



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 12:24 am GMT

PDB ID : 3LN6  
Title : Crystal structure of a bifunctional glutathione synthetase from *Streptococcus agalactiae*  
Authors : Stout, J.; Vergauwen, B.; Savvides, S.N.  
Deposited on : 2010-02-02  
Resolution : 2.95 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

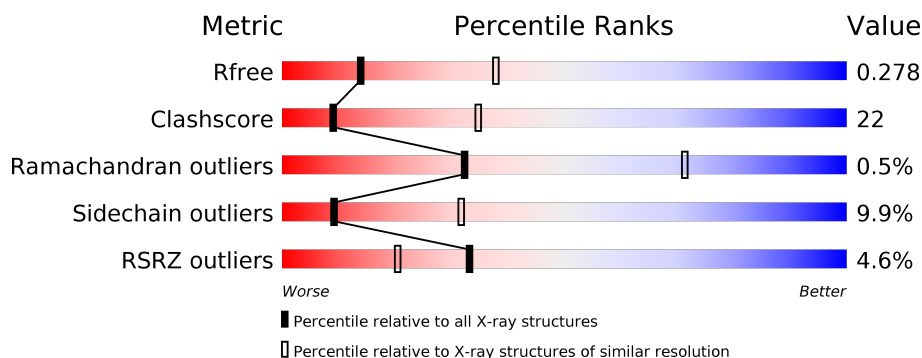
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.95 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	2395 (3.00-2.92)
Clashscore	112137	2773 (3.00-2.92)
Ramachandran outliers	110173	2680 (3.00-2.92)
Sidechain outliers	110143	2683 (3.00-2.92)
RSRZ outliers	101464	2421 (3.00-2.92)

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	750	<div> <div>5%</div> <div>60%</div> <div>35%</div> <div>..</div> </div>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 5533 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 Glutathione biosynthesis bifunctional protein gshAB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	743	Total	C	N	O	S	0	5	0
			5493	3487	927	1063	16			

- 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		

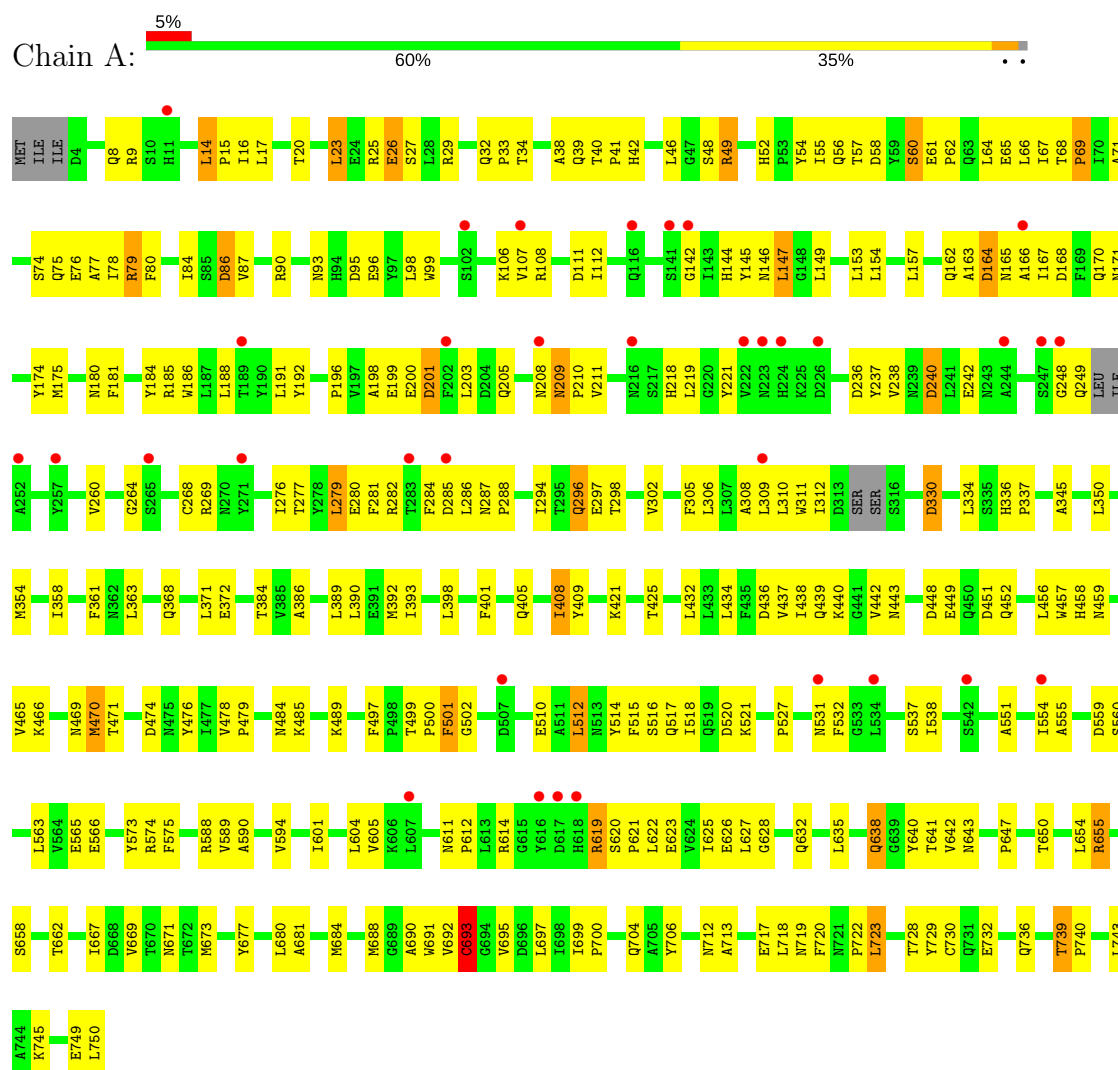
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	35	Total	O	0	0
			35	35		

