



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:45 PM GMT

PDB ID : 4G0I  
Title : Glutathionyl-Hydroquinone Reductase, YqjG of Escherichia coli  
Authors : Green, A.R.; Hayes, R.P.; Xun, L.; Kang, C.  
Deposited on : 2012-07-09  
Resolution : 2.05 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](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

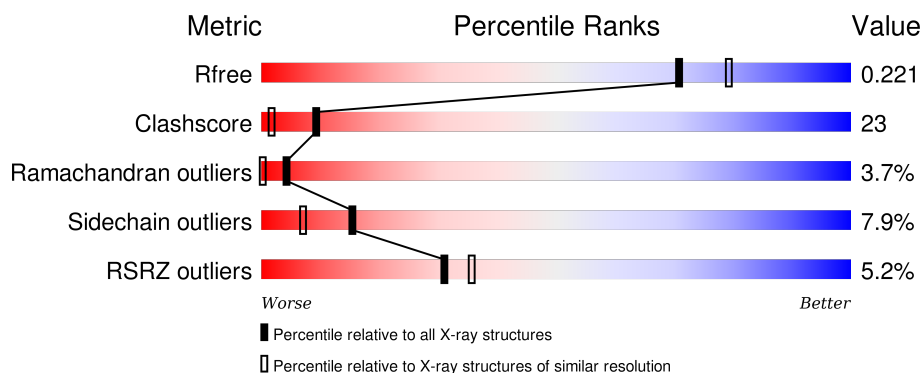
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.05 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1192 (2.04-2.04)
Clashscore	102246	1269 (2.04-2.04)
Ramachandran outliers	100387	1258 (2.04-2.04)
Sidechain outliers	100360	1258 (2.04-2.04)
RSRZ outliers	91569	1194 (2.04-2.04)

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	328	<div> <div>4%</div> <div>63%</div> <div>25%</div> <div>9%</div> <div>.</div> </div>
1	B	328	<div> <div>6%</div> <div>63%</div> <div>26%</div> <div>9%</div> <div>.</div> </div>

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	402	-	-	-	X
2	SO4	B	402	-	-	-	X
3	MES	A	407	-	-	X	X
3	MES	A	408	-	-	-	X
3	MES	B	407	-	-	-	X

## 2 Entry composition [i](#)

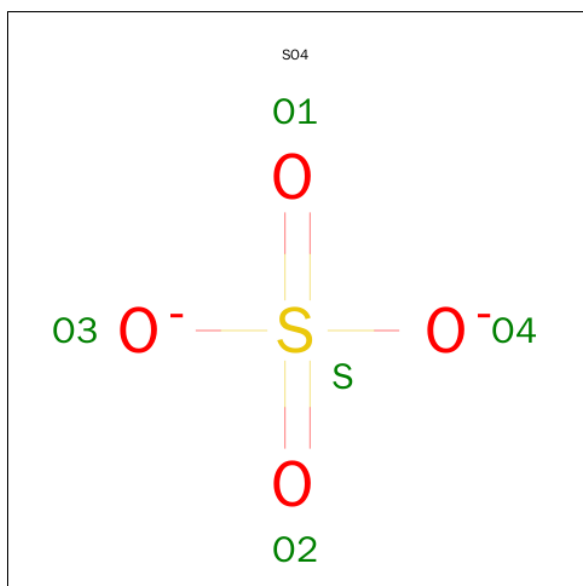
There are 4 unique types of molecules in this entry. The entry contains 5699 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 protein yqjG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	327	Total	C	N	O	S	0	1	0
			2649	1701	456	486	6			
1	B	327	Total	C	N	O	S	0	1	0
			2649	1701	456	486	6			

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



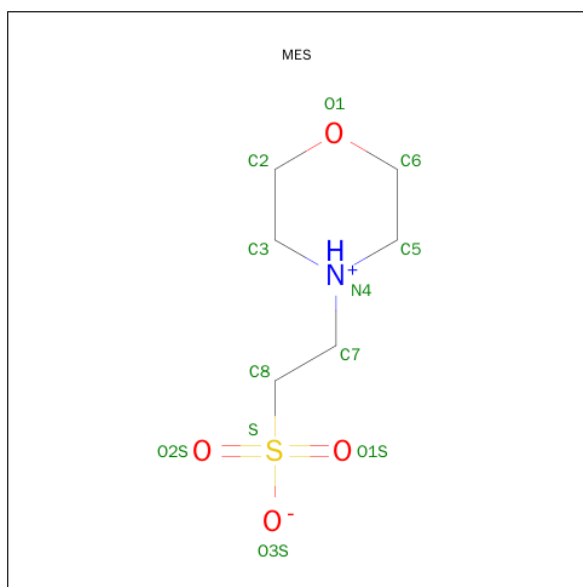
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

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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	B	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	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

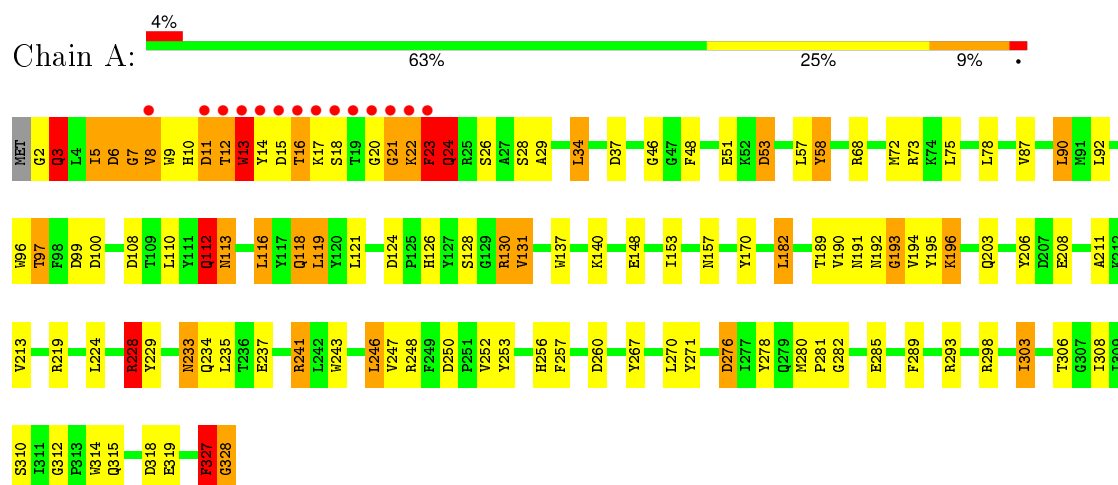
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	160	Total 160	O 160	0	0
4	B	145	Total 145	O 145	0	0

