0
2	SO4	E	6100	-	-	0/0/0/0	0/0/0/0
2	SO4	F	3606	-	-	0/0/0/0	0/0/0/0
2	SO4	F	4700	-	-	0/0/0/0	0/0/0/0
2	SO4	G	3605	-	-	0/0/0/0	0/0/0/0
2	SO4	G	3704	-	-	0/0/0/0	0/0/0/0
2	SO4	G	4900	-	-	0/0/0/0	0/0/0/0
2	SO4	H	3604	-	-	0/0/0/0	0/0/0/0
2	SO4	H	6101	-	-	0/0/0/0	0/0/0/0

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3600	SO4	O1-S	-3.30	1.35	1.47
2	D	3601	SO4	O1-S	-3.26	1.36	1.47
2	F	3606	SO4	O1-S	-2.95	1.37	1.47
2	G	3605	SO4	O2-S	-2.74	1.37	1.47
2	D	3601	SO4	O2-S	-2.48	1.38	1.47
2	B	3603	SO4	O4-S	-2.42	1.38	1.47
2	E	3607	SO4	O1-S	-2.42	1.38	1.47
2	B	3603	SO4	O2-S	-2.21	1.39	1.47
2	A	3602	SO4	O3-S	-2.18	1.39	1.47
2	E	3607	SO4	O4-S	-2.18	1.39	1.47
2	H	3604	SO4	O1-S	-2.18	1.39	1.47
2	H	3604	SO4	O2-S	-2.10	1.40	1.47
2	H	3604	SO4	O3-S	-2.10	1.39	1.47
2	A	3602	SO4	O1-S	-2.06	1.40	1.47
2	D	3601	SO4	O4-S	-2.04	1.40	1.47
2	C	3600	SO4	O3-S	-2.00	1.40	1.47
2	C	5000	SO4	O2-S	2.27	1.54	1.47

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	D	3800	SO4	O2-S-O1	-4.23	96.10	109.50
2	D	3601	SO4	O2-S-O1	-2.85	100.46	109.50
2	B	3701	SO4	O2-S-O1	-2.49	101.62	109.50
2	E	5001	SO4	O2-S-O1	-2.35	102.03	109.50
2	G	4900	SO4	O2-S-O1	-2.07	102.94	109.50
2	B	3603	SO4	O2-S-O1	-2.06	102.96	109.50
2	C	5000	SO4	O2-S-O1	-2.05	102.99	109.50
2	F	4700	SO4	O4-S-O3	2.03	117.25	108.98
2	G	3704	SO4	O2-S-O1	2.50	117.41	109.50

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	3701	SO4	1	0
2	C	5000	SO4	2	0
2	G	4900	SO4	1	0
2	H	6101	SO4	2	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	292/293 (99%)	0.59	36 (12%) <b>5</b> <b>6</b>	11, 20, 41, 60	0
1	B	292/293 (99%)	0.50	35 (11%) <b>6</b> <b>6</b>	9, 19, 44, 63	0
1	C	293/293 (100%)	0.44	27 (9%) <b>11</b> <b>12</b>	9, 20, 43, 65	0
1	D	292/293 (99%)	0.62	33 (11%) <b>7</b> <b>7</b>	10, 21, 47, 72	0
1	E	292/293 (99%)	0.65	26 (8%) <b>12</b> <b>13</b>	10, 23, 45, 67	0
1	F	293/293 (100%)	0.42	19 (6%) <b>22</b> <b>25</b>	8, 16, 43, 69	0
1	G	292/293 (99%)	0.49	26 (8%) <b>12</b> <b>13</b>	8, 16, 38, 66	0
1	H	292/293 (99%)	0.59	32 (10%) <b>7</b> <b>8</b>	10, 20, 42, 52	0
All	All	2338/2344 (99%)	0.54	234 (10%) <b>9</b> <b>10</b>	8, 19, 43, 72	0

All (234) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	13	GLY	12.4
1	A	13	GLY	11.2
1	B	13	GLY	10.4
1	F	13	GLY	9.7
1	E	193	PRO	9.3
1	E	13	GLY	8.2
1	B	16	LEU	8.2
1	D	15	ARG	8.2
1	E	12	SER	8.1
1	C	13	GLY	7.9
1	E	194	ARG	7.3
1	E	195	GLY	7.2
1	F	14	THR	7.1
1	H	11	GLY	6.6
1	H	12	SER	6.3
1	G	12	SER	6.2

