



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:21 AM UTC

PDB ID : 4G0I / pdb_00004g0i
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

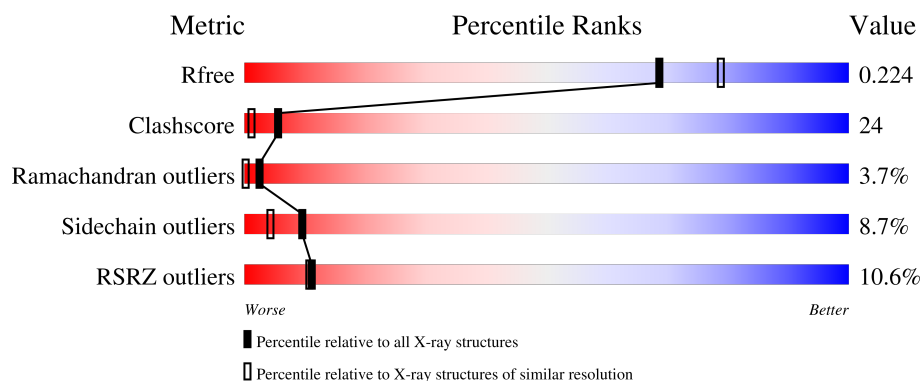
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	328	9% 55% 31% 9% .
1	B	328	12% 53% 31% 14% .

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
3	MES	A	407	-	-	X	-
3	MES	A	408	-	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 (CCD ID: SO4) (formula: O₄S).



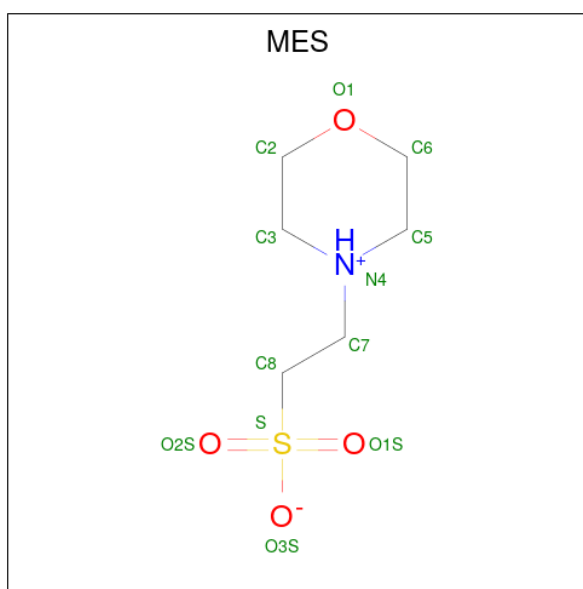
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

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 (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



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		

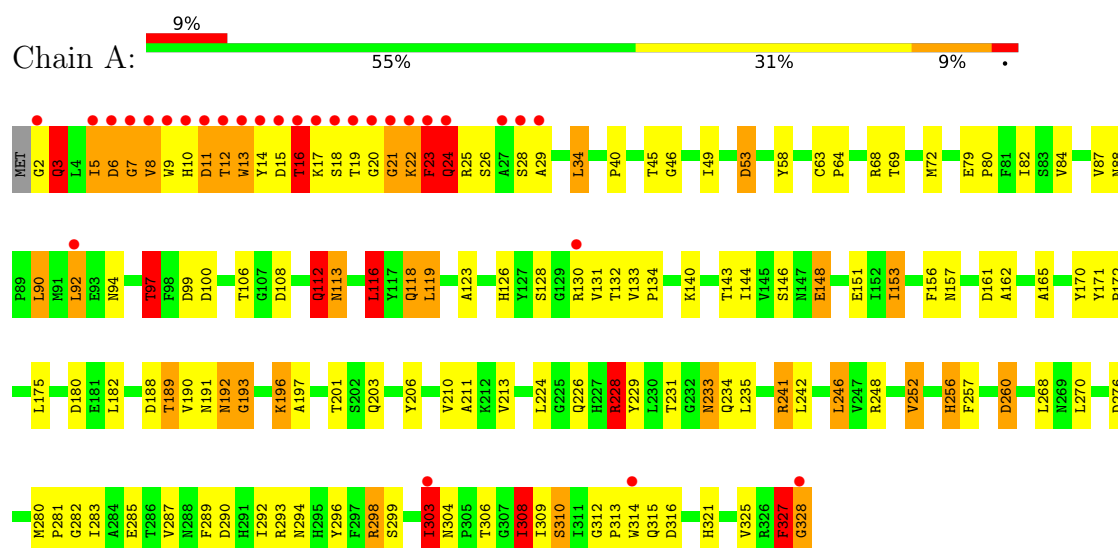
- Molecule 4 is water.

