



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 09:02 pm GMT

PDB ID : 4G0K  
Title : Glutathionyl-hydroquinone reductase, YqjG, of E.coli complexed with GS-menadione  
Authors : Green, A.R.; Hayes, R.P.; Xun, L.; Kang, C.  
Deposited on : 2012-07-09  
Resolution : 2.56 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

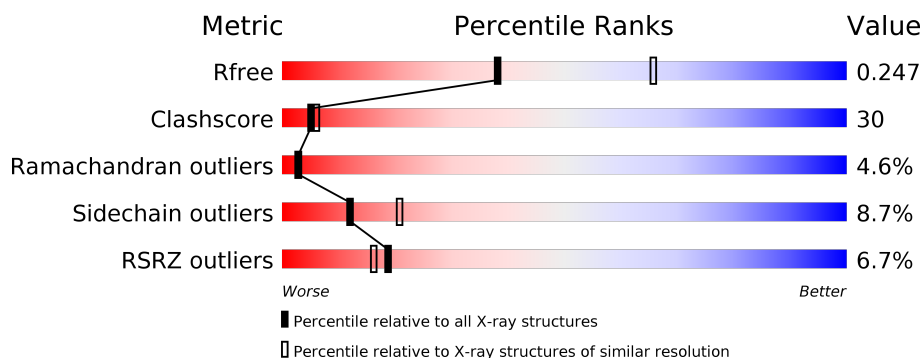
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.56 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))
$R_{free}$	100719	3689 (2.60-2.52)
Clashscore	112137	4096 (2.60-2.52)
Ramachandran outliers	110173	4037 (2.60-2.52)
Sidechain outliers	110143	4037 (2.60-2.52)
RSRZ outliers	101464	3700 (2.60-2.52)

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>6%</div> <div>55%</div> <div>35%</div> <div>8%</div> </div>
1	B	328	<div> <div>7%</div> <div>57%</div> <div>35%</div> <div>6%</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
2	SO4	B	408	-	-	X	-
3	MES	A	408	-	-	-	X
3	MES	A	409	-	-	-	X
3	MES	A	410	-	-	-	X
3	MES	B	409	-	-	-	X
4	OVS	A	411	-	-	X	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5616 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
			2644	1698	453	486	7			
1	B	327	Total	C	N	O	S	0	1	0
			2644	1698	453	486	7			

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



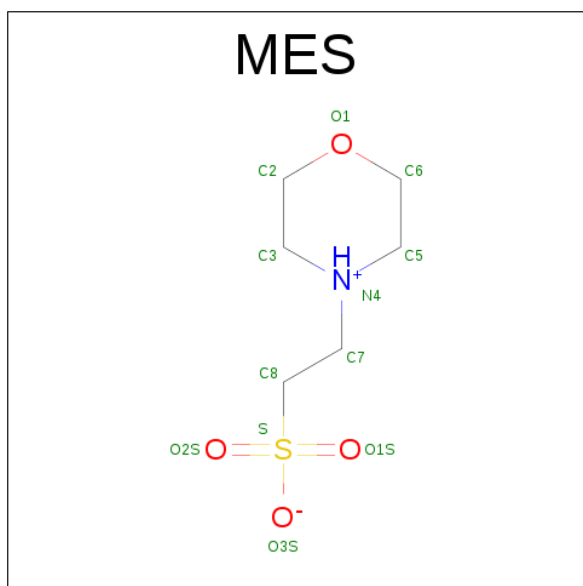
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

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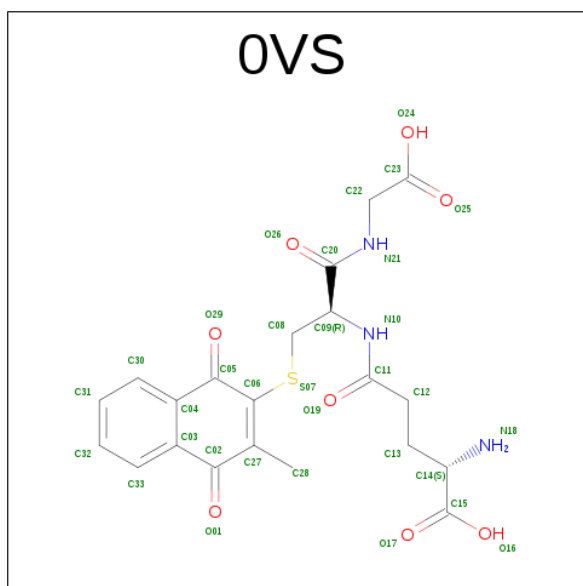
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	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	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 L-GAMMA-GLUTAMYL-S-(3-METHYL-1,4-DIOXO-1,4-DIHYDRO NAPHTHALEN-2-YL)-L-CYSTEINYLGLYCINE (three-letter code: 0VS) (formula:  $C_{21}H_{23}N_3O_8S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			33	21	3	8	1		
4	B	1	Total	C	N	O	S	0	0
			33	21	3	8	1		

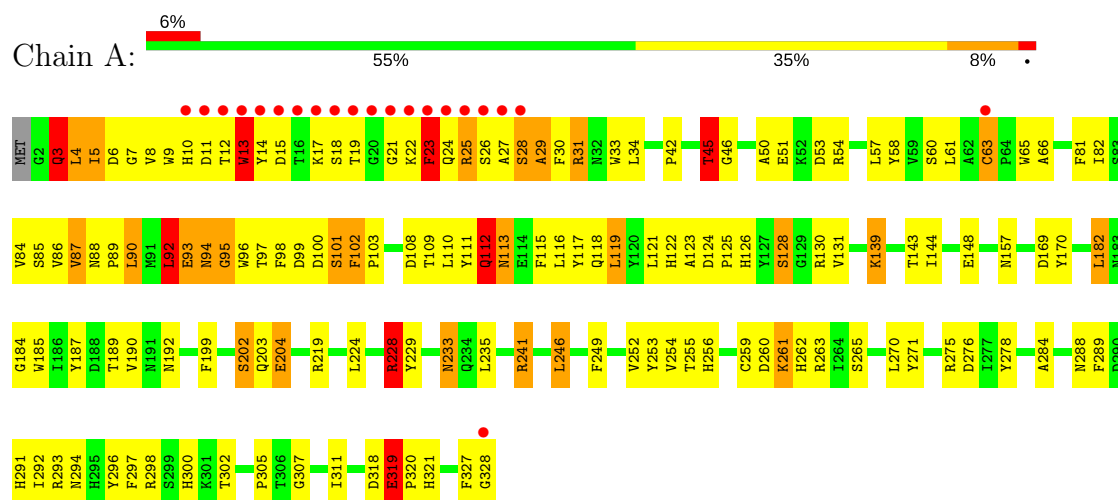
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	79	Total	O	0	0
			79	79		
5	B	60	Total	O	0	0
			60	60		