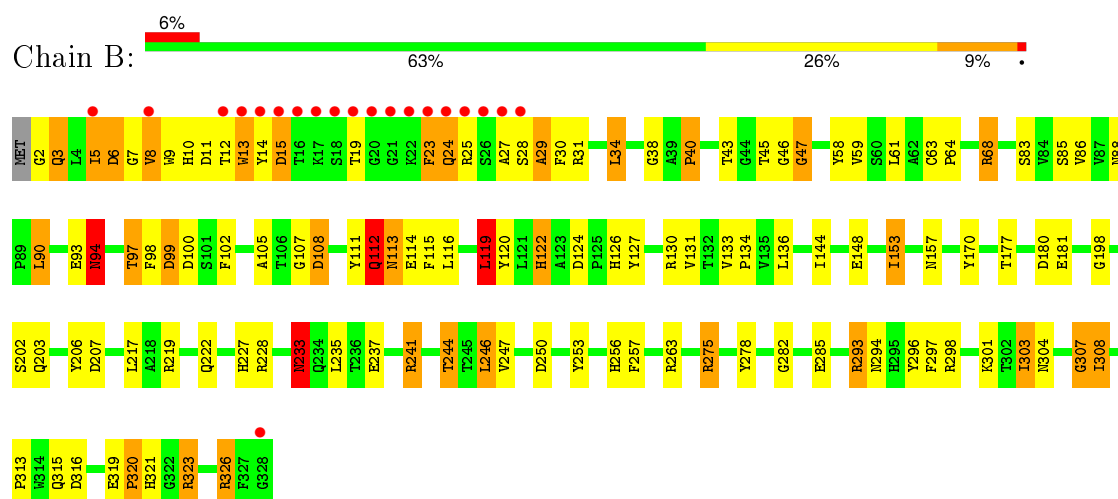
### 3 Residue-property plots [i](#)

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: protein yqjG



#### • Molecule 1: protein yqjG



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	149.15Å 149.15Å 105.34Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.80 – 2.05 48.82 – 2.05	Depositor EDS
% Data completeness (in resolution range)	87.4 (48.80-2.05) 87.4 (48.82-2.05)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.66 (at 2.05Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.6.1_357)	Depositor
R, $R_{free}$	0.196 , 0.227 0.193 , 0.221	Depositor DCC
$R_{free}$ test set	1761 reflections (2.36%)	DCC
Wilson B-factor (Å <sup>2</sup> )	35.6	Xtriage
Anisotropy	0.176	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 46.9	EDS
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 83027 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5699	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	30/2732 (1.1%)	1.58	42/3719 (1.1%)
1	B	1.62	25/2732 (0.9%)	1.47	26/3719 (0.7%)
All	All	1.63	55/5464 (1.0%)	1.52	68/7438 (0.9%)

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	285	GLU	CD-OE2	13.42	1.40	1.25
1	B	148	GLU	CD-OE2	9.47	1.36	1.25
1	A	327	PHE	C-O	9.30	1.41	1.23
1	A	278	TYR	CD1-CE1	8.91	1.52	1.39
1	B	63	CYS	CB-SG	8.70	1.97	1.82
1	B	285	GLU	CG-CD	8.58	1.64	1.51
1	A	51	GLU	CG-CD	8.11	1.64	1.51
1	A	194	VAL	CB-CG2	-7.92	1.36	1.52
1	A	247	VAL	CB-CG1	-7.59	1.36	1.52
1	B	93	GLU	CB-CG	7.55	1.66	1.52
1	B	233	ASN	CB-CG	7.38	1.68	1.51
1	B	285	GLU	CD-OE1	7.32	1.33	1.25
1	A	131	VAL	CB-CG1	7.24	1.68	1.52
1	A	319	GLU	CD-OE2	7.22	1.33	1.25
1	A	87	VAL	CA-CB	-7.04	1.40	1.54
1	B	253	TYR	CB-CG	6.91	1.62	1.51
1	B	114	GLU	CG-CD	6.87	1.62	1.51
1	A	319	GLU	CG-CD	6.80	1.62	1.51
1	A	228	ARG	CG-CD	-6.72	1.35	1.51
1	B	253	TYR	CD2-CE2	6.72	1.49	1.39
1	B	237	GLU	CG-CD	6.65	1.61	1.51
1	A	228	ARG	CD-NE	-6.59	1.35	1.46
1	B	253	TYR	CE1-CZ	6.43	1.47	1.38
1	B	282	GLY	C-O	-6.42	1.13	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	278	TYR	CD2-CE2	6.32	1.48	1.39
1	A	213	VAL	CA-CB	-6.30	1.41	1.54
1	B	296	TYR	CD2-CE2	6.27	1.48	1.39
1	A	113	ASN	CG-OD1	6.11	1.37	1.24
1	B	83	SER	CB-OG	6.07	1.50	1.42
1	A	58	TYR	CE1-CZ	6.05	1.46	1.38
1	A	118	GLN	CB-CG	6.01	1.68	1.52
1	A	271	TYR	CD1-CE1	5.92	1.48	1.39
1	B	85	SER	CA-CB	5.92	1.61	1.52
1	B	90	LEU	CG-CD1	5.90	1.73	1.51
1	B	153	ILE	CB-CG2	5.77	1.70	1.52
1	A	96	TRP	CB-CG	5.73	1.60	1.50
1	B	148	GLU	CG-CD	5.70	1.60	1.51
1	A	211	ALA	CA-CB	5.66	1.64	1.52
1	A	72	MET	CG-SD	5.51	1.95	1.81
1	B	307	GLY	C-O	5.47	1.32	1.23
1	A	253	TYR	CD2-CE2	5.46	1.47	1.39
1	A	267	TYR	CE2-CZ	-5.45	1.31	1.38
1	A	250	ASP	CB-CG	5.39	1.63	1.51
1	B	181	GLU	CG-CD	5.39	1.60	1.51
1	A	208	GLU	CD-OE2	5.24	1.31	1.25
1	A	137	TRP	CG-CD1	5.24	1.44	1.36
1	A	312	GLY	C-O	5.17	1.31	1.23
1	A	267	TYR	CE1-CZ	5.16	1.45	1.38
1	B	90	LEU	CG-CD2	5.16	1.71	1.51
1	A	48	PHE	CE1-CZ	5.13	1.47	1.37
1	B	250	ASP	CG-OD2	5.13	1.37	1.25
1	A	195	TYR	CD2-CE2	5.12	1.47	1.39
1	A	237	GLU	CG-CD	5.07	1.59	1.51
1	A	243	TRP	CB-CG	5.06	1.59	1.50
1	B	58	TYR	CD1-CE1	5.03	1.46	1.39