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

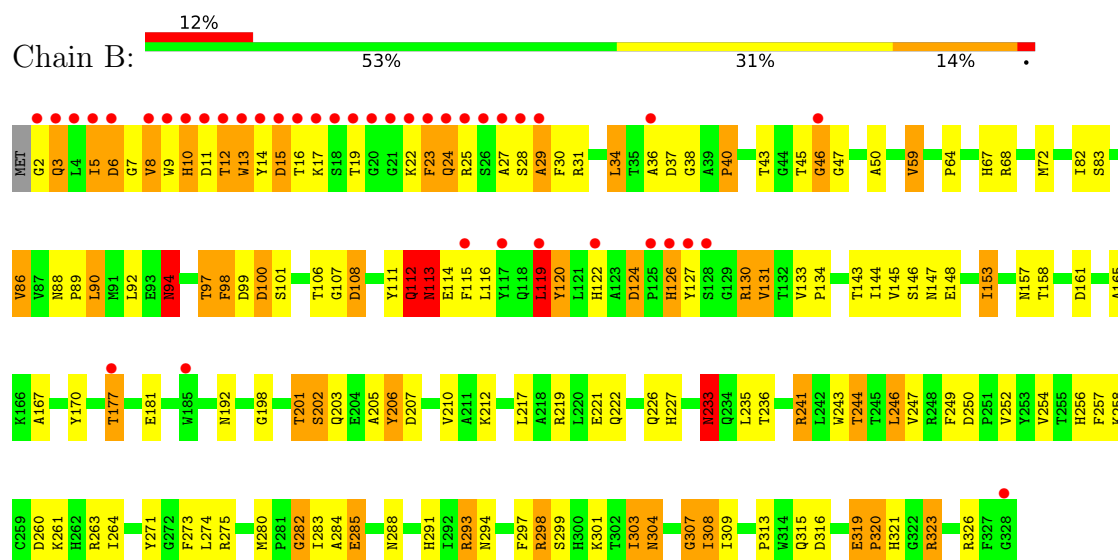
3 Residue-property plots

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

• Molecule 1: 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, α , β , γ	149.15Å 149.15Å 105.34Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.80 – 2.05 48.80 – 2.05	Depositor EDS
% Data completeness (in resolution range)	87.4 (48.80-2.05) 87.2 (48.80-2.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.66 (at 2.05Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, R_{free}	0.196 , 0.227 0.196 , 0.224	Depositor DCC
R_{free} test set	1979 reflections (2.38%)	wwPDB-VP
Wilson B-factor (Å ²)	35.6	Xtriage
Anisotropy	0.176	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5699	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, 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	1.97	55/2732 (2.0%)	1.82	72/3719 (1.9%)
1	B	1.95	58/2732 (2.1%)	1.74	47/3719 (1.3%)
All	All	1.96	113/5464 (2.1%)	1.78	119/7438 (1.6%)