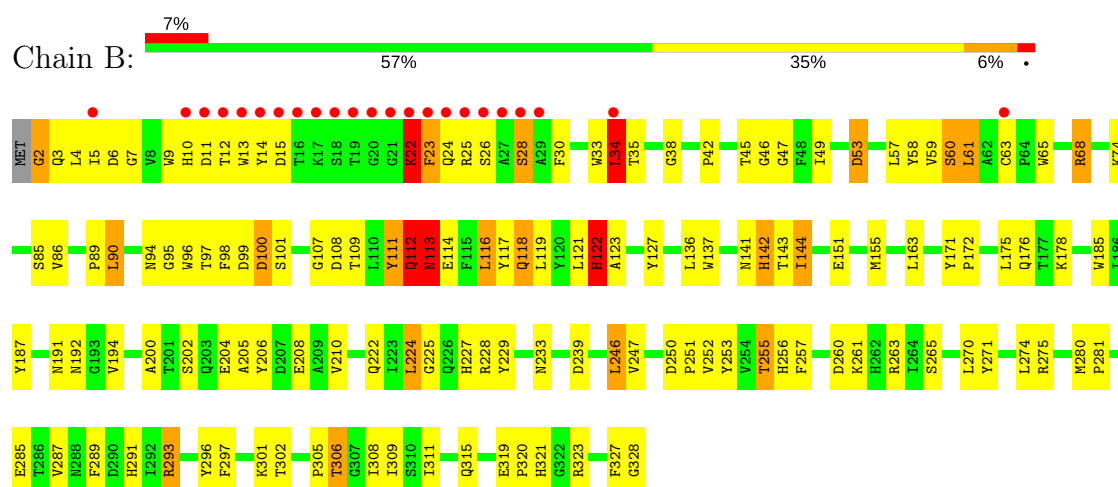
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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, $\alpha$ , $\beta$ , $\gamma$	148.41Å 148.41Å 105.17Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.67 – 2.56 48.67 – 2.56	Depositor EDS
% Data completeness (in resolution range)	91.2 (48.67-2.56) 91.3 (48.67-2.56)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.93 (at 2.54Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, $R_{free}$	0.191 , 0.238 0.189 , 0.247	Depositor DCC
$R_{free}$ test set	1706 reflections (4.78%)	DCC
Wilson B-factor (Å <sup>2</sup> )	46.4	Xtriage
Anisotropy	0.154	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 54.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.024 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5616	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.14% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: 0VS, 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	1.34	12/2727 (0.4%)	1.17	16/3714 (0.4%)
1	B	1.31	12/2727 (0.4%)	1.18	14/3714 (0.4%)
All	All	1.32	24/5454 (0.4%)	1.18	30/7428 (0.4%)

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	204	GLU	CD-OE1	18.39	1.45	1.25
1	A	204	GLU	CD-OE2	16.90	1.44	1.25
1	B	204	GLU	CD-OE2	15.92	1.43	1.25
1	B	204	GLU	CD-OE1	13.95	1.41	1.25
1	A	185	TRP	CB-CG	-10.37	1.31	1.50
1	B	185	TRP	CB-CG	-10.27	1.31	1.50
1	B	204	GLU	CB-CG	9.62	1.70	1.52
1	A	63[A]	CYS	CB-SG	-8.76	1.67	1.82
1	A	63[B]	CYS	CB-SG	-8.76	1.67	1.82
1	B	204	GLU	CG-CD	8.56	1.64	1.51
1	A	319	GLU	CG-CD	8.18	1.64	1.51
1	A	204	GLU	CG-CD	7.79	1.63	1.51
1	A	259	CYS	CB-SG	-7.03	1.70	1.82
1	B	233	ASN	CB-CG	6.75	1.66	1.51
1	A	204	GLU	CB-CG	6.55	1.64	1.52
1	A	319	GLU	CD-OE2	6.34	1.32	1.25
1	A	84	VAL	CB-CG2	6.14	1.65	1.52
1	B	113	ASN	CB-CG	6.13	1.65	1.51
1	B	113	ASN	CG-OD1	6.03	1.37	1.24
1	A	148	GLU	CD-OE2	5.92	1.32	1.25
1	B	90	LEU	CG-CD2	5.66	1.72	1.51
1	B	2	GLY	C-O	5.52	1.32	1.23
1	B	247	VAL	CB-CG1	-5.28	1.41	1.52
1	B	247	VAL	CA-CB	5.17	1.65	1.54

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	293	ARG	NE-CZ-NH1	-9.18	115.71	120.30
1	A	34	LEU	CB-CG-CD2	-8.88	95.91	111.00
1	A	228	ARG	NE-CZ-NH1	7.89	124.25	120.30
1	A	228	ARG	NE-CZ-NH2	-7.73	116.43	120.30
1	B	263	ARG	NE-CZ-NH2	-7.41	116.59	120.30
1	B	228	ARG	NE-CZ-NH1	-7.20	116.70	120.30
1	A	113	ASN	CB-CA-C	-7.08	96.24	110.40
1	B	260	ASP	CB-CG-OD1	6.93	124.54	118.30
1	A	57	LEU	CB-CG-CD2	-6.58	99.81	111.00
1	B	250	ASP	CB-CG-OD2	6.53	124.17	118.30
1	A	92	LEU	CA-CB-CG	6.39	129.99	115.30
1	B	250	ASP	CB-CG-OD1	-6.38	112.55	118.30
1	A	90	LEU	N-CA-CB	-6.27	97.86	110.40
1	B	34	LEU	CB-CG-CD1	-6.15	100.54	111.00
1	A	31	ARG	NE-CZ-NH2	-6.05	117.28	120.30
1	B	61	LEU	CB-CG-CD2	-5.97	100.85	111.00
1	B	53	ASP	CB-CG-OD1	-5.91	112.99	118.30
1	B	57	LEU	CB-CG-CD2	-5.91	100.96	111.00
1	A	241	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	A	90	LEU	CA-CB-CG	-5.75	102.08	115.30
1	A	263	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	A	139	LYS	CD-CE-NZ	5.43	124.18	111.70
1	A	219	ARG	NE-CZ-NH1	-5.40	117.60	120.30
1	B	155	MET	CG-SD-CE	-5.37	91.61	100.20
1	A	45	THR	CB-CA-C	-5.35	97.16	111.60
1	A	182	LEU	CA-CB-CG	5.32	127.54	115.30
1	B	163	LEU	CB-CG-CD2	-5.28	102.03	111.00
1	B	224	LEU	CA-CB-CG	5.16	127.17	115.30
1	B	68	ARG	NE-CZ-NH1	-5.07	117.77	120.30
1	A	219	ARG	NE-CZ-NH2	5.02	122.81	120.30

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	2644	0	2530	173	0
1	B	2644	0	2530	143	0
2	A	35	0	0	0	0
2	B	40	0	0	2	0
3	A	36	0	36	12	0
3	B	12	0	12	0	0
4	A	33	0	21	10	0
4	B	33	0	21	4	0
5	A	79	0	0	8	2
5	B	60	0	0	8	2
All	All	5616	0	5150	314	2

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 30.