### 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: Glutathione biosynthesis bifunctional protein gshAB



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	143.02Å 143.02Å 211.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.95 29.61 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (20.00-2.95) 99.7 (29.61-2.90)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.11 (at 2.90Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.253 , 0.286 0.244 , 0.278	Depositor DCC
$R_{free}$ test set	1180 reflections (5.05%)	DCC
Wilson B-factor (Å <sup>2</sup> )	76.2	Xtriage
Anisotropy	0.013	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 69.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.015 for -1/2*h-1/2*k-1/2*l,-1/2*h-1/2*k+1/2*l,-h+k 0.003 for -1/2*h+1/2*k-1/2*l,1/2*h-1/2*k-1/2*l,-h-k	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	5533	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.41% 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: SO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.66	2/5627 (0.0%)	0.73	0/7696

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	693	CYS	CB-SG	-7.69	1.69	1.82
1	A	730	CYS	CB-SG	-6.17	1.71	1.82

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	5493	0	4883	232	0
2	A	5	0	0	0	0
3	A	35	0	0	5	0
All	All	5533	0	4883	232	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 22.

All (232) 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:693:CYS:SG	1:A:718:LEU:HD11	2.16	0.85
1:A:196:PRO:HA	1:A:211:VAL:O	1.85	0.76
1:A:208:ASN:O	1:A:209:ASN:HB2	1.84	0.76
1:A:60:SER:HB2	1:A:62:PRO:HD2	1.68	0.75
1:A:165:ASN:HB3	1:A:168:ASP:H	1.55	0.72
1:A:238:VAL:HA	1:A:268:CYS:SG	2.30	0.71
1:A:308:ALA:HB2	1:A:354:MET:HG2	1.73	0.69
1:A:26:GLU:HG3	1:A:142:GLY:O	1.93	0.69
1:A:184:TYR:HB3	1:A:350:LEU:HD11	1.73	0.69
1:A:501:PHE:CD1	1:A:566:GLU:HB2	2.27	0.69
1:A:677:TYR:CE1	1:A:706:TYR:HB2	2.28	0.68
1:A:692:VAL:HG12	1:A:692:VAL:O	1.94	0.68
1:A:61:GLU:HB3	1:A:62:PRO:HD3	1.75	0.67
1:A:209:ASN:HB3	1:A:210:PRO:HD2	1.79	0.64
1:A:264:GLY:HA3	1:A:277:THR:HB	1.79	0.64
1:A:478:VAL:HG13	1:A:720:PHE:CG	2.33	0.64
1:A:501:PHE:CE1	1:A:566:GLU:HB2	2.32	0.64
1:A:605:VAL:HG21	1:A:627:LEU:HD21	1.80	0.64
1:A:489:LYS:HG3	1:A:499:THR:HG21	1.81	0.63