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	228	ARG	NE-CZ-NH1	22.45	131.52	120.30
1	A	241	ARG	NE-CZ-NH1	20.59	130.59	120.30
1	B	241	ARG	NE-CZ-NH1	16.88	128.74	120.30
1	B	241	ARG	NE-CZ-NH2	-16.23	112.19	120.30
1	A	241	ARG	NE-CZ-NH2	-13.31	113.64	120.30
1	B	90	LEU	CB-CG-CD2	13.28	133.58	111.00
1	B	293	ARG	NE-CZ-NH1	-12.11	114.24	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	248	ARG	NE-CZ-NH2	10.03	125.31	120.30
1	A	90	LEU	CB-CG-CD2	-9.57	94.73	111.00
1	A	68	ARG	NE-CZ-NH2	-9.38	115.61	120.30
1	A	90	LEU	CA-CB-CG	-9.03	94.52	115.30
1	A	327	PHE	CB-CA-C	-8.83	92.74	110.40
1	A	328	GLY	N-CA-C	-8.40	92.10	113.10
1	B	90	LEU	CD1-CG-CD2	-8.32	85.53	110.50
1	A	248	ARG	NE-CZ-NH1	-7.81	116.39	120.30
1	B	246	LEU	CB-CG-CD1	7.73	124.15	111.00
1	A	119	LEU	CA-CB-CG	-7.59	97.83	115.30
1	B	119	LEU	CA-CB-CG	-7.55	97.94	115.30
1	A	228	ARG	NH1-CZ-NH2	-7.20	111.48	119.40
1	A	228	ARG	NE-CZ-NH2	-7.18	116.71	120.30
1	B	228	ARG	NE-CZ-NH1	-7.08	116.76	120.30
1	B	326	ARG	NE-CZ-NH1	7.08	123.84	120.30
1	B	275	ARG	NE-CZ-NH1	-7.01	116.80	120.30
1	A	37	ASP	CB-CG-OD2	6.92	124.53	118.30
1	B	124	ASP	CB-CG-OD1	-6.69	112.28	118.30
1	B	90	LEU	CB-CG-CD1	-6.67	99.65	111.00
1	A	246	LEU	CB-CG-CD1	6.66	122.32	111.00
1	A	327	PHE	CA-C-N	-6.50	103.19	116.20
1	B	136	LEU	CB-CG-CD2	-6.43	100.06	111.00
1	A	7	GLY	N-CA-C	-6.43	97.03	113.10
1	A	219	ARG	NE-CZ-NH1	-6.38	117.11	120.30
1	B	97	THR	N-CA-CB	-6.33	98.28	110.30
1	A	276	ASP	CB-CG-OD1	6.16	123.84	118.30
1	A	182	LEU	CB-CG-CD1	6.11	121.39	111.00
1	A	46	GLY	C-N-CA	-6.08	109.53	122.30
1	B	68	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	A	34	LEU	CB-CG-CD1	-6.07	100.68	111.00
1	A	29	ALA	C-N-CA	-6.06	106.54	121.70
1	B	180	ASP	CB-CG-OD1	5.91	123.62	118.30
1	B	90	LEU	CA-CB-CG	-5.91	101.72	115.30
1	A	73	ARG	NE-CZ-NH1	5.89	123.25	120.30
1	B	99	ASP	CB-CG-OD2	5.82	123.53	118.30
1	A	97	THR	OG1-CB-CG2	5.79	123.31	110.00
1	A	193	GLY	N-CA-C	-5.73	98.77	113.10
1	A	121	LEU	CB-CG-CD2	5.73	120.74	111.00
1	A	124	ASP	CB-CG-OD2	-5.67	113.19	118.30
1	B	47	GLY	N-CA-C	-5.66	98.94	113.10
1	A	78	LEU	CA-CB-CG	-5.64	102.33	115.30
1	B	61	LEU	CB-CG-CD2	-5.59	101.50	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	327	PHE	N-CA-CB	5.58	120.65	110.60
1	A	110	LEU	CB-CG-CD2	5.55	120.44	111.00
1	A	130	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	A	318	ASP	CB-CG-OD2	-5.47	113.38	118.30
1	A	57	LEU	CB-CG-CD2	-5.42	101.78	111.00
1	B	94	ASN	N-CA-C	5.42	125.63	111.00
1	B	293	ARG	CG-CD-NE	-5.41	100.44	111.80
1	B	323	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	A	278	TYR	CD1-CE1-CZ	-5.38	114.96	119.80
1	A	327	PHE	N-CA-C	-5.34	96.59	111.00
1	A	124	ASP	CB-CG-OD1	5.32	123.08	118.30
1	B	247	VAL	CG1-CB-CG2	-5.18	102.62	110.90
1	B	296	TYR	CB-CG-CD1	-5.18	117.89	121.00
1	A	196	LYS	CD-CE-NZ	5.17	123.58	111.70
1	A	53	ASP	CB-CG-OD2	-5.11	113.70	118.30
1	A	75	LEU	CB-CG-CD2	5.05	119.59	111.00
1	A	90	LEU	CD1-CG-CD2	-5.04	95.38	110.50
1	B	105	ALA	N-CA-CB	5.01	117.12	110.10
1	A	306	THR	CA-CB-CG2	-5.01	105.39	112.40

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	2649	0	2537	142	0
1	B	2649	0	2536	97	0
2	A	30	0	0	0	0
2	B	30	0	0	0	0
3	A	24	0	24	11	0
3	B	12	0	12	2	0
4	A	160	0	0	5	0
4	B	145	0	0	7	0
All	All	5699	0	5109	239	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 23.