All (314) 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:63[A]:CYS:SG	1:A:66:ALA:HB3	1.84	1.17
1:A:26:SER:HB2	1:A:128:SER:O	1.44	1.16
1:A:27:ALA:O	1:A:29:ALA:N	1.89	1.05
1:A:22:LYS:C	1:A:23:PHE:CD1	2.30	1.05
1:B:85:SER:OG	1:B:109:THR:HG22	1.55	1.02
1:B:255:THR:CG2	5:B:511:HOH:O	2.06	1.01
1:B:255:THR:HG23	5:B:511:HOH:O	1.61	1.00
1:A:131:VAL:HG12	1:A:131:VAL:O	1.61	0.99
1:A:260:ASP:OD2	1:B:255:THR:HG21	1.63	0.98
1:A:23:PHE:HA	1:A:24:GLN:HB2	1.44	0.97
1:B:97:THR:HG22	1:B:99:ASP:H	1.28	0.96
1:B:24:GLN:HG2	1:B:25:ARG:HG3	1.50	0.93
1:A:22:LYS:C	1:A:23:PHE:HD1	1.72	0.91
1:A:26:SER:CB	1:A:128:SER:O	2.17	0.91
1:A:63[A]:CYS:SG	1:A:66:ALA:CB	2.59	0.90
1:A:97:THR:HG22	1:A:99:ASP:H	1.37	0.87
1:A:22:LYS:O	1:A:23:PHE:HD1	1.58	0.86
1:B:100:ASP:OD1	1:B:101:SER:N	2.10	0.84
1:B:321:HIS:CD2	1:B:323:ARG:H	1.96	0.83
1:A:318:ASP:OD1	5:A:544:HOH:O	1.95	0.83
1:A:27:ALA:C	1:A:29:ALA:H	1.78	0.83
1:A:199:PHE:HZ	1:A:300:HIS:HD1	1.23	0.82
1:A:327:PHE:HB3	1:A:328:GLY:HA3	1.59	0.82
1:A:24:GLN:H	1:A:27:ALA:H	1.24	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:ASP:CG	1:B:101:SER:H	1.84	0.81
1:A:260:ASP:O	1:A:261:LYS:CB	2.29	0.80
1:B:34:LEU:HD12	1:B:34:LEU:C	2.02	0.80
1:B:4:LEU:HD13	1:B:117:TYR:HB2	1.64	0.78
1:B:321:HIS:HD2	1:B:323:ARG:H	1.30	0.77
1:A:89:PRO:HG3	1:A:291:HIS:ND1	1.99	0.77
1:B:113:ASN:ND2	1:B:118:GLN:HB3	1.99	0.77
1:A:97:THR:CG2	1:A:99:ASP:H	1.97	0.76
1:A:51:GLU:O	5:A:548:HOH:O	2.02	0.76
1:A:202:SER:HB2	3:A:409:MES:O2S	1.85	0.76
1:B:111:TYR:HE2	1:B:137:TRP:CZ2	2.03	0.76
1:A:199:PHE:HZ	1:A:300:HIS:ND1	1.83	0.76
1:B:9:TRP:HE1	1:B:94:ASN:HA	1.51	0.76
1:A:260:ASP:O	1:A:261:LYS:HB2	1.87	0.74
1:A:9:TRP:CZ2	1:A:94:ASN:HA	2.23	0.74
1:B:202:SER:HB2	2:B:408:SO4:O2	1.87	0.74
1:B:60:SER:OG	5:B:507:HOH:O	2.06	0.74
1:B:256:HIS:HD2	1:B:257:PHE:CE1	2.07	0.73
1:B:306:THR:HB	1:B:308:ILE:HG12	1.71	0.73
1:B:5:ILE:HD12	1:B:10:HIS:CD2	2.25	0.72
1:A:24:GLN:C	1:A:26:SER:H	1.91	0.72
3:A:408:MES:H51	3:A:408:MES:O3S	1.90	0.72
1:B:224:LEU:HD12	1:B:270:LEU:HD23	1.72	0.71
1:B:97:THR:HG22	1:B:99:ASP:N	2.04	0.71
1:B:122:HIS:O	1:B:122:HIS:ND1	2.24	0.70
1:A:131:VAL:CG1	1:A:131:VAL:O	2.36	0.70
1:A:130:ARG:HD2	4:A:411:OVS:O24	1.91	0.70
1:A:27:ALA:C	1:A:29:ALA:N	2.41	0.70
1:B:33:TRP:CE2	1:B:42:PRO:HD2	2.27	0.70
1:A:113:ASN:O	5:A:538:HOH:O	2.09	0.69
1:B:256:HIS:HD2	1:B:257:PHE:CD1	2.10	0.69
1:A:30:PHE:C	1:A:31:ARG:HG2	2.11	0.69
1:A:45:THR:HG22	1:A:46:GLY:H	1.58	0.69
1:B:111:TYR:O	1:B:113:ASN:N	2.23	0.69
1:A:24:GLN:O	1:A:27:ALA:N	2.27	0.68
1:A:23:PHE:N	1:A:23:PHE:CD1	2.62	0.68
1:A:130:ARG:CD	4:A:411:OVS:O24	2.42	0.67
1:A:284:ALA:HB2	5:A:517:HOH:O	1.93	0.67
1:A:184:GLY:HA2	3:A:410:MES:H61	1.77	0.67
1:A:327:PHE:CB	1:A:328:GLY:HA3	2.22	0.67
1:A:108:ASP:HB3	1:A:112:GLN:HA	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:ASN:H	1:A:233:ASN:HD22	1.42	0.67
1:A:9:TRP:CE2	1:A:94:ASN:HA	2.29	0.67
1:A:110:LEU:HB3	1:A:111:TYR:CE1	2.30	0.67
1:B:275:ARG:HG3	1:B:275:ARG:HH11	1.58	0.67
1:A:24:GLN:C	1:A:26:SER:N	2.43	0.67
1:B:113:ASN:HB3	1:B:118:GLN:OE1	1.94	0.67
1:A:60:SER:HB3	1:A:63[A]:CYS:SG	2.34	0.66
1:A:9:TRP:NE1	1:A:94:ASN:HA	2.11	0.66
1:B:256:HIS:CD2	1:B:257:PHE:CE1	2.85	0.65
1:A:111:TYR:CD1	1:A:111:TYR:N	2.62	0.65
1:B:137:TRP:CE3	1:B:144:ILE:HD13	2.32	0.65
1:A:278:TYR:O	5:A:517:HOH:O	2.14	0.65
1:A:260:ASP:O	1:B:311:ILE:CG2	2.44	0.65
1:B:111:TYR:CD1	1:B:111:TYR:N	2.61	0.64
1:B:30:PHE:HB3	1:B:144:ILE:CG2	2.27	0.64
1:B:30:PHE:HB3	1:B:144:ILE:HG21	1.78	0.64
1:A:24:GLN:O	1:A:26:SER:N	2.30	0.64
1:A:100:ASP:O	5:A:537:HOH:O	2.15	0.63
1:B:255:THR:HG22	5:B:511:HOH:O	1.84	0.62
1:B:9:TRP:NE1	1:B:94:ASN:HA	2.14	0.61
1:B:74:LYS:HE3	1:B:285:GLU:OE1	2.00	0.61
1:A:115:PHE:CB	1:A:117:TYR:CE2	2.84	0.61
1:A:235:LEU:H	3:A:408:MES:H31	1.65	0.61
1:B:108:ASP:OD1	1:B:108:ASP:C	2.39	0.61
1:B:2:GLY:CA	1:B:9:TRP:CH2	2.84	0.60
1:A:256:HIS:HB2	1:A:297:PHE:CE1	2.36	0.60
1:B:121:LEU:C	1:B:123:ALA:H	2.05	0.60
1:A:229:TYR:OH	5:A:549:HOH:O	2.12	0.60
1:B:321:HIS:HD2	1:B:323:ARG:HB2	1.67	0.60
1:B:112:GLN:CD	1:B:112:GLN:H	2.04	0.59
1:A:110:LEU:HB3	1:A:111:TYR:CD1	2.37	0.59
1:A:305:PRO:HG3	1:B:305:PRO:CG	2.33	0.59
1:A:3:GLN:HG2	1:A:14:TYR:CB	2.32	0.59
1:B:187:TYR:O	1:B:192:ASN:HB2	2.03	0.59
1:A:288:ASN:OD1	1:A:291:HIS:HD2	1.86	0.58
1:A:9:TRP:CZ2	1:A:95:GLY:N	2.71	0.58
1:A:228:ARG:HD2	1:A:229:TYR:CZ	2.38	0.58
1:A:288:ASN:O	1:A:292:ILE:HG13	2.03	0.58
1:B:33:TRP:NE1	1:B:42:PRO:HD2	2.18	0.58
1:A:275:ARG:NH2	1:A:321:HIS:HA	2.18	0.57