All (113) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	327	PHE	C-O	14.09	1.41	1.23
1	A	213	VAL	CA-CB	-11.01	1.41	1.54
1	A	87	VAL	CA-CB	-10.65	1.40	1.54
1	A	49	ILE	CA-CB	10.08	1.65	1.54
1	B	291	HIS	CA-C	-8.55	1.42	1.52
1	B	236	THR	CA-C	-8.29	1.42	1.52
1	B	285	GLU	CD-OE2	7.93	1.40	1.25
1	B	202	SER	N-CA	-7.88	1.36	1.46
1	A	228	ARG	CD-NE	-7.86	1.35	1.46
1	B	252	VAL	CA-C	-7.84	1.42	1.52
1	B	282	GLY	C-O	-7.80	1.13	1.23
1	A	69	THR	N-CA	7.78	1.55	1.46
1	B	92	LEU	CA-C	7.71	1.58	1.53
1	B	288	ASN	C-O	7.69	1.32	1.24
1	B	283	ILE	CA-CB	-7.67	1.44	1.54
1	A	90	LEU	CA-CB	7.39	1.63	1.53
1	A	16	THR	CA-CB	7.29	1.65	1.53
1	A	113	ASN	CG-OD1	7.28	1.37	1.23
1	B	98	PHE	CA-C	-7.23	1.42	1.52
1	B	143	THR	CA-C	7.20	1.61	1.52
1	A	211	ALA	CA-CB	7.07	1.64	1.53
1	A	79	GLU	C-O	-7.01	1.17	1.24
1	B	86	VAL	CA-CB	7.01	1.62	1.54
1	B	323	ARG	CA-C	6.98	1.62	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	88	ASN	CA-C	6.94	1.61	1.53
1	B	177	THR	CA-C	6.93	1.61	1.52
1	A	290	ASP	N-CA	6.56	1.54	1.46
1	B	146	SER	C-O	6.52	1.31	1.23
1	A	153	ILE	CG1-CD1	-6.52	1.26	1.51
1	B	273	PHE	N-CA	6.49	1.54	1.46
1	A	106	THR	CA-C	6.42	1.61	1.52
1	B	90	LEU	CG-CD1	6.41	1.73	1.52
1	B	309	ILE	CA-C	6.40	1.60	1.53
1	B	233	ASN	CB-CG	6.39	1.68	1.52
1	B	274	LEU	C-O	6.37	1.31	1.24
1	B	59	VAL	CA-CB	6.32	1.64	1.54
1	A	79	GLU	CA-C	6.29	1.60	1.52
1	B	307	GLY	C-O	6.29	1.32	1.23
1	A	123	ALA	CA-C	-6.27	1.44	1.52
1	A	292	ILE	CA-CB	6.24	1.61	1.54
1	B	250	ASP	CG-OD2	6.21	1.37	1.25
1	B	284	ALA	C-O	-6.17	1.17	1.24
1	B	131	VAL	CA-C	6.16	1.59	1.53
1	B	16	THR	CA-C	6.00	1.60	1.52
1	A	143	THR	CA-CB	-6.00	1.44	1.53
1	A	133	VAL	CA-C	5.97	1.59	1.52
1	A	143	THR	CA-C	5.97	1.60	1.52
1	B	124	ASP	N-CA	5.97	1.51	1.46
1	A	188	ASP	N-CA	-5.95	1.39	1.46
1	B	260	ASP	CA-C	-5.94	1.45	1.52
1	B	254	VAL	CA-CB	5.91	1.61	1.54
1	B	16	THR	CA-CB	5.90	1.62	1.53
1	A	312	GLY	C-O	5.89	1.31	1.24
1	A	72	MET	CG-SD	5.89	1.95	1.80
1	A	260	ASP	CA-C	5.83	1.60	1.52
1	A	228	ARG	CG-CD	-5.76	1.35	1.52
1	B	12	THR	CA-CB	5.75	1.63	1.53
1	A	252	VAL	C-O	-5.74	1.17	1.24
1	B	130	ARG	CA-C	5.69	1.59	1.52
1	A	156	PHE	C-O	-5.66	1.17	1.24
1	B	94	ASN	CA-C	5.66	1.60	1.52
1	A	19	THR	CA-CB	5.66	1.62	1.53
1	A	226	GLN	N-CA	5.65	1.53	1.46
1	B	148	GLU	CD-OE2	5.64	1.36	1.25
1	B	148	GLU	CA-C	5.63	1.60	1.52
1	B	247	VAL	N-CA	-5.63	1.40	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	72	MET	SD-CE	-5.58	1.65	1.79
1	B	90	LEU	CG-CD2	5.57	1.71	1.52
1	B	126	HIS	CA-CB	5.52	1.61	1.53
1	A	296	TYR	N-CA	5.52	1.53	1.46
1	B	153	ILE	CB-CG2	5.51	1.70	1.52
1	B	261	LYS	CA-C	5.50	1.60	1.52
1	A	308	ILE	CA-C	5.50	1.59	1.52
1	A	309	ILE	CA-CB	5.50	1.60	1.53
1	B	106	THR	CA-C	5.48	1.60	1.52
1	B	280	MET	SD-CE	5.45	1.93	1.79
1	A	118	GLN	CB-CG	5.44	1.68	1.52
1	A	256	HIS	N-CA	5.43	1.52	1.46
1	A	63	CYS	CA-C	5.43	1.60	1.52
1	A	304	ASN	CA-C	5.43	1.59	1.52
1	A	196	LYS	CG-CD	5.42	1.68	1.52
1	B	161	ASP	C-O	-5.40	1.17	1.24
1	B	17	LYS	CA-C	5.39	1.59	1.52
1	A	313	PRO	CA-C	-5.38	1.46	1.52
1	A	69	THR	C-O	-5.37	1.17	1.24
1	B	50	ALA	C-O	-5.37	1.17	1.23
1	B	226	GLN	CA-C	5.35	1.59	1.52
1	A	45	THR	CA-C	5.34	1.61	1.53
1	B	67	HIS	C-O	-5.31	1.17	1.24
1	B	82	ILE	CA-CB	-5.30	1.47	1.54
1	A	180	ASP	C-O	-5.30	1.17	1.24
1	A	132	THR	CA-CB	-5.28	1.45	1.53
1	A	246	LEU	C-O	5.27	1.30	1.24
1	B	304	ASN	C-O	5.26	1.30	1.24
1	A	210	VAL	N-CA	-5.25	1.40	1.46
1	B	249	PHE	CA-CB	-5.24	1.45	1.53
1	A	294	ASN	CA-C	-5.21	1.46	1.52
1	B	147	ASN	CA-C	-5.20	1.46	1.52
1	A	34	LEU	CG-CD1	-5.19	1.35	1.52
1	A	161	ASP	CA-C	5.17	1.59	1.52
1	B	145	VAL	CA-CB	5.16	1.61	1.54
1	B	246	LEU	CA-CB	-5.16	1.45	1.53
1	B	167	ALA	CA-CB	5.15	1.61	1.53
1	B	89	PRO	C-O	5.12	1.30	1.24
1	B	285	GLU	CG-CD	5.11	1.64	1.52
1	A	84	VAL	CA-CB	5.10	1.62	1.54
1	B	243	TRP	C-O	-5.09	1.18	1.24
1	A	321	HIS	CA-CB	-5.07	1.46	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	242	LEU	CA-CB	5.06	1.61	1.53
1	A	144	ILE	CA-C	-5.04	1.46	1.52
1	A	68	ARG	N-CA	-5.04	1.40	1.46
1	B	165	ALA	CA-C	5.04	1.58	1.52
1	A	64	PRO	C-O	5.01	1.29	1.24