1:A:749:GLU:HG2	1:A:750:LEU:H	1.64	0.63
1:A:236:ASP:O	1:A:240:ASP:HB2	1.98	0.63
1:A:27:SER:HB3	1:A:98:LEU:HD23	1.82	0.62
1:A:93:ASN:HB2	1:A:96:GLU:HG3	1.83	0.60
1:A:75:GLN:HA	1:A:296:GLN:OE1	2.01	0.60
1:A:502:GLY:HA3	1:A:565:GLU:HA	1.83	0.60
1:A:284:PHE:HE2	1:A:302:VAL:HG21	1.67	0.59
1:A:590:ALA:HB1	1:A:655:ARG:O	2.01	0.59
1:A:601:ILE:HA	1:A:604:LEU:HD12	1.85	0.58
1:A:186:TRP:CH2	1:A:345:ALA:HB1	2.38	0.58
1:A:384[A]:THR:HG23	1:A:386:ALA:N	2.19	0.58
1:A:49[B]:ARG:NH1	1:A:61:GLU:OE1	2.37	0.58
1:A:218:HIS:CG	1:A:219:LEU:N	2.71	0.58
1:A:619:ARG:NE	1:A:619:ARG:HA	2.19	0.58
1:A:437:VAL:HG13	1:A:442:VAL:HB	1.87	0.57
1:A:448:ASP:OD1	1:A:451:ASP:HB2	2.05	0.57
1:A:108:ARG:HB3	1:A:111:ASP:CB	2.34	0.56
1:A:209:ASN:HB3	1:A:210:PRO:CD	2.34	0.56
1:A:706:TYR:HD1	1:A:712:ASN:HB3	1.70	0.56
1:A:469:ASN:ND2	1:A:722:PRO:HD2	2.19	0.56
1:A:448:ASP:O	1:A:449:GLU:HB3	2.04	0.56
1:A:39:GLN:NE2	1:A:111:ASP:HA	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:680:LEU:HG	1:A:684:MET:HE2	1.89	0.55
1:A:199:GLU:O	1:A:200:GLU:OE1	2.24	0.55
1:A:439:GLN:HG3	1:A:440:LYS:N	2.20	0.55
1:A:669:VAL:O	1:A:669:VAL:HG12	2.06	0.55
1:A:147:LEU:HD22	1:A:306:LEU:CD1	2.36	0.55
1:A:499:THR:HG22	1:A:500:PRO:O	2.07	0.55
1:A:61:GLU:N	1:A:62:PRO:CD	2.69	0.54
1:A:458:HIS:O	1:A:459:ASN:HB2	2.06	0.54
1:A:54:TYR:CD1	1:A:69:PRO:HD3	2.42	0.54
1:A:26:GLU:O	1:A:286:LEU:HD11	2.08	0.54
1:A:641:THR:HG22	1:A:643:ASN:H	1.73	0.54
1:A:693:CYS:SG	1:A:718:LEU:CD1	2.95	0.54
1:A:611:ASN:HB3	1:A:614:ARG:HG3	1.88	0.54
1:A:66:LEU:HD12	1:A:66:LEU:N	2.23	0.54
1:A:590:ALA:HA	1:A:658:SER:HA	1.91	0.53
1:A:723:LEU:HD21	3:A:752:HOH:O	2.08	0.53
1:A:285:ASP:O	1:A:286:LEU:C	2.46	0.53
1:A:384[A]:THR:HG23	1:A:386:ALA:H	1.73	0.53
1:A:451:ASP:O	1:A:452:GLN:HB2	2.08	0.53
1:A:80:PHE:O	1:A:84:ILE:HG12	2.07	0.53
1:A:86:ASP:OD2	1:A:90:ARG:NH2	2.42	0.53
1:A:484:ASN:O	1:A:485:LYS:CB	2.57	0.53
1:A:54:TYR:HB3	1:A:84:ILE:HD12	1.90	0.53
1:A:79:ARG:HG3	1:A:80:PHE:N	2.24	0.53
1:A:478:VAL:HB	1:A:479:PRO:HD3	1.91	0.52
1:A:16:ILE:HG23	1:A:17:LEU:HD22	1.91	0.52
1:A:66:LEU:H	1:A:66:LEU:HD12	1.74	0.52
1:A:336:HIS:CD2	1:A:337:PRO:HD2	2.44	0.52
1:A:32:GLN:HB3	1:A:33:PRO:HD3	1.92	0.52
1:A:248:GLY:O	1:A:249:GLN:O	2.28	0.52
1:A:86:ASP:OD1	1:A:421:LYS:HG3	2.10	0.52