1:A:22:LYS:HA	1:A:23:PHE:CE1	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:321:HIS:CD2	1:B:323:ARG:HB2	2.40	0.57
1:A:123:ALA:O	1:A:124:ASP:HB2	2.05	0.57
1:A:3:GLN:HG2	1:A:14:TYR:HB2	1.86	0.57
1:B:30:PHE:CG	1:B:144:ILE:HG21	2.40	0.57
1:B:137:TRP:HE3	1:B:144:ILE:CD1	2.18	0.57
1:B:38:GLY:O	1:B:47:GLY:HA2	2.05	0.57
1:A:5:ILE:O	1:A:7:GLY:N	2.38	0.57
1:A:241:ARG:HH12	3:A:410:MES:H72	1.70	0.56
1:A:4:LEU:HD12	1:A:9:TRP:HA	1.86	0.56
1:A:157:ASN:HD21	1:A:170:TYR:H	1.53	0.56
1:B:256:HIS:HB2	1:B:297:PHE:CE1	2.41	0.56
1:A:275:ARG:HH21	1:A:321:HIS:HA	1.71	0.56
1:A:224:LEU:HD12	1:A:270:LEU:HD23	1.88	0.56
1:B:65:TRP:CZ3	4:B:410:OVS:H7	2.41	0.56
1:A:125:PRO:HB2	1:A:126:HIS:CD2	2.42	0.55
1:B:289:PHE:O	1:B:293:ARG:HG3	2.06	0.55
1:A:233:ASN:N	1:A:233:ASN:HD22	2.04	0.55
1:A:89:PRO:HG3	1:A:291:HIS:CG	2.42	0.55
1:B:33:TRP:CD1	1:B:33:TRP:N	2.74	0.55
1:A:12:THR:O	1:A:14:TYR:CD2	2.60	0.55
1:A:10:HIS:CD2	1:A:15:ASP:OD1	2.59	0.55
1:B:3:GLN:O	1:B:9:TRP:CE3	2.60	0.55
1:B:256:HIS:CD2	1:B:257:PHE:CD1	2.95	0.54
1:B:123:ALA:HB1	1:B:143:THR:HG22	1.89	0.54
1:B:137:TRP:CE3	1:B:144:ILE:CD1	2.90	0.54
1:B:45:THR:C	1:B:46:GLY:O	2.46	0.54
1:A:157:ASN:HD21	1:A:169:ASP:HA	1.72	0.54
1:A:260:ASP:O	1:B:311:ILE:HG23	2.07	0.54
1:B:2:GLY:HA2	1:B:9:TRP:CH2	2.43	0.54
1:A:189:THR:OG1	1:A:190:VAL:HG23	2.08	0.54
1:B:137:TRP:CZ3	1:B:144:ILE:HD13	2.43	0.54
1:B:256:HIS:CE1	1:B:296:TYR:O	2.61	0.54
1:A:97:THR:HG22	1:A:99:ASP:N	2.15	0.54
1:B:14:TYR:O	1:B:14:TYR:CG	2.61	0.54
1:A:111:TYR:HD1	1:A:111:TYR:N	2.06	0.53
1:A:115:PHE:CD2	1:A:117:TYR:CE2	2.95	0.53
1:A:157:ASN:ND2	1:A:170:TYR:H	2.05	0.53
1:B:98:PHE:CZ	1:B:116:LEU:HD23	2.44	0.53
1:A:22:LYS:CA	1:A:23:PHE:CD1	2.92	0.53
1:A:294:ASN:OD1	1:A:298:ARG:HD3	2.09	0.53
1:B:202:SER:HB2	2:B:408:SO4:S	2.48	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:THR:HG23	1:B:14:TYR:HE2	1.74	0.53
1:B:9:TRP:CZ2	1:B:94:ASN:O	2.62	0.53
1:A:102:PHE:CD2	1:A:103:PRO:HD2	2.43	0.52
1:A:9:TRP:HE1	1:A:94:ASN:HA	1.73	0.52
4:B:410:OVS:C08	4:B:410:OVS:H5	2.39	0.52
1:A:87:VAL:HG21	1:A:96:TRP:CE3	2.44	0.52
1:A:130:ARG:HD3	4:A:411:OVS:O24	2.10	0.52
1:B:30:PHE:CB	1:B:144:ILE:HG21	2.40	0.52
1:B:97:THR:HG22	1:B:99:ASP:CB	2.40	0.52
1:A:110:LEU:C	1:A:111:TYR:HD1	2.13	0.51
1:B:206:TYR:CD2	1:B:206:TYR:C	2.84	0.51
1:B:222:GLN:O	1:B:225:GLY:HA3	2.10	0.51
1:A:130:ARG:HH11	4:A:411:OVS:H4	1.75	0.51
1:A:65:TRP:CZ3	4:A:411:OVS:H5	2.45	0.51
1:A:85:SER:OG	1:A:109:THR:HB	2.10	0.51
1:B:63[B]:CYS:SG	1:B:96:TRP:CZ2	3.04	0.51
1:B:151:GLU:OE1	5:B:532:HOH:O	2.19	0.51
1:A:33:TRP:CD1	1:A:42:PRO:HD2	2.45	0.51
1:A:60:SER:O	1:A:63[A]:CYS:SG	2.69	0.51
1:A:124:ASP:OD1	1:A:124:ASP:C	2.48	0.50
1:A:4:LEU:O	1:A:128:SER:HA	2.11	0.50
1:A:187:TYR:O	1:A:192:ASN:HB2	2.11	0.50
1:B:59:VAL:O	1:B:86:VAL:HA	2.11	0.50
1:B:14:TYR:O	1:B:14:TYR:CD1	2.64	0.50
1:A:261:LYS:HG2	1:A:262:HIS:CD2	2.47	0.50
1:B:2:GLY:C	1:B:9:TRP:CH2	2.85	0.50
1:A:289:PHE:O	1:A:293:ARG:HG3	2.11	0.50
1:A:110:LEU:HD21	1:A:139:LYS:HE2	1.92	0.49
1:A:24:GLN:HG2	1:A:25:ARG:H	1.76	0.49
1:A:288:ASN:OD1	1:A:291:HIS:CD2	2.65	0.49
1:B:275:ARG:HG3	1:B:275:ARG:NH1	2.26	0.49
1:B:22:LYS:HE3	1:B:22:LYS:HA	1.95	0.49
1:B:121:LEU:C	1:B:123:ALA:N	2.66	0.49
1:A:9:TRP:CZ2	1:A:94:ASN:CA	2.93	0.49
1:B:4:LEU:HD23	1:B:127:TYR:HD2	1.78	0.48
1:A:26:SER:O	1:A:27:ALA:C	2.51	0.48
1:A:50:ALA:O	1:A:51:GLU:HB3	2.13	0.48
1:A:5:ILE:HB	1:A:10:HIS:CD2	2.49	0.48
1:B:265:SER:HA	1:B:271:TYR:CG	2.48	0.48
1:B:65:TRP:CZ3	4:B:410:OVS:C28	2.97	0.48
1:A:311:ILE:HD11	1:B:261:LYS:HD2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:315:GLN:NE2	5:B:510:HOH:O	2.46	0.48
1:B:112:GLN:NE2	1:B:112:GLN:H	2.10	0.48
1:A:199:PHE:HZ	1:A:300:HIS:CE1	2.31	0.48
1:A:311:ILE:HG12	1:A:311:ILE:O	2.14	0.48
1:A:228:ARG:HD3	1:A:276:ASP:OD2	2.14	0.48
1:A:241:ARG:HH22	3:A:410:MES:H51	1.79	0.48
1:A:292:ILE:O	1:A:296:TYR:HD2	1.97	0.47
1:A:311:ILE:CD1	1:B:261:LYS:HD2	2.43	0.47
1:A:115:PHE:CG	1:A:117:TYR:CE2	3.02	0.47
1:A:54:ARG:O	1:A:139:LYS:HB2	2.15	0.47
1:B:172:PRO:HG2	1:B:175:LEU:HD12	1.95	0.47
1:B:98:PHE:HB3	1:B:108:ASP:H	1.78	0.47
1:B:5:ILE:CD1	1:B:10:HIS:CD2	2.95	0.47
1:B:58:TYR:CD1	1:B:85:SER:HB2	2.49	0.47
1:A:24:GLN:CG	1:A:25:ARG:H	2.28	0.47
1:A:13:TRP:C	1:A:15:ASP:HA	2.35	0.47
1:A:9:TRP:HZ2	1:A:95:GLY:N	2.11	0.47
1:B:34:LEU:HD12	1:B:35:THR:N	2.29	0.47
1:A:113:ASN:HB3	1:A:118:GLN:OE1	2.15	0.47
1:A:184:GLY:HA2	3:A:410:MES:C6	2.45	0.47
1:B:246:LEU:HA	1:B:246:LEU:HD12	1.51	0.47