All (239) 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:7:GLY:CA	1:A:8:VAL:HB	1.68	1.21
1:A:235:LEU:H	3:A:408:MES:H51	1.06	1.14
1:A:23:PHE:HA	1:A:24:GLN:CG	1.78	1.12
1:A:22:LYS:HG3	1:A:24:GLN:HA	1.28	1.11
1:A:7:GLY:HA2	1:A:8:VAL:CB	1.81	1.10
1:A:3:GLN:NE2	1:A:23:PHE:HD1	1.53	1.07
1:A:13:TRP:O	1:A:15:ASP:HA	1.55	1.07
1:A:22:LYS:C	1:A:24:GLN:HA	1.78	1.04
1:A:22:LYS:HG3	1:A:24:GLN:CA	1.87	1.03
1:A:23:PHE:HA	1:A:24:GLN:HG3	1.43	0.99
1:A:3:GLN:HE21	1:A:23:PHE:HD1	1.03	0.92
1:B:321:HIS:HD2	1:B:323:ARG:H	1.13	0.91
1:B:97:THR:HG22	1:B:99:ASP:H	1.34	0.91
1:A:13:TRP:C	1:A:15:ASP:HA	1.89	0.91
1:A:3:GLN:NE2	1:A:23:PHE:CD1	2.38	0.91
1:A:22:LYS:HE2	1:A:22:LYS:O	1.69	0.90
1:A:6:ASP:O	1:A:126:HIS:HA	1.69	0.90
1:A:23:PHE:N	1:A:24:GLN:HG2	1.87	0.89
1:A:97:THR:HG23	1:A:99:ASP:H	1.40	0.87
1:B:7:GLY:HA2	1:B:8:VAL:HB	1.55	0.87
1:A:235:LEU:N	3:A:408:MES:H51	1.90	0.87
1:A:15:ASP:OD1	1:A:16:THR:N	2.06	0.86
1:A:97:THR:CG2	1:A:99:ASP:H	1.87	0.86
1:A:7:GLY:HA2	1:A:8:VAL:HB	0.90	0.86
1:B:321:HIS:CD2	1:B:323:ARG:H	1.94	0.85
1:A:12:THR:O	1:A:14:TYR:CD2	2.30	0.84
1:A:22:LYS:O	1:A:24:GLN:HA	1.78	0.83
1:A:6:ASP:H	1:A:7:GLY:HA2	1.43	0.83
1:A:23:PHE:CA	1:A:24:GLN:CG	2.57	0.82
1:A:192:ASN:O	1:A:196:LYS:HE3	1.78	0.81
1:A:23:PHE:HD2	1:A:23:PHE:H	1.25	0.81
1:A:22:LYS:CG	1:A:24:GLN:O	2.30	0.80
1:B:13:TRP:HB2	1:B:15:ASP:OD2	1.81	0.80
1:A:11:ASP:O	1:A:12:THR:OG1	2.00	0.80
1:A:22:LYS:O	1:A:22:LYS:CE	2.30	0.80
1:A:6:ASP:H	1:A:7:GLY:CA	1.95	0.79
1:A:22:LYS:O	1:A:22:LYS:CG	2.30	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:TRP:O	1:A:15:ASP:CA	2.30	0.79
1:A:22:LYS:O	1:A:22:LYS:CD	2.30	0.79
1:A:22:LYS:O	1:A:24:GLN:CA	2.30	0.79
1:B:198:GLY:O	1:B:303:ILE:HD11	1.82	0.78
1:B:7:GLY:HA2	1:B:8:VAL:CB	2.14	0.78
1:A:17:LYS:HG3	1:A:18:SER:H	1.49	0.78
1:B:7:GLY:CA	1:B:8:VAL:HB	2.13	0.78
1:A:235:LEU:H	3:A:408:MES:C5	1.94	0.75
1:B:97:THR:CG2	1:B:99:ASP:H	2.00	0.75
1:A:23:PHE:HA	1:A:24:GLN:CB	2.17	0.75
1:A:189:THR:OG1	1:A:190:VAL:HG23	1.86	0.75
1:A:8:VAL:O	1:A:8:VAL:HG12	1.85	0.75
1:A:22:LYS:HG3	1:A:24:GLN:C	2.08	0.74
1:B:64:PRO:HB3	1:B:244:THR:HG23	1.67	0.74
1:A:6:ASP:N	1:A:7:GLY:CA	2.51	0.74
1:B:2:GLY:O	1:B:3:GLN:HB2	1.87	0.73
1:A:193:GLY:HA2	1:A:196:LYS:HD2	1.70	0.73
1:A:148:GLU:OE2	4:A:641:HOH:O	2.07	0.73
1:B:7:GLY:CA	1:B:8:VAL:CB	2.67	0.73
1:A:233:ASN:ND2	1:A:234:GLN:HE21	1.87	0.72
1:A:22:LYS:CD	1:A:24:GLN:O	2.38	0.72
1:B:28:SER:O	1:B:29:ALA:HB3	1.88	0.72
1:B:6:ASP:H	1:B:7:GLY:CA	2.03	0.71
1:A:328:GLY:O	4:A:655:HOH:O	2.08	0.71
1:B:315:GLN:NE2	4:B:524:HOH:O	2.23	0.71
1:A:22:LYS:HD3	1:A:24:GLN:O	1.90	0.71
1:A:13:TRP:O	1:A:15:ASP:CG	2.30	0.70
1:A:12:THR:O	1:A:14:TYR:HD2	1.74	0.70
1:A:10:HIS:O	1:A:12:THR:N	2.25	0.69
1:A:8:VAL:HG13	1:A:10:HIS:NE2	2.07	0.69
1:A:203:GLN:H	3:A:407:MES:H71	1.58	0.69
1:A:234:GLN:OE1	3:A:408:MES:H71	1.94	0.68
1:A:22:LYS:O	1:A:22:LYS:HG3	1.91	0.68
1:B:68:ARG:HE	1:B:244:THR:HG21	1.60	0.67
1:A:5:ILE:O	1:A:128:SER:OG	2.08	0.67
1:A:12:THR:C	1:A:14:TYR:HD2	1.98	0.66
1:B:40:PRO:HD3	1:B:46:GLY:HA3	1.77	0.66
1:A:22:LYS:C	1:A:24:GLN:CA	2.59	0.66
1:A:26:SER:HB2	1:A:128:SER:O	1.95	0.66
1:A:6:ASP:N	1:A:7:GLY:HA2	2.10	0.66
1:B:316:ASP:OD1	1:B:319:GLU:HG2	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:LYS:O	1:A:24:GLN:N	2.28	0.65
1:A:192:ASN:HD22	1:A:196:LYS:HE3	1.61	0.65
1:A:23:PHE:N	1:A:23:PHE:CD2	2.56	0.65
1:A:23:PHE:CA	1:A:24:GLN:HG2	2.26	0.65