All (119) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	123	ALA	N-CA-C	-12.07	98.68	113.41
1	B	90	LEU	CD1-CG-CD2	-11.48	85.53	110.80
1	A	29	ALA	CA-C-N	-10.85	106.54	123.24
1	A	29	ALA	C-N-CA	-10.85	106.54	123.24
1	A	228	ARG	NE-CZ-NH1	10.02	131.52	121.50
1	A	298	ARG	N-CA-C	9.52	121.73	111.36
1	B	124	ASP	CA-C-N	-9.33	110.17	121.00
1	B	124	ASP	C-N-CA	-9.33	110.17	121.00
1	A	241	ARG	NE-CZ-NH1	9.09	130.59	121.50
1	B	192	ASN	N-CA-C	-8.89	102.35	113.55
1	A	25	ARG	N-CA-C	-8.79	102.33	113.23
1	A	189	THR	N-CA-C	-8.59	102.81	113.38
1	B	299	SER	N-CA-C	-8.28	103.77	114.04
1	A	46	GLY	CA-C-N	-8.28	109.53	122.69
1	A	46	GLY	C-N-CA	-8.28	109.53	122.69
1	A	325	VAL	CB-CA-C	-8.26	103.37	111.30
1	A	327	PHE	N-CA-C	-8.16	96.59	109.23
1	B	241	ARG	NE-CZ-NH2	-7.79	112.19	119.20
1	B	97	THR	N-CA-CB	-7.71	98.28	111.69
1	B	90	LEU	CB-CG-CD2	7.63	133.58	110.70
1	A	327	PHE	CB-CA-C	-7.58	92.74	109.56
1	B	271	TYR	N-CA-C	-7.53	102.43	111.69
1	B	37	ASP	N-CA-C	7.33	122.41	113.17
1	A	328	GLY	N-CA-C	-7.31	92.10	113.30
1	B	293	ARG	NE-CZ-NH1	-7.26	114.24	121.50
1	B	241	ARG	NE-CZ-NH1	7.24	128.74	121.50
1	A	53	ASP	N-CA-C	7.02	121.18	112.47
1	A	90	LEU	CD1-CG-CD2	-7.01	95.38	110.80
1	A	97	THR	OG1-CB-CG2	7.00	123.31	109.30
1	B	94	ASN	N-CA-C	6.96	125.63	110.80
1	A	231	THR	N-CA-C	-6.85	104.12	113.30
1	A	303	ILE	CB-CA-C	-6.82	103.70	111.55
1	A	248	ARG	NE-CZ-NH2	6.79	125.31	119.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	126	HIS	N-CA-C	-6.73	103.66	112.41
1	B	92	LEU	N-CA-C	6.71	114.28	108.78
1	A	299	SER	CA-C-N	-6.69	113.82	122.79
1	A	299	SER	C-N-CA	-6.69	113.82	122.79
1	A	94	ASN	N-CA-C	6.67	121.27	113.20
1	B	264	ILE	N-CA-C	-6.56	102.86	111.05
1	B	201	THR	N-CA-C	-6.55	105.86	114.31
1	A	327	PHE	O-C-N	6.44	130.74	123.27
1	B	46	GLY	N-CA-C	-6.43	102.76	112.41
1	A	252	VAL	CA-C-N	-6.28	110.77	120.31
1	A	252	VAL	C-N-CA	-6.28	110.77	120.31
1	A	90	LEU	CA-CB-CG	-6.22	94.52	116.30
1	A	82	ILE	CB-CA-C	-6.20	102.05	110.42
1	B	83	SER	N-CA-C	-6.19	101.35	110.52
1	B	298	ARG	N-CA-C	6.19	120.67	113.18
1	A	119	LEU	N-CA-C	-6.19	104.61	111.36
1	B	210	VAL	CA-C-N	-6.19	110.90	120.31
1	B	210	VAL	C-N-CA	-6.19	110.90	120.31
1	A	241	ARG	NE-CZ-NH2	-6.17	113.64	119.20
1	A	283	ILE	CB-CA-C	-6.15	102.98	111.65
1	A	92	LEU	N-CA-C	6.08	113.77	108.78
1	A	193	GLY	N-CA-C	-6.08	98.77	113.18
1	A	189	THR	CA-C-N	-6.03	111.12	121.97
1	A	189	THR	C-N-CA	-6.03	111.12	121.97
1	A	228	ARG	NH1-CZ-NH2	-6.01	111.48	119.30
1	B	250	ASP	CA-C-N	-5.92	113.72	119.87