3:A:408:MES:C5	3:A:408:MES:O3S	2.63	0.47
1:B:34:LEU:HD23	1:B:136:LEU:HD21	1.97	0.47
1:A:4:LEU:HD13	1:A:9:TRP:HE3	1.79	0.46
1:B:85:SER:OG	1:B:109:THR:CG2	2.46	0.46
1:A:204:GLU:N	3:A:409:MES:O2S	2.34	0.46
1:B:297:PHE:CD2	1:B:309:ILE:HG23	2.51	0.46
1:B:187:TYR:HA	1:B:191:ASN:HB2	1.97	0.46
1:B:98:PHE:O	1:B:107:GLY:HA2	2.15	0.46
1:B:321:HIS:HD2	1:B:323:ARG:N	2.06	0.46
4:B:410:OVS:H8	4:B:410:OVS:H5	1.98	0.46
1:A:115:PHE:HB3	1:A:117:TYR:CD2	2.51	0.46
1:A:124:ASP:HA	1:A:125:PRO:HD2	1.65	0.46
1:A:110:LEU:CD2	1:A:139:LYS:HE2	2.46	0.46
1:A:319:GLU:HA	1:A:320:PRO:HD2	1.62	0.46
1:B:287:VAL:O	1:B:287:VAL:HG12	2.14	0.46
1:A:307:GLY:O	5:A:547:HOH:O	2.21	0.46
1:B:96:TRP:N	5:B:520:HOH:O	2.29	0.46
1:B:108:ASP:O	1:B:112:GLN:HA	2.16	0.45
1:A:311:ILE:HD13	1:B:261:LYS:HB2	1.98	0.45
1:B:97:THR:C	1:B:99:ASP:H	2.20	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:ASP:OD2	1:A:101:SER:OG	2.23	0.45
1:B:194:VAL:O	1:B:257:PHE:CD2	2.69	0.45
1:B:97:THR:CG2	1:B:99:ASP:HB2	2.47	0.45
1:A:143:THR:HB	1:A:144:ILE:H	1.62	0.45
1:A:246:LEU:HD12	1:A:246:LEU:HA	1.79	0.45
1:A:81:PHE:O	1:A:82:ILE:HG12	2.17	0.45
1:B:205:ALA:O	1:B:208:GLU:HB3	2.16	0.45
3:A:410:MES:H81	3:A:410:MES:H32	1.72	0.45
1:A:22:LYS:HA	1:A:23:PHE:CD1	2.52	0.45
1:B:111:TYR:HE2	1:B:137:TRP:HZ2	1.57	0.45
1:B:30:PHE:CG	1:B:144:ILE:CG2	3.00	0.45
1:A:119:LEU:HD22	1:A:119:LEU:HA	1.56	0.45
1:B:22:LYS:HA	1:B:22:LYS:CE	2.47	0.45
1:A:63[B]:CYS:SG	4:A:411:OVS:H8	2.57	0.44
1:A:65:TRP:CH2	4:A:411:OVS:H7	2.53	0.44
1:B:12:THR:HG23	1:B:14:TYR:CE2	2.50	0.44
1:B:4:LEU:HD21	1:B:121:LEU:CD2	2.47	0.44
1:B:141:ASN:O	1:B:142:HIS:C	2.56	0.44
1:B:97:THR:CG2	1:B:99:ASP:CB	2.96	0.44
1:A:121:LEU:HA	1:A:124:ASP:O	2.18	0.44
1:A:228:ARG:HH11	1:A:276:ASP:CG	2.20	0.44
1:B:251:PRO:HG2	1:B:289:PHE:CE1	2.53	0.44
1:B:2:GLY:HA2	1:B:9:TRP:CZ2	2.53	0.44
1:B:5:ILE:O	1:B:7:GLY:N	2.51	0.44
1:B:98:PHE:CG	1:B:108:ASP:HB2	2.52	0.44
1:B:327:PHE:HA	1:B:328:GLY:HA2	1.43	0.44
1:B:98:PHE:CD2	1:B:108:ASP:HB2	2.53	0.44
1:A:202:SER:HA	3:A:409:MES:H71	2.00	0.43
1:B:319:GLU:HA	1:B:320:PRO:HD2	1.81	0.43
1:A:92:LEU:H	1:A:92:LEU:HD23	1.82	0.43
1:A:12:THR:O	1:A:14:TYR:N	2.52	0.43
1:B:98:PHE:HB2	1:B:114:GLU:HA	1.99	0.43
1:B:97:THR:CG2	1:B:99:ASP:H	2.14	0.43
1:A:305:PRO:HG3	1:B:305:PRO:HG3	1.99	0.43
1:A:5:ILE:HD13	1:A:5:ILE:HA	1.92	0.43
1:A:9:TRP:HZ2	1:A:95:GLY:H	1.67	0.43
1:B:89:PRO:HG3	1:B:291:HIS:ND1	2.34	0.43
1:A:93:GLU:H	1:A:93:GLU:CD	2.21	0.43
1:A:26:SER:HB3	1:A:128:SER:O	2.14	0.43
1:A:88:ASN:HB2	1:A:99:ASP:O	2.18	0.43
1:B:229:TYR:HB3	1:B:239:ASP:OD1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:265:SER:HA	1:B:271:TYR:CD1	2.53	0.43
1:B:30:PHE:HB3	1:B:144:ILE:HG22	2.00	0.43
1:A:254:VAL:HG12	1:A:255:THR:N	2.33	0.42
1:A:61:LEU:HD23	1:A:61:LEU:HA	1.37	0.42
1:B:95:GLY:HA3	5:B:520:HOH:O	2.18	0.42
1:A:14:TYR:HD1	1:A:14:TYR:O	2.01	0.42
1:B:3:GLN:NE2	1:B:14:TYR:CD1	2.87	0.42
1:A:252:VAL:HG11	1:A:296:TYR:CG	2.55	0.42
1:B:246:LEU:HB3	1:B:274:LEU:HD13	2.00	0.42
1:A:24:GLN:NE2	1:A:25:ARG:HD3	2.34	0.42
1:B:30:PHE:CD1	1:B:144:ILE:HB	2.54	0.42
1:A:58:TYR:CE2	1:A:119:LEU:HD11	2.55	0.42
1:A:23:PHE:HA	1:A:24:GLN:CB	2.25	0.42
1:A:296:TYR:O	1:A:300:HIS:CD2	2.72	0.42
1:B:171:TYR:CD2	1:B:176:GLN:NE2	2.88	0.42
1:A:86:VAL:HG12	1:A:87:VAL:O	2.20	0.42
1:B:3:GLN:O	1:B:9:TRP:CZ3	2.73	0.42
1:A:4:LEU:CD1	1:A:9:TRP:HE3	2.33	0.41
1:B:26:SER:C	1:B:28:SER:H	2.23	0.41
1:A:110:LEU:C	1:A:111:TYR:CD1	2.92	0.41
1:A:115:PHE:HB2	1:A:117:TYR:CE2	2.55	0.41
1:A:233:ASN:H	1:A:233:ASN:ND2	2.11	0.41
1:B:280:MET:HA	1:B:281:PRO:HD3	1.90	0.41
1:B:306:THR:HB	1:B:308:ILE:CG1	2.47	0.41
1:A:249:PHE:HA	1:A:253:TYR:CD2	2.56	0.41
1:A:265:SER:HA	1:A:271:TYR:CG	2.56	0.41
1:A:97:THR:CG2	1:A:98:PHE:N	2.83	0.41
1:A:113:ASN:OD1	1:A:118:GLN:HB3	2.20	0.41
1:B:61:LEU:HD23	1:B:61:LEU:HA	1.85	0.41
1:B:194:VAL:HG21	1:B:253:TYR:CD2	2.56	0.41
1:B:23:PHE:HA	1:B:24:GLN:HA	1.86	0.41
1:A:27:ALA:O	1:A:28:SER:C	2.57	0.41
1:A:65:TRP:CZ3	4:A:411:OVS:C28	3.04	0.41
1:A:26:SER:CB	1:A:128:SER:C	2.88	0.41
4:A:411:OVS:O17	4:A:411:OVS:C12	2.69	0.41
1:A:115:PHE:CD2	1:A:117:TYR:CZ	3.09	0.40
1:A:130:ARG:NH1	4:A:411:OVS:H4	2.35	0.40
1:B:98:PHE:HB3	1:B:108:ASP:N	2.37	0.40
1:A:276:ASP:HA	1:A:321:HIS:CD2	2.56	0.40
1:B:224:LEU:HD12	1:B:270:LEU:CD2	2.47	0.40
1:A:92:LEU:HB2	1:A:93:GLU:H	1.73	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:ARG:HH22	1:B:191:ASN:ND2	2.19	0.40
1:A:203:GLN:H	3:A:409:MES:H71	1.86	0.40
1:B:28:SER:C	1:B:30:PHE:H	2.25	0.40