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Mol	Chain	Res	Type	RSRZ
1	G	15	ARG	6.2
1	G	16	LEU	5.7
1	D	22	ALA	5.7
1	B	193	PRO	5.7
1	C	193	PRO	5.6
1	B	275	LEU	5.5
1	D	14	THR	5.5
1	D	194	ARG	5.5
1	D	195	GLY	5.4
1	D	192	SER	5.4
1	C	12	SER	5.4
1	G	14	THR	5.3
1	A	16	LEU	5.3
1	D	193	PRO	5.2
1	C	14	THR	5.2
1	E	11	GLY	5.2
1	E	15	ARG	5.1
1	B	15	ARG	5.1
1	B	191	PRO	5.1
1	H	23	ILE	5.0
1	E	14	THR	5.0
1	D	11	GLY	5.0
1	B	194	ARG	5.0
1	A	195	GLY	4.9
1	D	197	LEU	4.9
1	C	195	GLY	4.9
1	D	16	LEU	4.8
1	F	193	PRO	4.7
1	C	191	PRO	4.6
1	A	23	ILE	4.5
1	E	164	LEU	4.5
1	C	11	GLY	4.4
1	D	23	ILE	4.4
1	C	15	ARG	4.4
1	B	12	SER	4.4
1	A	192	SER	4.4
1	G	195	GLY	4.3
1	G	194[A]	ARG	4.3
1	A	12	SER	4.2
1	D	164	LEU	4.2
1	D	12	SER	4.2
1	H	22	ALA	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	14	THR	4.0
1	E	192	SER	4.0
1	H	265	ALA	4.0
1	G	17	HIS	4.0
1	G	193	PRO	3.9
1	H	273	ALA	3.9
1	E	191	PRO	3.9
1	B	266	ALA	3.9
1	A	15	ARG	3.9
1	A	193	PRO	3.9
1	H	195	GLY	3.8
1	C	194	ARG	3.8
1	F	192	SER	3.8
1	A	277	LYS	3.8
1	F	11	GLY	3.8
1	H	152	GLN	3.8
1	A	191	PRO	3.7
1	F	277	LYS	3.6
1	G	270	LYS	3.6
1	G	192	SER	3.6
1	C	1	MET	3.6
1	C	277	LYS	3.6
1	H	194	ARG	3.6
1	F	23	ILE	3.6
1	G	23	ILE	3.6
1	A	270	LYS	3.6
1	G	18	PRO	3.5
1	B	277	LYS	3.5
1	A	14	THR	3.5
1	D	277	LYS	3.5
1	C	273	ALA	3.5
1	H	192	SER	3.5
1	B	276	ALA	3.5
1	F	15	ARG	3.5
1	H	277	LYS	3.5
1	B	265	ALA	3.4
1	A	197	LEU	3.4
1	B	17	HIS	3.3
1	C	192	SER	3.4
1	E	84	SER	3.4
1	D	84	SER	3.3
1	E	16	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	H	288	LEU	3.3
1	C	16	LEU	3.2
1	A	266	ALA	3.2
1	E	196	GLU	3.2
1	B	192	SER	3.2
1	F	164	LEU	3.2
1	E	277	LYS	3.2
1	C	275	LEU	3.2
1	B	195	GLY	3.2
1	E	23	ILE	3.2
1	A	265	ALA	3.1
1	A	11	GLY	3.1
1	H	193	PRO	3.0
1	C	86	ASP	3.0
1	E	10	GLY	3.0
1	G	13	GLY	3.0
1	H	279	GLY	2.9
1	C	276	ALA	2.9
1	H	276	ALA	2.9
1	F	1	MET	2.9
1	A	194	ARG	2.9
1	G	275	LEU	2.9
1	E	289	THR	2.9
1	A	288	LEU	2.9
1	G	277	LYS	2.8
1	F	191	PRO	2.8
1	A	269	GLU	2.8
1	F	195	GLY	2.8
1	D	266	ALA	2.8
1	B	270	LYS	2.8
1	H	278	ASN	2.8
1	F	265	ALA	2.8
1	H	85	PRO	2.8
1	F	12	SER	2.8
1	B	269	GLU	2.7
1	D	187	ARG	2.7
1	D	191	PRO	2.7
1	D	190	LYS	2.7
1	B	23	ILE	2.7
1	C	269	GLU	2.7
1	G	11	GLY	2.7
1	A	190	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	H	275	LEU	2.6
1	D	85	PRO	2.6
1	H	21	LEU	2.6
1	A	276	ALA	2.6
1	D	19	ALA	2.6
1	D	127	GLN	2.6
1	H	84	SER	2.6
1	B	22	ALA	2.6
1	E	258	TYR	2.6
1	A	272	ALA	2.5
1	A	273	ALA	2.5
1	G	21	LEU	2.5
1	H	272	ALA	2.5