1	B	250	ASP	C-N-CA	-5.92	113.72	119.87
1	B	158	THR	CB-CA-C	-5.89	101.56	109.16
1	B	10	HIS	N-CA-C	5.89	119.05	107.98
1	B	258	LYS	CA-C-N	-5.79	113.07	122.34
1	B	258	LYS	C-N-CA	-5.79	113.07	122.34
1	A	162	ALA	N-CA-C	-5.79	105.99	113.16
1	A	46	GLY	N-CA-C	-5.76	104.86	112.81
1	A	287	VAL	CA-C-N	-5.75	114.67	122.95
1	A	287	VAL	C-N-CA	-5.75	114.67	122.95
1	B	113	ASN	CB-CG-ND2	5.72	124.98	116.40
1	B	205	ALA	N-CA-C	-5.71	104.69	111.03
1	A	172	PRO	CA-C-N	-5.67	113.05	119.28
1	A	172	PRO	C-N-CA	-5.67	113.05	119.28
1	A	116	LEU	N-CA-C	-5.66	105.11	111.28
1	A	171	TYR	CA-C-N	-5.63	114.58	120.38
1	A	171	TYR	C-N-CA	-5.63	114.58	120.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	7	GLY	N-CA-C	-5.61	97.03	113.30
1	A	92	LEU	CB-CA-C	-5.60	109.00	117.07
1	B	153	ILE	N-CA-C	-5.58	103.96	111.44
1	B	221	GLU	N-CA-C	-5.58	105.35	111.82
1	B	206	TYR	CA-C-N	-5.57	112.25	120.38
1	B	206	TYR	C-N-CA	-5.57	112.25	120.38
1	A	119	LEU	CA-C-N	-5.54	112.42	120.29
1	A	119	LEU	C-N-CA	-5.54	112.42	120.29
1	A	192	ASN	CB-CA-C	-5.49	101.84	110.85
1	A	197	ALA	N-CA-C	-5.49	104.70	111.40
1	B	36	ALA	N-CA-C	-5.48	105.85	112.54
1	B	120	TYR	N-CA-C	-5.46	105.48	111.82
1	A	228	ARG	CB-CG-CD	5.39	123.70	111.30
1	B	100	ASP	N-CA-C	5.38	119.16	112.59
1	A	90	LEU	CB-CG-CD2	-5.32	94.73	110.70
1	A	148	GLU	CA-C-N	5.28	127.67	120.54
1	A	148	GLU	C-N-CA	5.28	127.67	120.54
1	A	119	LEU	CA-CB-CG	-5.28	97.83	116.30
1	A	228	ARG	CA-CB-CG	-5.25	103.59	114.10
1	B	293	ARG	CG-CD-NE	-5.25	100.44	112.00
1	B	119	LEU	CA-CB-CG	-5.24	97.94	116.30
1	A	252	VAL	CB-CA-C	-5.23	102.71	111.29
1	A	134	PRO	CA-C-N	-5.22	115.73	122.99
1	A	134	PRO	C-N-CA	-5.22	115.73	122.99
1	B	181	GLU	N-CA-C	-5.20	105.50	111.07
1	B	114	GLU	N-CA-C	-5.20	107.96	114.56
1	A	146	SER	CA-C-N	-5.16	113.10	122.50
1	A	146	SER	C-N-CA	-5.16	113.10	122.50
1	A	40	PRO	CB-CA-C	-5.16	104.22	110.98
1	B	285	GLU	N-CA-C	-5.16	106.94	113.18
1	B	97	THR	OG1-CB-CG2	5.14	119.58	109.30
1	A	268	LEU	CB-CA-C	-5.14	102.75	110.92
1	A	175	LEU	N-CA-C	-5.13	105.92	113.61
1	A	80	PRO	CB-CA-C	-5.13	104.57	111.85
1	A	310	SER	CB-CA-C	5.11	117.93	109.70
1	A	248	ARG	NE-CZ-NH1	-5.11	116.39	121.50
1	A	306	THR	N-CA-C	5.11	118.77	112.54
1	A	151	GLU	N-CA-C	-5.10	106.22	112.90
1	B	101	SER	CB-CA-C	-5.09	104.94	111.50
1	A	116	LEU	CB-CA-C	-5.08	102.37	110.79
1	B	319	GLU	CA-C-N	5.06	126.17	119.84
1	B	319	GLU	C-N-CA	5.06	126.17	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	165	ALA	N-CA-C	-5.02	103.52	110.35
1	B	59	VAL	N-CA-CB	-5.00	104.89	112.35