1:A:21:GLY:O	1:A:24:GLN:NE2	2.30	0.65
1:A:22:LYS:HE2	1:A:22:LYS:C	2.17	0.64
1:A:13:TRP:O	1:A:15:ASP:CB	2.45	0.64
1:A:6:ASP:H	1:A:8:VAL:HB	1.61	0.64
1:B:321:HIS:HD2	1:B:323:ARG:N	1.90	0.64
1:B:241:ARG:HD2	4:B:594:HOH:O	1.98	0.62
1:A:15:ASP:O	1:A:17:LYS:N	2.32	0.62
1:A:113:ASN:OD1	1:A:118:GLN:CB	2.48	0.62
1:A:8:VAL:HG13	1:A:10:HIS:CE1	2.35	0.61
1:B:6:ASP:O	1:B:126:HIS:CA	2.47	0.61
1:A:12:THR:O	1:A:14:TYR:N	2.30	0.61
1:A:157:ASN:HD21	1:A:170:TYR:H	1.49	0.61
1:A:14:TYR:HA	1:A:15:ASP:HB2	1.82	0.61
1:A:5:ILE:HG13	1:A:10:HIS:CD2	2.36	0.60
1:B:157:ASN:ND2	1:B:170:TYR:H	1.98	0.60
1:B:304:ASN:ND2	1:B:307:GLY:HA2	2.17	0.60
1:A:22:LYS:HE2	1:A:22:LYS:CA	2.31	0.60
1:B:298:ARG:O	1:B:301:LYS:HE2	2.03	0.58
1:B:6:ASP:H	1:B:7:GLY:HA3	1.66	0.58
1:A:282:GLY:O	1:A:285:GLU:HG2	2.04	0.58
1:A:5:ILE:HG13	1:A:10:HIS:HD2	1.68	0.58
1:A:8:VAL:CG1	1:A:10:HIS:NE2	2.66	0.58
1:B:6:ASP:O	1:B:126:HIS:HA	2.04	0.58
1:A:23:PHE:N	1:A:23:PHE:HD2	1.96	0.57
1:A:112:GLN:CD	1:A:112:GLN:N	2.57	0.57
1:B:28:SER:O	1:B:29:ALA:CB	2.52	0.57
1:B:235:LEU:H	3:B:407:MES:H82	1.69	0.57
1:B:7:GLY:HA2	1:B:8:VAL:CG2	2.35	0.56
1:A:289:PHE:O	1:A:293:ARG:HG3	2.05	0.56
1:A:113:ASN:OD1	1:A:118:GLN:HB3	2.05	0.56
1:B:275:ARG:HG3	1:B:275:ARG:HH11	1.71	0.56
1:B:6:ASP:N	1:B:7:GLY:CA	2.65	0.56
1:A:23:PHE:N	1:A:24:GLN:HA	2.20	0.56
1:B:6:ASP:O	1:B:126:HIS:C	2.44	0.56
1:A:203:GLN:N	3:A:407:MES:H71	2.20	0.56
1:A:23:PHE:CA	1:A:24:GLN:CB	2.83	0.55
1:B:2:GLY:N	1:B:14:TYR:CE2	2.74	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:233:ASN:O	3:B:407:MES:H31	2.06	0.55
1:A:22:LYS:HG3	1:A:24:GLN:O	2.02	0.55
1:B:198:GLY:O	1:B:303:ILE:CD1	2.53	0.55
1:A:315:GLN:OE1	4:A:564:HOH:O	2.18	0.55
1:A:97:THR:HG22	1:A:99:ASP:H	1.70	0.54
1:B:24:GLN:N	1:B:27:ALA:HB2	2.22	0.54
1:B:97:THR:HG22	1:B:99:ASP:N	2.15	0.54
1:B:304:ASN:HD22	1:B:307:GLY:HA2	1.72	0.54
1:A:203:GLN:HB3	3:A:407:MES:H82	1.90	0.53
1:B:206:TYR:O	1:B:207:ASP:C	2.41	0.53
1:A:140:LYS:NZ	4:A:595:HOH:O	2.42	0.53
1:B:9:TRP:HE1	1:B:94:ASN:HA	1.72	0.53
1:B:133:VAL:HB	1:B:134:PRO:HA	1.91	0.53
1:A:113:ASN:OD1	1:A:118:GLN:HB2	2.07	0.53
1:A:228:ARG:HD2	1:A:229:TYR:CZ	2.44	0.52
1:A:228:ARG:HD3	1:A:276:ASP:OD2	2.10	0.52
1:A:10:HIS:C	1:A:12:THR:H	2.13	0.52
1:B:5:ILE:HG22	1:B:6:ASP:N	2.24	0.52
1:A:241:ARG:HD2	4:A:615:HOH:O	2.09	0.52
1:A:17:LYS:CG	1:A:18:SER:H	2.14	0.51
1:B:38:GLY:O	1:B:47:GLY:HA2	2.09	0.51
1:A:7:GLY:CA	1:A:8:VAL:CB	2.46	0.51
1:B:9:TRP:NE1	1:B:94:ASN:HA	2.26	0.49
1:A:314:TRP:O	1:A:315:GLN:HB3	2.11	0.49
1:B:12:THR:O	1:B:14:TYR:CD2	2.66	0.49
1:A:108:ASP:HB3	1:A:112:GLN:HA	1.93	0.49
1:A:224:LEU:HD12	1:A:270:LEU:HD23	1.93	0.49
1:A:13:TRP:O	1:A:15:ASP:OD1	2.30	0.49
1:B:304:ASN:HD21	1:B:308:ILE:N	2.11	0.49
1:B:24:GLN:HG2	1:B:25:ARG:HG3	1.95	0.49
1:B:256:HIS:HD2	1:B:257:PHE:CE1	2.31	0.49
1:A:157:ASN:ND2	1:A:170:TYR:H	2.09	0.49
1:B:5:ILE:CG2	1:B:6:ASP:N	2.73	0.48
1:B:157:ASN:HD21	1:B:170:TYR:H	1.61	0.48
1:B:256:HIS:CD2	1:B:257:PHE:CE1	3.01	0.48
1:A:327:PHE:CB	1:A:328:GLY:HA2	2.38	0.48
1:A:256:HIS:HD2	1:A:257:PHE:CE1	2.31	0.48
1:A:15:ASP:CG	1:A:16:THR:H	2.10	0.48
1:A:17:LYS:HG3	1:A:18:SER:N	2.22	0.48
1:B:88:ASN:HB2	1:B:99:ASP:O	2.13	0.48
1:B:319:GLU:OE2	1:B:320:PRO:HD2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:VAL:O	1:A:192:ASN:N	2.46	0.48
1:A:92:LEU:HD22	1:A:92:LEU:N	2.29	0.48
1:B:59:VAL:O	1:B:86:VAL:HA	2.13	0.48