1	D	189	LEU	2.5
1	E	278	ASN	2.5
1	D	276	ALA	2.5
1	F	123	GLY	2.5
1	H	222	ALA	2.5
1	B	190	LYS	2.5
1	H	13	GLY	2.5
1	B	11	GLY	2.5
1	A	17	HIS	2.4
1	B	152	GLN	2.4
1	B	113	TYR	2.4
1	E	57	PRO	2.4
1	B	267	GLN	2.4
1	H	269	GLU	2.4
1	C	270	LYS	2.4
1	G	22	ALA	2.4
1	A	267	GLN	2.4
1	H	270	LYS	2.4
1	D	21	LEU	2.4
1	B	222	ALA	2.4
1	A	85	PRO	2.4
1	C	196	GLU	2.4
1	B	285	LYS	2.4
1	C	266	ALA	2.4
1	D	196	GLU	2.3
1	A	187	ARG	2.3
1	E	2	LYS	2.3
1	A	275	LEU	2.3
1	A	18	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	276	ALA	2.3
1	C	197	LEU	2.2
1	D	24	SER	2.2
1	E	129	GLN	2.2
1	B	278	ASN	2.2
1	H	266	ALA	2.2
1	C	164	LEU	2.2
1	D	270	LYS	2.2
1	H	224	LEU	2.2
1	C	127	GLN	2.2
1	H	223	TRP	2.2
1	C	285	LYS	2.2
1	B	288	LEU	2.2
1	F	289	THR	2.2
1	B	259	ARG	2.2
1	B	261	LYS	2.2
1	H	258	TYR	2.2
1	B	289	THR	2.2
1	F	275	LEU	2.2
1	F	194	ARG	2.2
1	A	172	VAL	2.2
1	F	250	VAL	2.2
1	H	65	GLN	2.1
1	E	265	ALA	2.1
1	G	19	ALA	2.1
1	A	223	TRP	2.1
1	G	7	ILE	2.1
1	H	264	ASP	2.1
1	C	189	LEU	2.1
1	A	136	ALA	2.1
1	C	17	HIS	2.1
1	D	269	GLU	2.1
1	D	285	LYS	2.1
1	B	258	TYR	2.1
1	E	197	LEU	2.1
1	G	191	PRO	2.1
1	D	118	PHE	2.1
1	H	238	PHE	2.1
1	D	112	LEU	2.1
1	G	265	ALA	2.1
1	A	196	GLU	2.0
1	A	287	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	189	LEU	2.0
1	G	106	LEU	2.0
1	A	279	GLY	2.0
1	A	83	PRO	2.0
1	B	279	GLY	2.0
1	E	119	HIS	2.0
1	G	6	ILE	2.0
1	G	239	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	SO4	C	3600	5/5	0.99	0.11	0.39	27,31,35,37	0
2	SO4	G	3605	5/5	0.99	0.13	0.31	27,28,31,31	0
2	SO4	H	6101	5/5	0.89	0.23	0.12	50,58,59,65	0
2	SO4	D	3601	5/5	0.99	0.11	-0.02	25,28,30,34	0
2	SO4	B	3701	5/5	0.98	0.11	-0.10	55,57,58,59	0
2	SO4	A	3602	5/5	0.99	0.12	-0.17	25,26,29,29	0
2	SO4	E	3607	5/5	0.98	0.11	-0.22	25,27,31,32	0
2	SO4	H	3604	5/5	0.99	0.13	-0.24	29,30,30,31	0
2	SO4	F	3606	5/5	0.99	0.11	-0.24	22,28,31,32	0
2	SO4	G	3704	5/5	0.96	0.10	-0.34	47,50,52,56	0
2	SO4	B	3603	5/5	0.99	0.12	-0.58	28,30,32,33	0
2	SO4	D	3800	5/5	0.97	0.09	-1.04	48,52,56,56	0
2	SO4	C	3702	5/5	0.94	0.23	-	53,58,58,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SO4	E	6100	5/5	0.93	0.27	-	45,47,49,51	0
2	SO4	G	4900	5/5	0.93	0.15	-	59,60,61,63	0
2	SO4	E	5001	5/5	0.91	0.16	-	45,46,50,50	0
2	SO4	F	4700	5/5	0.89	0.17	-	42,52,58,59	0
2	SO4	D	3703	5/5	0.92	0.25	-	52,59,62,64	0
2	SO4	A	3700	5/5	0.98	0.09	-	45,47,52,55	0
2	SO4	C	5000	5/5	0.92	0.18	-	41,48,52,53	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.