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	149	0
1	B	2649	0	2536	99	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	248	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 24.

All (248) 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:22:LYS:C	1:A:24:GLN:HA	1.78	1.09
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:HG3	1:A:24:GLN:CA	1.87	1.03
1:A:23:PHE:HA	1:A:24:GLN:HG3	1.43	0.99

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:TRP:C	1:A:15:ASP:HA	1.89	0.96
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:3:GLN:NE2	1:A:23:PHE:CD1	2.38	0.91
1:A:22:LYS:O	1:A:22:LYS:HE2	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:H	1:A:23:PHE:HD2	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:HG3	1:A:24:GLN:C	2.08	0.79
1:A:22:LYS:O	1:A:22:LYS:CG	2.30	0.79
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:13:TRP:O	1:A:15:ASP:CG	2.30	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:PRO:HB3	1:B:244:THR:HG23	1.67	0.74
1:A:22:LYS:C	1:A:24:GLN:CA	2.59	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:12:THR:C	1:A:14:TYR:HD2	1.98	0.71
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:22:LYS:C	1:A:22:LYS:HE2	2.17	0.69
1:A:22:LYS:HG3	1:A:22:LYS:O	1.91	0.68
1:A:234:GLN:OE1	3:A:408:MES:H71	1.94	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:B:40:PRO:HD3	1:B:46:GLY:HA3	1.77	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
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: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:A:112:GLN:CD	1:A:112:GLN:N	2.57	0.62
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:6:ASP:O	1:B:126:HIS:C	2.44	0.59
1:A:11:ASP:C	1:A:12:THR:HG1	2.08	0.59
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:206:TYR:O	1:B:207:ASP:C	2.41	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: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:A:10:HIS:C	1:A:12:THR:H	2.13	0.56
1:B:6:ASP:N	1:B:7:GLY:CA	2.65	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
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:A:315:GLN:OE1	4:A:564:HOH:O	2.18	0.55
1:B:198:GLY:O	1:B:303:ILE:CD1	2.53	0.55
1:A:97:THR:HG22	1:A:99:ASP:H	1.70	0.54
1:A:23:PHE:N	1:A:24:GLN:HA	2.20	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:9:TRP:HE1	1:B:94:ASN:HA	1.72	0.53
1:A:15:ASP:CG	1:A:16:THR:H	2.10	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:22:LYS:O	1:A:23:PHE:C	2.53	0.52
1:A:228:ARG:HD2	1:A:229:TYR:CZ	2.44	0.52
1:B:108:ASP:C	1:B:108:ASP:OD1	2.51	0.52
1:A:228:ARG:HD3	1:A:276:ASP:OD2	2.10	0.52
1:A:22:LYS:CG	1:A:24:GLN:C	2.78	0.52
1:A:241:ARG:HD2	4:A:615:HOH:O	2.09	0.52
1:B:5:ILE:HG22	1:B:6:ASP:N	2.24	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:A:10:HIS:C	1:A:12:THR:N	2.67	0.50
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: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:B:12:THR:O	1:B:14:TYR:CD2	2.66	0.49
1:A:13:TRP:O	1:A:15:ASP:OD1	2.30	0.49
1:B:24:GLN:HG2	1:B:25:ARG:HG3	1.95	0.49
1:B:304:ASN:HD21	1:B:308:ILE:N	2.11	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: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:A:206:TYR:CD2	1:A:206:TYR:C	2.92	0.48
1:B:319:GLU:OE2	1:B:320:PRO:HD2	2.13	0.48
1:A:92:LEU:N	1:A:92:LEU:HD22	2.29	0.48
1:A:190:VAL:O	1:A:192:ASN:N	2.46	0.48
1:B:59:VAL:O	1:B:86:VAL:HA	2.13	0.48
1:A:140:LYS:NZ	4:A:595:HOH:O	2.42	0.48
1:A:203:GLN:H	3:A:407:MES:C7	2.25	0.48
1:A:12:THR:C	1:A:14:TYR:N	2.72	0.47
1:A:260:ASP:O	1:B:263[A]:ARG:NH2	2.48	0.47
1:A:233:ASN:C	1:A:233:ASN:HD22	2.22	0.47
1:B:14:TYR:HA	1:B:15:ASP:HB2	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:308:ILE:HD13	1:B:203:GLN:HA	1.96	0.47
1:B:98:PHE:CD2	1:B:108:ASP:N	2.83	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:A:116:LEU:HD13	1:A:131:VAL:HG12	1.97	0.46
1:B:130:ARG:HG2	4:B:625:HOH:O	2.14	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: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: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:233:ASN:ND2	1:A:233:ASN:C	2.74	0.45
1:A:190:VAL:C	1:A:192:ASN:N	2.73	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:112:GLN:N	1:B:112:GLN:CD	2.74	0.44
1:A:99:ASP:OD2	1:A:99:ASP:C	2.61	0.44
1:B:5:ILE:HG22	1:B:8:VAL:HB	2.00	0.44
1:A:12:THR:C	1:A:14:TYR:H	2.21	0.44
1:A:11:ASP:C	1:A:12:THR:OG1	2.57	0.44
1:B:19:THR:HG22	1:B:19:THR:O	2.18	0.44
1:B:30:PHE:HB3	1:B:144:ILE:HG22	1.99	0.44
1:B:94:ASN:OD1	1:B:115:PHE:CZ	2.71	0.44
1:B:111:TYR:O	1:B:112:GLN:HG2	2.17	0.44
1:B:282:GLY:HA2	1:B:285:GLU:CD	2.43	0.43
1:B:177:THR:HG22	4:B:546:HOH:O	2.18	0.43
1:A:12:THR:CA	1:A:14:TYR:HD2	2.31	0.43
3:A:408:MES:H52	3:A:408:MES:H81	1.20	0.43
1:B:3:GLN:HE22	1:B:23:PHE:HE1	1.65	0.43
1:A:15:ASP:O	1:A:16:THR:C	2.61	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:SER:HB2	1:B:31:ARG:HG3	2.01	0.42
1:A:316:ASP:OD1	1:A:316:ASP:C	2.62	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:A:327:PHE:C	1:A:328:GLY:O	2.55	0.41
1:B:113:ASN:ND2	1:B:119:LEU:HG	2.35	0.41
1:B:217:LEU:HD23	1:B:217:LEU:HA	1.59	0.41
1:A:58:TYR:CE2	1:A:119:LEU:HD13	2.56	0.41
1:B:293:ARG:HH11	1:B:293:ARG:HD3	1.63	0.41
1:A:92:LEU:HD13	1:A:92:LEU:HA	1.86	0.41
1:B:68:ARG:CZ	1:B:241:ARG:HG2	2.51	0.41
1:B:256:HIS:HD2	1:B:257:PHE:CD1	2.38	0.41
1:A:12:THR:C	1:A:14:TYR:CD2	2.83	0.41
1:B:34:LEU:HA	1:B:34:LEU:HD12	1.73	0.41
1:B:124:ASP:C	1:B:124:ASP:OD1	2.63	0.41
1:A:100:ASP:OD1	1:A:100:ASP:N	2.51	0.41
1:B:256:HIS:CD2	1:B:257:PHE:CD1	3.09	0.40
1:B:94:ASN:OD1	1:B:115:PHE:CE1	2.74	0.40
1:A:303:ILE:HG21	1:A:303:ILE:HD13	1.67	0.40
1:B:30:PHE:CD2	1:B:30:PHE:N	2.88	0.40
1:B:120:TYR:CD2	1:B:131:VAL:HG13	2.56	0.40
1:A:2:GLY:HA2	1:A:9:TRP:CH2	2.57	0.40
1:A:192:ASN:O	1:A:192:ASN:ND2	2.54	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%)	2	0
1	B	326/328 (99%)	289 (89%)	26 (8%)	11 (3%)	3	0
All	All	652/656 (99%)	577 (88%)	51 (8%)	24 (4%)	2	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%)	254 (91%)	24 (9%)	10	4
1	B	278/278 (100%)	254 (91%)	24 (9%)	10	4
All	All	556/556 (100%)	508 (91%)	48 (9%)	9	4