1:A:551:ALA:O	1:A:554:ILE:HG22	2.10	0.52
1:A:284:PHE:CE2	1:A:302:VAL:HG21	2.44	0.51
1:A:87:VAL:HG21	1:A:438:ILE:HB	1.91	0.51
1:A:501:PHE:C	1:A:501:PHE:CD2	2.83	0.51
1:A:619:ARG:HA	1:A:619:ARG:HE	1.74	0.51
1:A:368:GLN:O	1:A:372:GLU:HG2	2.10	0.51
1:A:34:THR:O	1:A:34:THR:HG22	2.10	0.51
1:A:268:CYS:O	1:A:269:ARG:CB	2.57	0.51
1:A:514:TYR:O	1:A:517:GLN:N	2.44	0.51
1:A:29:ARG:HG3	1:A:62:PRO:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:TYR:HD1	1:A:279:LEU:HD22	1.74	0.51
1:A:436:ASP:OD1	1:A:739:THR:HB	2.11	0.51
1:A:611:ASN:ND2	1:A:612:PRO:HD2	2.26	0.50
1:A:358:ILE:HG23	1:A:363:LEU:HB2	1.93	0.50
1:A:476:TYR:O	1:A:479:PRO:HD2	2.11	0.50
1:A:697:LEU:HD22	1:A:713:ALA:HB1	1.94	0.50
1:A:8:GLN:HG2	1:A:9:ARG:N	2.27	0.50
1:A:181:PHE:O	1:A:185:ARG:HB2	2.11	0.49
1:A:337:PRO:HB3	1:A:386:ALA:HB1	1.93	0.49
1:A:66:LEU:HB3	1:A:84:ILE:HG21	1.94	0.49
1:A:667:ILE:HA	1:A:732:GLU:O	2.12	0.49
1:A:25:ARG:O	1:A:65:GLU:HA	2.12	0.49
1:A:611:ASN:CG	1:A:612:PRO:HD2	2.33	0.49
1:A:655:ARG:HG3	1:A:662:THR:HB	1.95	0.49
1:A:501:PHE:C	1:A:501:PHE:HD2	2.15	0.49
1:A:390:LEU:O	1:A:393:ILE:HG22	2.13	0.49
1:A:147:LEU:HD22	1:A:306:LEU:HD13	1.95	0.48
1:A:717:GLU:CG	1:A:718:LEU:N	2.75	0.48
1:A:56:GLN:O	1:A:64:LEU:HD12	2.13	0.48
1:A:655:ARG:CG	1:A:655:ARG:HH21	2.27	0.48
1:A:99:TRP:HD1	3:A:754:HOH:O	1.96	0.48
1:A:287:ASN:HA	1:A:288:PRO:HD3	1.65	0.48
1:A:620:SER:HB2	1:A:621:PRO:HD2	1.96	0.48
1:A:614:ARG:NH1	1:A:623:GLU:O	2.47	0.48
1:A:690:ALA:HB1	1:A:693:CYS:HB3	1.96	0.48
1:A:181:PHE:CE2	1:A:281:PHE:HD1	2.32	0.48
1:A:638:GLN:HB3	1:A:640:TYR:HD2	1.79	0.48
1:A:673:MET:CE	1:A:699:ILE:HD13	2.44	0.48
1:A:717:GLU:HG2	1:A:718:LEU:N	2.29	0.48
1:A:166:ALA:O	1:A:170:GLN:HG3	2.14	0.47
1:A:180:ASN:HB3	1:A:309:LEU:HD22	1.96	0.47
1:A:465:VAL:HG12	1:A:471:THR:HG22	1.96	0.47
1:A:54:TYR:O	1:A:66:LEU:HA	2.14	0.47
1:A:393:ILE:CG1	1:A:398:LEU:HG	2.44	0.47
1:A:162:GLN:HG2	1:A:164:ASP:H	1.79	0.47
1:A:26:GLU:HA	1:A:64:LEU:O	2.15	0.47
1:A:66:LEU:HD23	1:A:84:ILE:HG22	1.96	0.47
1:A:739:THR:OG1	1:A:740:PRO:HD3	2.14	0.47
1:A:501:PHE:CG	1:A:566:GLU:HB2	2.50	0.47
1:A:632:GLN:O	1:A:635:LEU:HB2	2.14	0.47
1:A:188:LEU:HD11	1:A:305:PHE:CD2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:690:ALA:CB	1:A:693:CYS:HB3	2.45	0.47
1:A:32:GLN:N	1:A:33:PRO:CD	2.78	0.47