1:B:108:ASP:OD1	1:B:108:ASP:C	2.51	0.48
1:A:22:LYS:O	1:A:23:PHE:C	2.53	0.48
1:A:203:GLN:H	3:A:407:MES:C7	2.25	0.48
1:A:260:ASP:O	1:B:263[A]:ARG:NH2	2.48	0.47
1:B:14:TYR:HA	1:B:15:ASP:HB2	1.96	0.47
1:B:113:ASN:HD22	1:B:119:LEU:CD1	2.27	0.47
1:A:97:THR:CG2	1:A:99:ASP:HB3	2.45	0.47
3:A:407:MES:H51	3:A:407:MES:H81	1.62	0.47
1:A:192:ASN:O	1:A:196:LYS:CE	2.58	0.47
1:B:98:PHE:CD2	1:B:108:ASP:N	2.83	0.47
1:A:308:ILE:HD13	1:B:203:GLN:HA	1.96	0.47
1:A:12:THR:HA	1:A:14:TYR:CD2	2.50	0.47
1:B:6:ASP:O	1:B:127:TYR:N	2.47	0.46
1:B:294:ASN:O	1:B:298:ARG:HB2	2.14	0.46
1:B:130:ARG:HG2	4:B:625:HOH:O	2.14	0.46
1:A:116:LEU:HD13	1:A:131:VAL:HG12	1.97	0.46
1:A:23:PHE:N	1:A:24:GLN:CA	2.78	0.46
1:B:256:HIS:HB2	1:B:297:PHE:CE1	2.51	0.46
1:A:10:HIS:C	1:A:12:THR:N	2.67	0.46
1:A:327:PHE:HB3	1:A:328:GLY:HA2	1.98	0.46
1:B:7:GLY:HA2	1:B:8:VAL:HG23	1.98	0.45
1:A:280:MET:HA	1:A:281:PRO:HD3	1.78	0.45
1:A:14:TYR:N	1:A:15:ASP:HA	2.21	0.45
1:B:263[A]:ARG:CZ	1:B:313:PRO:HB3	2.47	0.45
1:A:203:GLN:CB	3:A:407:MES:H82	2.46	0.45
1:A:26:SER:CB	1:A:128:SER:O	2.63	0.45
1:B:24:GLN:H	1:B:27:ALA:HB2	1.82	0.45
1:B:98:PHE:O	1:B:107:GLY:HA2	2.17	0.45
1:B:5:ILE:HG22	1:B:8:VAL:HB	2.00	0.44
1:B:19:THR:HG22	1:B:19:THR:O	2.18	0.44
1:B:94:ASN:OD1	1:B:115:PHE:CZ	2.71	0.44
1:B:30:PHE:HB3	1:B:144:ILE:HG22	1.99	0.44
1:B:111:TYR:O	1:B:112:GLN:HG2	2.17	0.44
1:B:177:THR:HG22	4:B:546:HOH:O	2.18	0.43
1:A:206:TYR:CD2	1:A:206:TYR:C	2.92	0.43
1:A:12:THR:CA	1:A:14:TYR:HD2	2.31	0.43
3:A:408:MES:H81	3:A:408:MES:H52	1.20	0.43
1:B:3:GLN:HE22	1:B:23:PHE:HE1	1.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:THR:C	1:A:14:TYR:N	2.72	0.43
1:A:233:ASN:C	1:A:233:ASN:HD22	2.22	0.43
1:B:8:VAL:HG12	1:B:10:HIS:CE1	2.54	0.43
1:B:219:ARG:NH2	1:B:222:GLN:OE1	2.52	0.42
1:A:22:LYS:CG	1:A:24:GLN:HA	2.21	0.42
1:B:28:SER:HB2	1:B:31:ARG:HG3	2.01	0.42
1:A:327:PHE:C	1:A:328:GLY:O	2.55	0.42
1:B:40:PRO:HG3	1:B:46:GLY:H	1.85	0.42
1:B:112:GLN:NE2	4:B:633:HOH:O	2.51	0.42
1:B:2:GLY:N	1:B:14:TYR:HE2	2.16	0.42
1:B:326:ARG:HD2	4:B:553:HOH:O	2.20	0.42
1:B:233:ASN:H	1:B:233:ASN:HD22	1.67	0.42
1:A:20:GLY:HA2	1:A:21:GLY:HA3	1.68	0.42
1:B:45:THR:O	4:B:508:HOH:O	2.21	0.42
1:A:2:GLY:HA2	1:A:9:TRP:CZ2	2.55	0.42
1:B:31:ARG:O	1:B:43:THR:OG1	2.32	0.42
1:B:6:ASP:H	1:B:7:GLY:HA2	1.82	0.41
1:A:6:ASP:O	1:A:126:HIS:CA	2.55	0.41
1:A:256:HIS:CD2	1:A:257:PHE:CE1	3.08	0.41
1:B:113:ASN:ND2	1:B:119:LEU:HG	2.35	0.41
1:B:217:LEU:HA	1:B:217:LEU:HD23	1.59	0.41
1:A:58:TYR:CE2	1:A:119:LEU:HD13	2.56	0.41
1:B:293:ARG:HD3	1:B:293:ARG:HH11	1.63	0.41
1:B:68:ARG:CZ	1:B:241:ARG:HG2	2.51	0.41
1:A:92:LEU:HA	1:A:92:LEU:HD13	1.86	0.41
1:B:256:HIS:HD2	1:B:257:PHE:CD1	2.38	0.41
1:B:34:LEU:HD12	1:B:34:LEU:HA	1.73	0.41
1:A:100:ASP:N	1:A:100:ASP:OD1	2.51	0.41
1:B:256:HIS:CD2	1:B:257:PHE:CD1	3.09	0.40
1:A:233:ASN:ND2	1:A:233:ASN:C	2.74	0.40
1:B:94:ASN:OD1	1:B:115:PHE:CE1	2.74	0.40
1:A:190:VAL:C	1:A:192:ASN:N	2.73	0.40
1:B:30:PHE:N	1:B:30:PHE:CD2	2.88	0.40
1:B:120:TYR:CD2	1:B:131:VAL:HG13	2.56	0.40
1:A:303:ILE:HD13	1:A:303:ILE:HG21	1.67	0.40
1:A:192:ASN:O	1:A:192:ASN:ND2	2.54	0.40
1:B:112:GLN:CD	1:B:112:GLN:N	2.74	0.40
1:A:2:GLY:HA2	1:A:9:TRP:CH2	2.57	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	326/328 (99%)	288 (88%)	25 (8%)	13 (4%)	4	0
1	B	326/328 (99%)	289 (89%)	26 (8%)	11 (3%)	5	0
All	All	652/656 (99%)	577 (88%)	51 (8%)	24 (4%)	4	0