All (2) 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)
5:A:564:HOH:O	5:B:544:HOH:O[4_456]	1.93	0.27
5:A:574:HOH:O	5:B:554:HOH:O[4_456]	2.13	0.07

## 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%)	276 (85%)	33 (10%)	17 (5%)		
1	B	326/328 (99%)	269 (82%)	44 (14%)	13 (4%)		
All	All	652/656 (99%)	545 (84%)	77 (12%)	30 (5%)		

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	ASP
1	A	11	ASP
1	A	13	TRP
1	A	19	THR
1	A	28	SER
1	A	29	ALA
1	A	87	VAL
1	A	112	GLN
1	A	261	LYS

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Mol	Chain	Res	Type
1	B	6	ASP
1	B	11	ASP
1	B	28	SER
1	B	100	ASP
1	B	112	GLN
1	B	113	ASN
1	A	3	GLN
1	A	18	SER
1	A	25	ARG
1	A	92	LEU
1	A	95	GLY
1	B	22	LYS
1	B	122	HIS
1	A	21	GLY
1	A	23	PHE
1	B	142	HIS
1	B	118	GLN
1	A	17	LYS
1	B	15	ASP
1	B	200	ALA
1	B	252	VAL

### 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%)	252 (91%)	26 (9%)	10	17
1	B	278/278 (100%)	256 (92%)	22 (8%)	14	26
All	All	556/556 (100%)	508 (91%)	48 (9%)	12	21

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	4	LEU

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Mol	Chain	Res	Type
1	A	5	ILE
1	A	8	VAL
1	A	13	TRP
1	A	23	PHE
1	A	45	THR
1	A	53	ASP
1	A	90	LEU
1	A	92	LEU
1	A	93	GLU
1	A	94	ASN
1	A	101	SER
1	A	102	PHE
1	A	112	GLN
1	A	116	LEU
1	A	119	LEU
1	A	122	HIS
1	A	128	SER
1	A	182	LEU
1	A	202	SER
1	A	228	ARG
1	A	233	ASN
1	A	246	LEU
1	A	302	THR
1	A	319	GLU
1	B	13	TRP
1	B	22	LYS
1	B	23	PHE
1	B	34	LEU
1	B	49	ILE
1	B	53	ASP
1	B	60	SER
1	B	90	LEU
1	B	111	TYR
1	B	112	GLN
1	B	116	LEU
1	B	119	LEU
1	B	122	HIS
1	B	144	ILE
1	B	178	LYS
1	B	210	VAL
1	B	227	HIS
1	B	246	LEU