1:A:78:ILE:HG13	1:A:296:GLN:HG2	1.97	0.46
1:A:145:TYR:HB2	1:A:284:PHE:CE1	2.50	0.46
1:A:443:ASN:HB3	1:A:457:TRP:CZ2	2.49	0.46
1:A:16:ILE:HA	1:A:153:LEU:HD13	1.96	0.46
1:A:443:ASN:HB3	1:A:457:TRP:CE2	2.50	0.46
1:A:667:ILE:O	1:A:669:VAL:HG23	2.15	0.46
1:A:614:ARG:HA	1:A:622:LEU:O	2.15	0.46
1:A:106:LYS:NZ	1:A:108:ARG:HB2	2.30	0.46
1:A:284:PHE:N	1:A:284:PHE:CD1	2.83	0.46
1:A:527:PRO:HB2	1:A:559:ASP:HB3	1.97	0.46
1:A:554:ILE:CG2	1:A:555:ALA:N	2.79	0.46
1:A:605:VAL:HG13	1:A:625:ILE:HB	1.98	0.46
1:A:432:LEU:HB2	1:A:739:THR:HG21	1.98	0.46
1:A:145:TYR:CB	1:A:284:PHE:CE1	2.99	0.45
1:A:8:GLN:HB2	1:A:311:TRP:CD1	2.51	0.45
1:A:575:PHE:N	1:A:575:PHE:CD2	2.83	0.45
1:A:700:PRO:HD2	1:A:712:ASN:O	2.16	0.45
1:A:146:ASN:OD1	1:A:280:GLU:HG3	2.16	0.45
1:A:514:TYR:O	1:A:517:GLN:HB3	2.17	0.45
1:A:71:ALA:HB3	1:A:77:ALA:HB2	1.98	0.45
1:A:77:ALA:O	1:A:80:PHE:HB2	2.16	0.45
1:A:478:VAL:HG13	1:A:720:PHE:CD2	2.52	0.45
1:A:512:LEU:HA	1:A:515:PHE:HB3	1.99	0.45
1:A:218:HIS:CD2	1:A:219:LEU:N	2.85	0.45
1:A:144:HIS:CE1	1:A:282:ARG:HD2	2.52	0.45
1:A:60:SER:HB3	1:A:112:ILE:HG23	1.99	0.45
1:A:393:ILE:CB	1:A:398:LEU:HG	2.47	0.45
1:A:489:LYS:HE3	1:A:499:THR:HG21	1.99	0.45
1:A:162:GLN:HG2	1:A:163:ALA:N	2.32	0.44
1:A:238:VAL:O	1:A:242:GLU:HG3	2.17	0.44
1:A:667:ILE:HG12	1:A:732:GLU:HB3	1.98	0.44
1:A:42:HIS:HB2	1:A:49[B]:ARG:HH11	1.81	0.44
1:A:443:ASN:HB2	1:A:457:TRP:O	2.17	0.44
1:A:474:ASP:OD1	1:A:691:TRP:HB3	2.16	0.44
1:A:466:LYS:O	1:A:470:MET:HB2	2.16	0.44
1:A:14:LEU:CD2	1:A:361:PHE:CE1	3.00	0.44
1:A:521:LYS:HG2	1:A:521:LYS:H	1.49	0.44
1:A:54:TYR:CE1	1:A:69:PRO:HD3	2.53	0.44
1:A:188:LEU:HG	1:A:305:PHE:CE2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:ILE:HG22	1:A:409:TYR:N	2.31	0.44
1:A:647:PRO:HB2	1:A:650:THR:OG1	2.18	0.44
1:A:334:LEU:HA	1:A:334:LEU:HD13	1.76	0.44
1:A:107:VAL:CB	1:A:200:GLU:HB2	2.48	0.44
1:A:209:ASN:CB	1:A:210:PRO:CD	2.94	0.44
1:A:392:MET:HB3	1:A:401:PHE:CD1	2.53	0.44
1:A:54:TYR:HA	1:A:67:ILE:O	2.17	0.44
1:A:620:SER:HB2	1:A:621:PRO:CD	2.48	0.44
1:A:654:LEU:N	1:A:654:LEU:HD22	2.32	0.44
1:A:628:GLY:O	1:A:632:GLN:HG3	2.18	0.44
1:A:61:GLU:N	1:A:62:PRO:HD2	2.33	0.43
1:A:310:LEU:HD23	1:A:310:LEU:HA	1.76	0.43
1:A:86:ASP:CG	1:A:421:LYS:HG3	2.38	0.43
1:A:198:ALA:HB1	1:A:201:ASP:HB2	2.00	0.43
1:A:641:THR:CG2	1:A:642:VAL:N	2.81	0.43