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	23	PHE
1	A	24	GLN
1	A	11	ASP
1	A	12	THR
1	A	16	THR
1	B	3	GLN
1	B	29	ALA
1	B	94	ASN
1	B	113	ASN
1	A	3	GLN
1	A	8	VAL
1	A	28	SER
1	B	8	VAL
1	B	11	ASP
1	B	15	ASP
1	B	24	GLN
1	B	108	ASP
1	B	122	HIS
1	A	13	TRP
1	A	112	GLN
1	A	191	ASN
1	B	112	GLN
1	A	252	VAL
1	A	21	GLY

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	278/278 (100%)	256 (92%)	22 (8%)	15	7
1	B	278/278 (100%)	256 (92%)	22 (8%)	15	7
All	All	556/556 (100%)	512 (92%)	44 (8%)	15	7

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	5	ILE
1	A	6	ASP
1	A	13	TRP
1	A	22	LYS
1	A	23	PHE
1	A	24	GLN
1	A	34	LEU
1	A	53	ASP
1	A	90	LEU
1	A	112	GLN
1	A	116	LEU
1	A	130	ARG
1	A	153	ILE
1	A	182	LEU
1	A	228	ARG
1	A	233	ASN
1	A	246	LEU
1	A	298	ARG
1	A	303	ILE
1	A	310	SER
1	A	327	PHE
1	B	5	ILE
1	B	6	ASP
1	B	13	TRP
1	B	23	PHE
1	B	34	LEU

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Mol	Chain	Res	Type
1	B	40	PRO
1	B	90	LEU
1	B	100	ASP
1	B	102	PHE
1	B	112	GLN
1	B	116	LEU
1	B	119	LEU
1	B	122	HIS
1	B	153	ILE
1	B	202	SER
1	B	227	HIS
1	B	233	ASN
1	B	244	THR
1	B	246	LEU
1	B	303	ILE
1	B	308	ILE
1	B	320	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	GLN
1	A	157	ASN
1	A	192	ASN
1	A	222	GLN
1	A	233	ASN
1	A	256	HIS
1	A	279	GLN
1	B	3	GLN
1	B	10	HIS
1	B	94	ASN
1	B	113	ASN
1	B	157	ASN
1	B	233	ASN
1	B	256	HIS
1	B	304	ASN
1	B	315	GLN
1	B	321	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 ⓘ

15 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	401	-	4,4,4	1.54	0	6,6,6	0.28	0
2	SO4	A	402	-	4,4,4	1.07	0	6,6,6	1.03	0
2	SO4	A	403	-	4,4,4	0.89	0	6,6,6	1.18	0
2	SO4	A	404	-	4,4,4	0.52	0	6,6,6	0.83	0
2	SO4	A	405	-	4,4,4	0.52	0	6,6,6	0.53	0
2	SO4	A	406	-	4,4,4	0.86	0	6,6,6	0.67	0
3	MES	A	407	-	11,12,12	1.50	2 (18%)	14,16,16	3.47	7 (50%)
3	MES	A	408	-	11,12,12	1.91	4 (36%)	14,16,16	5.75	10 (71%)
2	SO4	B	401	-	4,4,4	1.26	0	6,6,6	0.86	0
2	SO4	B	402	-	4,4,4	0.74	0	6,6,6	1.02	0
2	SO4	B	403	-	4,4,4	0.65	0	6,6,6	1.18	1 (16%)
2	SO4	B	404	-	4,4,4	0.41	0	6,6,6	0.39	0
2	SO4	B	405	-	4,4,4	0.80	0	6,6,6	0.76	0
2	SO4	B	406	-	4,4,4	0.85	0	6,6,6	0.47	0
3	MES	B	407	-	11,12,12	1.13	1 (9%)	14,16,16	4.37	9 (64%)