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Mol	Chain	Res	Type
1	B	255	THR
1	B	301	LYS
1	B	302	THR
1	B	306	THR

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

Mol	Chain	Res	Type
1	A	3	GLN
1	A	10	HIS
1	A	24	GLN
1	A	126	HIS
1	A	157	ASN
1	A	191	ASN
1	A	192	ASN
1	A	222	GLN
1	A	233	ASN
1	A	256	HIS
1	A	279	GLN
1	A	291	HIS
1	B	3	GLN
1	B	113	ASN
1	B	233	ASN
1	B	234	GLN
1	B	256	HIS
1	B	315	GLN
1	B	321	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

21 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	0.38	0	6,6,6	0.89	0
2	SO4	A	402	-	4,4,4	0.74	0	6,6,6	0.70	0
2	SO4	A	403	-	4,4,4	0.64	0	6,6,6	0.53	0
2	SO4	A	404	-	4,4,4	0.84	0	6,6,6	0.55	0
2	SO4	A	405	-	4,4,4	0.49	0	6,6,6	0.60	0
2	SO4	A	406	-	4,4,4	0.49	0	6,6,6	0.44	0
2	SO4	A	407	-	4,4,4	0.73	0	6,6,6	0.25	0
3	MES	A	408	-	12,12,12	2.10	2 (16%)	14,16,16	7.08	11 (78%)
3	MES	A	409	-	12,12,12	1.60	2 (16%)	14,16,16	3.22	7 (50%)
3	MES	A	410	-	12,12,12	1.57	2 (16%)	14,16,16	3.18	10 (71%)
4	OVS	A	411	-	26,34,34	1.94	5 (19%)	35,47,47	2.84	15 (42%)
2	SO4	B	401	-	4,4,4	0.40	0	6,6,6	0.55	0
2	SO4	B	402	-	4,4,4	0.74	0	6,6,6	0.50	0
2	SO4	B	403	-	4,4,4	0.42	0	6,6,6	0.39	0
2	SO4	B	404	-	4,4,4	0.39	0	6,6,6	0.49	0
2	SO4	B	405	-	4,4,4	0.55	0	6,6,6	0.68	0
2	SO4	B	406	-	4,4,4	0.55	0	6,6,6	0.30	0
2	SO4	B	407	-	4,4,4	0.71	0	6,6,6	0.82	0
2	SO4	B	408	-	4,4,4	0.50	0	6,6,6	0.66	0
3	MES	B	409	-	12,12,12	1.89	2 (16%)	14,16,16	2.92	6 (42%)
4	OVS	B	410	-	26,34,34	2.75	15 (57%)	35,47,47	3.66	17 (48%)

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
2	SO4	A	407	-	-	0/0/0/0	0/0/0/0
3	MES	A	408	-	-	0/6/14/14	0/1/1/1
3	MES	A	409	-	-	0/6/14/14	0/1/1/1
3	MES	A	410	-	-	0/6/14/14	0/1/1/1
4	OVS	A	411	-	-	0/21/47/47	0/2/2/2
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
2	SO4	B	407	-	-	0/0/0/0	0/0/0/0
2	SO4	B	408	-	-	0/0/0/0	0/0/0/0
3	MES	B	409	-	-	0/6/14/14	0/1/1/1
4	OVS	B	410	-	-	1/21/47/47	0/2/2/2

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	408	MES	C8-S	-5.22	1.69	1.77
3	B	409	MES	C8-S	-4.54	1.70	1.77
3	A	410	MES	C8-S	-3.17	1.72	1.77
3	A	409	MES	C8-S	-3.13	1.72	1.77
4	B	410	OVS	C09-N10	2.06	1.50	1.45
4	A	411	OVS	C33-C03	2.13	1.43	1.39
4	B	410	OVS	C03-C04	2.21	1.44	1.40
3	A	410	MES	O1S-S	2.28	1.51	1.45
3	B	409	MES	O2S-S	2.35	1.52	1.45
4	B	410	OVS	C33-C03	2.44	1.43	1.39
4	B	410	OVS	C30-C04	2.50	1.43	1.39
3	A	409	MES	O1S-S	2.60	1.52	1.45
4	B	410	OVS	C09-C20	2.66	1.60	1.52
4	B	410	OVS	C27-C02	2.74	1.54	1.48
4	A	411	OVS	C08-S07	3.00	1.85	1.81
4	B	410	OVS	C08-C09	3.02	1.61	1.53
4	B	410	OVS	C06-C27	3.16	1.41	1.36
4	B	410	OVS	O26-C20	3.19	1.29	1.23
4	B	410	OVS	C20-N21	3.37	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	410	0VS	C12-C11	3.43	1.58	1.51
3	A	408	MES	O1S-S	3.43	1.55	1.45
4	A	411	0VS	C06-C27	3.97	1.43	1.36
4	B	410	0VS	C04-C05	4.13	1.56	1.48
4	A	411	0VS	C06-S07	4.31	1.86	1.74
4	B	410	0VS	C06-S07	4.43	1.86	1.74
4	B	410	0VS	C11-N10	4.65	1.43	1.34
4	A	411	0VS	C11-N10	4.69	1.43	1.34
4	B	410	0VS	C08-S07	5.16	1.88	1.81