All (48) 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	22	LYS
1	A	23	PHE
1	A	24	GLN
1	A	34	LEU
1	A	53	ASP
1	A	90	LEU
1	A	97	THR
1	A	112	GLN
1	A	116	LEU
1	A	130	ARG
1	A	153	ILE
1	A	182	LEU
1	A	201	THR
1	A	228	ARG
1	A	233	ASN
1	A	246	LEU
1	A	298	ARG
1	A	303	ILE
1	A	308	ILE
1	A	310	SER
1	A	327	PHE
1	B	5	ILE
1	B	6	ASP
1	B	13	TRP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	22	LYS
1	B	23	PHE
1	B	34	LEU
1	B	40	PRO
1	B	72	MET
1	B	90	LEU
1	B	100	ASP
1	B	112	GLN
1	B	116	LEU
1	B	119	LEU
1	B	153	ILE
1	B	201	THR
1	B	202	SER
1	B	212	LYS
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	HIS
1	A	142	HIS
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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 oligosaccharides 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	B	406	-	4,4,4	0.72	0	6,6,6	0.37	0
2	SO4	B	403	-	4,4,4	0.55	0	6,6,6	1.13	0
2	SO4	A	406	-	4,4,4	0.71	0	6,6,6	1.00	0
2	SO4	A	401	-	4,4,4	1.02	0	6,6,6	0.38	0
2	SO4	B	405	-	4,4,4	0.73	0	6,6,6	0.90	0
2	SO4	B	402	-	4,4,4	0.60	0	6,6,6	1.26	1 (16%)
2	SO4	A	402	-	4,4,4	0.78	0	6,6,6	1.60	1 (16%)
2	SO4	A	403	-	4,4,4	0.73	0	6,6,6	1.74	2 (33%)
3	MES	A	408	-	12,12,12	2.21	6 (50%)	15,16,16	4.05	8 (53%)
2	SO4	B	404	-	4,4,4	0.09	0	6,6,6	0.44	0
2	SO4	A	404	-	4,4,4	0.06	0	6,6,6	0.59	0
3	MES	A	407	-	12,12,12	2.01	2 (16%)	15,16,16	2.84	8 (53%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	A	405	-	4,4,4	0.48	0	6,6,6	0.50	0
3	MES	B	407	-	12,12,12	1.54	3 (25%)	15,16,16	3.27	9 (60%)
2	SO4	B	401	-	4,4,4	0.81	0	6,6,6	1.47	2 (33%)

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
3	MES	A	407	-	-	1/6/14/14	0/1/1/1
3	MES	A	408	-	-	4/6/14/14	0/1/1/1
3	MES	B	407	-	-	4/6/14/14	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	407	MES	C8-S	-4.75	1.70	1.77
3	A	408	MES	O1S-S	4.23	1.57	1.45
3	B	407	MES	C8-S	-3.60	1.72	1.77
3	A	408	MES	C8-S	-3.29	1.73	1.77
3	A	408	MES	C5-C6	2.68	1.60	1.50
3	A	407	MES	O1S-S	2.47	1.52	1.45
3	A	408	MES	C3-N4	2.43	1.53	1.46
3	A	408	MES	O1-C6	2.32	1.51	1.42
3	B	407	MES	O2S-S	2.31	1.51	1.45
3	B	407	MES	O1S-S	2.16	1.51	1.45
3	A	408	MES	C3-C2	2.04	1.58	1.50

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	408	MES	O1S-S-C8	9.61	121.25	106.73
3	A	408	MES	C5-N4-C3	8.49	127.12	108.84
3	B	407	MES	C5-N4-C3	7.61	125.23	108.84
3	B	407	MES	O1S-S-C8	6.72	116.89	106.73
3	A	407	MES	C5-N4-C3	5.27	120.19	108.84
3	A	407	MES	O2S-S-C8	5.00	114.28	106.73
3	A	408	MES	O1-C6-C5	4.41	121.26	111.77
3	A	407	MES	O1-C2-C3	4.23	120.88	111.77
3	A	408	MES	C7-N4-C3	4.12	122.22	111.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	407	MES	O2S-S-O1S	-3.38	102.82	113.82
3	B	407	MES	C6-O1-C2	3.25	120.40	109.88
3	A	407	MES	C7-N4-C5	3.22	119.83	111.24
3	A	407	MES	C7-N4-C3	3.14	119.62	111.24
2	A	403	SO4	O3-S-O1	-3.02	93.76	109.56
3	A	408	MES	O2S-S-O1S	-3.00	104.08	113.82
3	A	408	MES	O3S-S-O2S	-2.90	104.13	111.40
3	A	408	MES	O2S-S-C8	2.90	111.11	106.73
3	B	407	MES	C7-N4-C5	2.84	118.81	111.24
2	A	403	SO4	O3-S-O2	2.77	124.05	109.56
2	B	401	SO4	O3-S-O1	-2.77	95.09	109.56
3	B	407	MES	O2S-S-C8	2.73	110.85	106.73
3	A	408	MES	C6-O1-C2	2.47	117.87	109.88
2	B	402	SO4	O4-S-O1	-2.41	96.95	109.56
3	A	407	MES	O3S-S-O2S	-2.41	105.37	111.40
3	A	407	MES	O2S-S-O1S	-2.32	106.28	113.82
3	A	407	MES	C6-C5-N4	2.31	113.63	110.12
2	A	402	SO4	O4-S-O1	-2.29	97.57	109.56
2	B	401	SO4	O4-S-O1	2.19	121.01	109.56
3	B	407	MES	O1-C6-C5	2.12	116.33	111.77
3	B	407	MES	O3S-S-O1S	-2.06	106.25	111.40
3	B	407	MES	C2-C3-N4	2.04	113.21	110.12