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	401	-	-	0/0/0/0	0/0/0/0
2	SO4	A	402	-	-	0/0/0/0	0/0/0/0
2	SO4	A	403	-	-	0/0/0/0	0/0/0/0
2	SO4	A	404	-	-	0/0/0/0	0/0/0/0
2	SO4	A	405	-	-	0/0/0/0	0/0/0/0
2	SO4	A	406	-	-	0/0/0/0	0/0/0/0
3	MES	A	407	-	-	0/6/14/14	0/1/1/1
3	MES	A	408	-	-	0/6/14/14	0/1/1/1
2	SO4	B	401	-	-	0/0/0/0	0/0/0/0
2	SO4	B	402	-	-	0/0/0/0	0/0/0/0
2	SO4	B	403	-	-	0/0/0/0	0/0/0/0
2	SO4	B	404	-	-	0/0/0/0	0/0/0/0
2	SO4	B	405	-	-	0/0/0/0	0/0/0/0
2	SO4	B	406	-	-	0/0/0/0	0/0/0/0
3	MES	B	407	-	-	0/6/14/14	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	407	MES	O2S-S	2.03	1.51	1.45
3	A	408	MES	O1-C6	2.16	1.51	1.42
3	A	407	MES	O1S-S	2.18	1.52	1.45
3	A	407	MES	O3S-S	2.28	1.52	1.46
3	A	408	MES	C3-N4	2.38	1.53	1.46
3	A	408	MES	C5-C6	2.53	1.60	1.50
3	A	408	MES	O1S-S	3.78	1.57	1.45

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	408	MES	C7-C8-S	-3.85	100.59	112.51
3	A	408	MES	O3S-S-O2S	-3.21	104.13	111.61
3	B	407	MES	O2S-S-O1S	-2.93	102.82	113.48
3	A	407	MES	O3S-S-O2S	-2.68	105.37	111.61
3	A	408	MES	O2S-S-O1S	-2.58	104.08	113.48
2	B	403	SO4	O4-S-O3	-2.44	99.07	108.98
3	B	407	MES	C7-C8-S	-2.36	105.21	112.51
3	B	407	MES	O3S-S-O1S	-2.30	106.25	111.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	408	MES	C7-N4-C5	-2.08	105.93	111.27
3	B	407	MES	C2-C3-N4	2.04	113.21	110.12
3	A	407	MES	C6-C5-N4	2.31	113.63	110.12
3	A	408	MES	C6-O1-C2	2.37	117.87	109.89
3	B	407	MES	C7-N4-C5	2.94	118.81	111.27
3	B	407	MES	C6-O1-C2	3.12	120.40	109.89
3	A	407	MES	C7-N4-C3	3.26	119.62	111.27
3	A	407	MES	C7-N4-C5	3.34	119.83	111.27
3	A	407	MES	O1-C2-C3	3.94	120.88	111.84
3	A	408	MES	O1-C6-C5	4.11	121.26	111.84
3	A	408	MES	C7-N4-C3	4.27	122.22	111.27
3	B	407	MES	O2S-S-C8	4.62	110.85	106.91
3	A	408	MES	O2S-S-C8	4.93	111.11	106.91
3	A	407	MES	C5-N4-C3	5.21	120.19	108.90
3	B	407	MES	C5-N4-C3	7.54	125.23	108.90
3	A	408	MES	C5-N4-C3	8.41	127.12	108.90
3	A	407	MES	O2S-S-C8	8.64	114.28	106.91
3	B	407	MES	O1S-S-C8	11.70	116.89	106.91
3	A	408	MES	O1S-S-C8	16.81	121.25	106.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	407	MES	6	0
3	A	408	MES	5	0
3	B	407	MES	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	327/328 (99%)	-0.15	14 (4%)	39 44	25, 40, 82, 143	0
1	B	327/328 (99%)	0.05	20 (6%)	25 28	27, 46, 109, 169	0
All	All	654/656 (99%)	-0.05	34 (5%)	31 36	25, 43, 99, 169	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	20	GLY	19.9
1	B	16	THR	15.2
1	B	17	LYS	12.5
1	B	18	SER	11.9
1	B	19	THR	11.4
1	B	23	PHE	9.0
1	B	21	GLY	8.4
1	A	23	PHE	8.0
1	B	14	TYR	7.5
1	B	28	SER	7.4
1	B	24	GLN	7.3
1	A	19	THR	7.1
1	B	25	ARG	6.7
1	A	14	TYR	6.5
1	B	13	TRP	5.8
1	B	26	SER	5.6
1	A	18	SER	5.2
1	B	12	THR	5.2
1	B	22	LYS	5.0
1	A	20	GLY	4.6
1	A	12	THR	4.5
1	A	22	LYS	4.1
1	B	15	ASP	4.1
1	A	16	THR	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	27	ALA	3.9
1	A	13	TRP	3.7
1	A	15	ASP	3.4
1	B	328	GLY	3.4
1	A	21	GLY	3.2
1	A	17	LYS	3.0
1	A	11	ASP	2.7
1	A	8	VAL	2.5
1	B	8	VAL	2.4
1	B	5	ILE	2.2

## 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
3	MES	B	407	12/12	0.80	0.63	51.10	62,118,129,148	0
3	MES	A	408	12/12	0.82	0.29	13.60	37,84,93,116	0
3	MES	A	407	12/12	0.76	0.50	11.40	49,101,133,157	0
2	SO4	A	402	5/5	0.87	0.26	10.34	51,86,93,142	0
2	SO4	B	402	5/5	0.91	0.21	7.88	39,81,98,128	0
2	SO4	B	403	5/5	0.99	0.09	0.68	53,66,68,84	0
2	SO4	B	404	5/5	0.96	0.09	-0.49	71,72,97,102	0
2	SO4	A	404	5/5	0.96	0.07	-2.16	67,76,104,116	0
2	SO4	A	403	5/5	0.94	0.08	-	59,60,76,83	0
2	SO4	A	401	5/5	0.86	0.30	-	61,68,116,142	0
2	SO4	A	406	5/5	0.89	0.13	-	66,81,102,122	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SO4	B	405	5/5	0.94	0.10	-	64,79,83,114	0
2	SO4	B	406	5/5	0.87	0.27	-	83,88,140,149	0
2	SO4	A	405	5/5	0.96	0.22	-	76,97,104,114	0
2	SO4	B	401	5/5	0.92	0.18	-	59,63,103,128	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.