1:A:350:LEU:O	1:A:354:MET:HG3	2.19	0.43
1:A:749:GLU:HG2	1:A:750:LEU:N	2.32	0.43
1:A:86:ASP:CG	1:A:421:LYS:CG	2.87	0.43
1:A:589:VAL:C	1:A:658:SER:HB2	2.39	0.43
1:A:432:LEU:CB	1:A:739:THR:HG21	2.48	0.43
1:A:181:PHE:CD2	1:A:260:VAL:HB	2.53	0.43
1:A:66:LEU:HB3	1:A:84:ILE:CG2	2.48	0.43
1:A:191:LEU:HA	1:A:191:LEU:HD23	1.72	0.43
1:A:469:ASN:HB2	1:A:692:VAL:HG11	2.01	0.43
1:A:297:GLU:CD	1:A:297:GLU:H	2.22	0.43
1:A:48:SER:O	1:A:52:HIS:HB2	2.18	0.43
1:A:23:LEU:O	1:A:68:THR:HG23	2.18	0.42
1:A:40:THR:CB	1:A:41:PRO:HD2	2.49	0.42
1:A:58:ASP:C	1:A:58:ASP:OD1	2.57	0.42
1:A:728:THR:HG22	1:A:729:TYR:CD1	2.54	0.42
1:A:739:THR:N	1:A:740:PRO:CD	2.83	0.42
1:A:588:ARG:HG3	3:A:775:HOH:O	2.19	0.42
1:A:434:LEU:HA	1:A:434:LEU:HD12	1.71	0.42
1:A:723:LEU:H	1:A:723:LEU:HG	1.59	0.42
1:A:149:LEU:HD12	1:A:154:LEU:HD21	2.02	0.42
1:A:171:ASN:OD1	1:A:276:ILE:CG1	2.68	0.42
1:A:167:ILE:CG1	1:A:168:ASP:N	2.83	0.41
1:A:237:TYR:CD2	1:A:237:TYR:C	2.93	0.41
1:A:573:TYR:CD2	1:A:699:ILE:HD12	2.55	0.41
1:A:181:PHE:CZ	1:A:281:PHE:HD1	2.38	0.41
1:A:49[B]:ARG:HH12	1:A:57:THR:HG21	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:HIS:HB3	1:A:330:ASP:OD1	2.20	0.41
1:A:489:LYS:HE3	1:A:499:THR:CG2	2.51	0.41
1:A:635:LEU:HA	1:A:635:LEU:HD23	1.82	0.41
1:A:205:GLN:HB3	1:A:208:ASN:HB3	2.03	0.41
1:A:38:ALA:O	1:A:39:GLN:HB2	2.21	0.41
1:A:497:PHE:CE2	1:A:684:MET:HG2	2.56	0.41
1:A:108:ARG:HB3	1:A:111:ASP:H	1.86	0.41
1:A:512:LEU:O	1:A:512:LEU:HG	2.21	0.41
1:A:518:ILE:HA	1:A:521:LYS:CE	2.50	0.41
1:A:574:ARG:HH22	1:A:719:ASN:HD22	1.68	0.41
1:A:681:ALA:O	1:A:695:VAL:HG21	2.21	0.41
1:A:501:PHE:CZ	1:A:566:GLU:HB2	2.56	0.41
1:A:260:VAL:HG13	1:A:260:VAL:O	2.21	0.41
1:A:192:TYR:CE2	1:A:298:THR:HG23	2.55	0.40
1:A:559:ASP:CG	1:A:560:SER:N	2.74	0.40
1:A:14:LEU:HA	1:A:15:PRO:HD3	1.91	0.40
1:A:49[A]:ARG:NH2	3:A:753:HOH:O	2.53	0.40
1:A:538:ILE:HG22	1:A:538:ILE:O	2.20	0.40
1:A:436:ASP:HB3	1:A:743:LEU:HD23	2.03	0.40
1:A:52:HIS:CE1	1:A:55:ILE:HB	2.57	0.40
1:A:185:ARG:O	1:A:186:TRP:C	2.59	0.40
1:A:389:LEU:HA	1:A:389:LEU:HD12	1.84	0.40
1:A:594:VAL:HG23	1:A:594:VAL:O	2.21	0.40
1:A:655:ARG:NH1	3:A:759:HOH:O	2.55	0.40
1:A:717:GLU:CG	1:A:718:LEU:H	2.34	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	742/750 (99%)	716 (96%)	22 (3%)	4 (0%)	32 71