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	407	MES	C8-C7-N4-C5
3	A	408	MES	C8-C7-N4-C5
3	A	408	MES	C7-C8-S-O2S
3	A	408	MES	C7-C8-S-O3S
3	B	407	MES	C7-C8-S-O2S
3	B	407	MES	C7-C8-S-O3S
3	B	407	MES	C8-C7-N4-C3
3	A	408	MES	C7-C8-S-O1S
3	B	407	MES	C7-C8-S-O1S

There are no ring outliers.

3 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	408	MES	5	0
3	A	407	MES	6	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	327/328 (99%)	0.17	29 (8%) 15 15	19, 40, 82, 143	1 (0%)
1	B	327/328 (99%)	0.52	40 (12%) 8 7	18, 46, 109, 169	1 (0%)
All	All	654/656 (99%)	0.35	69 (10%) 11 11	18, 43, 99, 169	2 (0%)

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	23	PHE	7.9
1	B	23	PHE	7.9
1	B	16	THR	6.3
1	B	13	TRP	6.3
1	A	14	TYR	5.7
1	B	5	ILE	5.5
1	A	13	TRP	5.2
1	B	12	THR	5.1
1	B	14	TYR	5.0
1	B	8	VAL	4.9
1	B	328	GLY	4.9
1	B	22	LYS	4.9
1	A	19	THR	4.8
1	A	20	GLY	4.7
1	A	12	THR	4.7
1	A	16	THR	4.7
1	B	10	HIS	4.7
1	B	26	SER	4.6
1	B	17	LYS	4.5
1	B	27	ALA	4.5
1	A	2	GLY	4.5
1	A	18	SER	4.3
1	B	28	SER	4.2
1	B	19	THR	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	11	ASP	4.0
1	A	22	LYS	3.8
1	A	8	VAL	3.8
1	B	9	TRP	3.7
1	A	15	ASP	3.7
1	A	328	GLY	3.6
1	A	11	ASP	3.6
1	B	126	HIS	3.5
1	A	5	ILE	3.4
1	B	21	GLY	3.4
1	A	17	LYS	3.3
1	B	18	SER	3.3
1	A	21	GLY	3.2
1	A	29	ALA	3.1
1	B	15	ASP	3.1
1	B	2	GLY	3.0
1	B	117	TYR	3.0
1	B	6	ASP	3.0
1	B	119	LEU	3.0
1	A	28	SER	2.9
1	B	20	GLY	2.9
1	A	10	HIS	2.9
1	B	122	HIS	2.9
1	A	303	ILE	2.8
1	B	24	GLN	2.8
1	B	29	ALA	2.8
1	B	36	ALA	2.7
1	A	314	TRP	2.7
1	A	7	GLY	2.5
1	A	27	ALA	2.5
1	B	177	THR	2.5
1	A	24	GLN	2.5
1	A	6	ASP	2.4
1	B	125	PRO	2.4
1	B	3	GLN	2.4
1	B	25	ARG	2.4
1	A	9	TRP	2.4
1	B	4	LEU	2.3
1	B	46	GLY	2.2
1	A	92	LEU	2.2
1	B	127	TYR	2.1
1	B	115	PHE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	130	ARG	2.1
1	B	128	SER	2.0
1	B	185	TRP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MES	B	407	12/12	0.66	0.32	62,118,129,148	0
3	MES	A	407	12/12	0.67	0.22	49,101,133,157	0
2	SO4	B	406	5/5	0.69	0.14	83,88,140,149	0
3	MES	A	408	12/12	0.73	0.25	37,84,93,116	0
2	SO4	A	401	5/5	0.78	0.13	61,68,116,142	0
2	SO4	B	401	5/5	0.78	0.12	59,63,103,128	0
2	SO4	A	405	5/5	0.79	0.08	76,97,104,114	0
2	SO4	A	402	5/5	0.84	0.12	51,86,93,142	0
2	SO4	A	406	5/5	0.86	0.09	66,81,102,122	0
2	SO4	A	403	5/5	0.88	0.12	59,60,76,83	0
2	SO4	B	405	5/5	0.88	0.07	64,79,83,114	0
2	SO4	B	402	5/5	0.90	0.12	39,81,98,128	0
2	SO4	A	404	5/5	0.90	0.09	67,76,104,116	0
2	SO4	B	404	5/5	0.93	0.09	71,72,97,102	0
2	SO4	B	403	5/5	0.95	0.08	53,66,68,84	0

6.5 Other polymers [i](#)

There are no such residues in this entry.