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	408	MES	O3S-S-C8	-9.03	94.95	106.06
4	B	410	0VS	O19-C11-N10	-8.45	108.38	122.97
4	A	411	0VS	C27-C06-C05	-6.83	115.87	121.64
4	B	410	0VS	C27-C06-C05	-6.26	116.35	121.64
4	A	411	0VS	O26-C20-N21	-5.94	111.63	123.07
4	A	411	0VS	C28-C27-C02	-5.78	106.55	116.23
4	B	410	0VS	O26-C20-N21	-4.55	114.30	123.07
3	A	409	MES	O3S-S-O2S	-3.41	103.55	111.37
4	A	411	0VS	O26-C20-C09	-3.27	113.39	120.43
4	B	410	0VS	O01-C02-C03	-3.07	116.51	121.55
4	B	410	0VS	C30-C04-C03	-3.05	115.80	119.26
3	A	410	MES	C6-C5-N4	-2.91	106.03	110.11
4	B	410	0VS	O29-C05-C06	-2.58	117.22	120.81
4	A	411	0VS	C04-C03-C02	-2.37	118.18	120.68
4	A	411	0VS	C08-C09-C20	-2.36	104.11	109.55
3	A	408	MES	O2S-S-O1S	-2.35	105.72	113.86
3	A	408	MES	O2S-S-C8	-2.32	104.80	106.79
3	A	410	MES	O3S-S-O1S	-2.28	106.14	111.37
4	A	411	0VS	O29-C05-C04	-2.20	117.93	121.55
3	B	409	MES	O2S-S-O1S	-2.12	106.52	113.86
4	B	410	0VS	C28-C27-C02	-2.02	112.85	116.23
3	A	410	MES	C2-C3-N4	2.00	112.92	110.11
3	A	408	MES	C7-N4-C3	2.06	116.55	111.26
4	A	411	0VS	C12-C11-N10	2.07	119.46	115.82
4	A	411	0VS	C13-C12-C11	2.22	118.19	113.18
4	B	410	0VS	C08-C09-C20	2.43	115.14	109.55
4	B	410	0VS	C33-C03-C04	2.48	122.07	119.26
3	A	409	MES	O2S-S-C8	2.48	108.92	106.79
4	A	411	0VS	C20-C09-N10	2.54	118.20	111.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	411	0VS	C22-N21-C20	2.63	125.96	122.39
3	A	410	MES	O1S-S-C8	2.73	109.14	106.79
3	A	408	MES	C6-O1-C2	2.74	119.17	109.89
3	B	409	MES	C6-O1-C2	2.80	119.35	109.89
3	A	410	MES	O1-C6-C5	2.81	118.11	111.83
3	A	410	MES	C7-N4-C5	2.87	118.60	111.26
3	A	409	MES	C7-N4-C5	2.89	118.66	111.26
3	A	408	MES	O3S-S-O2S	2.89	118.00	111.37
4	B	410	0VS	C09-C20-N21	2.95	122.53	116.51
3	A	409	MES	O1-C2-C3	3.01	118.55	111.83
3	A	410	MES	C7-N4-C3	3.01	118.97	111.26
3	A	408	MES	O1-C2-C3	3.09	118.74	111.83
4	B	410	0VS	C27-C06-S07	3.11	124.69	120.32
3	A	408	MES	C7-N4-C5	3.16	119.36	111.26
4	A	411	0VS	C27-C06-S07	3.23	124.85	120.32
4	A	411	0VS	C28-C27-C06	3.37	128.60	123.54
3	A	409	MES	C7-N4-C3	3.56	120.38	111.26
3	B	409	MES	O2S-S-C8	3.67	109.95	106.79
3	B	409	MES	C7-N4-C5	3.95	121.39	111.26
4	B	410	0VS	O01-C02-C27	4.11	125.33	120.31
3	A	410	MES	O2S-S-C8	4.20	110.40	106.79
3	A	408	MES	C2-C3-N4	4.29	116.12	110.11
4	B	410	0VS	C20-C09-N10	4.92	124.74	111.20
3	B	409	MES	C5-N4-C3	5.22	120.69	108.87
3	A	410	MES	C5-N4-C3	5.23	120.72	108.87
3	A	409	MES	C5-N4-C3	5.28	120.83	108.87
4	A	411	0VS	C08-S07-C06	5.48	122.46	104.43
4	B	410	0VS	C08-S07-C06	5.61	122.90	104.43
3	A	408	MES	C5-N4-C3	5.78	121.97	108.87
3	A	410	MES	O3S-S-C8	6.21	113.69	106.06
4	A	411	0VS	C06-C27-C02	6.26	124.77	120.21
3	B	409	MES	O3S-S-C8	6.42	113.95	106.06
4	B	410	0VS	C12-C11-N10	7.15	128.40	115.82
4	B	410	0VS	C06-C27-C02	7.16	125.43	120.21
3	A	409	MES	O3S-S-C8	7.60	115.40	106.06
4	B	410	0VS	C22-N21-C20	9.16	134.79	122.39
3	A	408	MES	O1S-S-C8	22.63	126.23	106.79

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	410	0VS	C27-C06-S07-C08

There are no ring outliers.

6 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	408	MES	3	0
3	A	409	MES	4	0
3	A	410	MES	5	0
4	A	411	0VS	10	0
2	B	408	SO4	2	0
4	B	410	0VS	4	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%)	0.13	21 (6%) 20 18	30, 47, 103, 142	0
1	B	327/328 (99%)	0.25	23 (7%) 17 15	33, 54, 126, 163	0
All	All	654/656 (99%)	0.19	44 (6%) 19 16	30, 51, 120, 163	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	19	THR	8.6
1	B	26	SER	6.9
1	A	15	ASP	6.9
1	B	21	GLY	6.8
1	B	17	LYS	6.8
1	A	23	PHE	6.6
1	A	16	THR	6.4
1	A	18	SER	6.1
1	A	17	LYS	6.1
1	B	16	THR	6.0
1	A	19	THR	6.0
1	A	11	ASP	5.9
1	A	21	GLY	5.8
1	B	18	SER	5.6
1	B	20	GLY	5.2
1	B	23	PHE	5.1
1	A	26	SER	5.0
1	B	28	SER	4.9
1	A	13	TRP	4.9
1	B	24	GLN	4.9
1	B	13	TRP	4.7
1	A	12	THR	4.7
1	B	27	ALA	4.6
1	A	328	GLY	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	14	TYR	4.2
1	A	20	GLY	4.1
1	A	27	ALA	4.0
1	A	28	SER	4.0
1	B	25	ARG	3.7
1	B	12	THR	3.6
1	A	10	HIS	3.3
1	B	22	LYS	3.1
1	A	22	LYS	3.0
1	B	15	ASP	2.9
1	B	11	ASP	2.8
1	B	14	TYR	2.7
1	A	24	GLN	2.6
1	B	5	ILE	2.5
1	B	29	ALA	2.4
1	B	10	HIS	2.4
1	B	63[A]	CYS	2.4
1	A	63[A]	CYS	2.2
1	A	25	ARG	2.2
1	B	34	LEU	2.1

## 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	A	410	12/12	0.85	0.44	21.09	64,92,102,116	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SO4	B	402	5/5	0.84	0.45	20.36	101,103,117,146	0
2	SO4	A	402	5/5	0.90	0.35	13.87	68,85,89,124	0
3	MES	B	409	12/12	0.85	0.41	13.33	68,87,98,119	0
3	MES	A	409	12/12	0.76	0.46	8.28	81,99,108,136	0
3	MES	A	408	12/12	0.92	0.27	7.39	53,72,83,93	0
4	OVS	B	410	33/33	0.80	0.21	0.54	71,87,102,108	0
4	OVS	A	411	33/33	0.89	0.18	0.36	52,95,112,119	0
2	SO4	A	403	5/5	0.94	0.14	-1.04	74,79,98,118	0
2	SO4	B	404	5/5	0.91	0.17	-	77,97,99,115	0
2	SO4	A	404	5/5	0.86	0.15	-	56,68,100,124	0
2	SO4	B	407	5/5	0.87	0.16	-	90,90,107,128	0
2	SO4	A	407	5/5	0.91	0.24	-	77,84,111,123	0
2	SO4	B	403	5/5	0.98	0.17	-	65,71,92,93	0
2	SO4	B	405	5/5	0.93	0.26	-	80,85,113,120	0
2	SO4	A	401	5/5	0.98	0.09	-	60,64,71,80	0
2	SO4	A	405	5/5	0.94	0.29	-	77,105,109,131	0
2	SO4	B	401	5/5	0.98	0.10	-	51,66,80,80	0
2	SO4	B	406	5/5	0.90	0.32	-	79,86,118,129	0
2	SO4	B	408	5/5	0.75	0.33	-	98,104,123,137	0
2	SO4	A	406	5/5	0.96	0.12	-	72,84,109,117	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.