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	209	ASN
1	A	312	ILE
1	A	531	ASN
1	A	69	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	502/669 (75%)	452 (90%)	50 (10%)	9 31

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LEU
1	A	20	THR
1	A	23	LEU
1	A	26	GLU
1	A	46	LEU
1	A	49[A]	ARG
1	A	49[B]	ARG
1	A	60	SER
1	A	74	SER
1	A	76	GLU
1	A	79	ARG
1	A	86	ASP
1	A	95	ASP
1	A	147	LEU
1	A	157	LEU
1	A	164	ASP
1	A	175	MET
1	A	201	ASP
1	A	203	LEU
1	A	221	TYR
1	A	240	ASP

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Mol	Chain	Res	Type
1	A	279	LEU
1	A	294	ILE
1	A	296	GLN
1	A	330	ASP
1	A	371	LEU
1	A	405	GLN
1	A	408	ILE
1	A	425	THR
1	A	456	LEU
1	A	470	MET
1	A	501	PHE
1	A	510	GLU
1	A	512	LEU
1	A	516	SER
1	A	520	ASP
1	A	532	PHE
1	A	537	SER
1	A	563	LEU
1	A	619	ARG
1	A	638	GLN
1	A	655	ARG
1	A	671	ASN
1	A	688	MET
1	A	693	CYS
1	A	704	GLN
1	A	723	LEU
1	A	736	GLN
1	A	739	THR
1	A	745	LYS

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

Mol	Chain	Res	Type
1	A	39	GLN
1	A	93	ASN
1	A	94	HIS
1	A	113	GLN
1	A	138	GLN
1	A	144	HIS
1	A	208	ASN
1	A	209	ASN
1	A	336	HIS

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Mol	Chain	Res	Type
1	A	403	GLN
1	A	405	GLN
1	A	458	HIS
1	A	592	ASN
1	A	610	GLN
1	A	657	ASN
1	A	671	ASN
1	A	679	GLN
1	A	736	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

1 ligand is 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	751	-	4,4,4	0.31	0	6,6,6	0.37	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means

no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	751	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	743/750 (99%)	0.01	34 (4%) 33 20	42, 91, 158, 211	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	223	ASN	6.1
1	A	189	THR	5.6
1	A	142	GLY	5.4
1	A	224	HIS	5.2
1	A	617	ASP	4.8
1	A	283	THR	4.2
1	A	247	SER	4.1
1	A	208	ASN	4.0
1	A	202	PHE	3.9
1	A	222	VAL	3.7
1	A	141	SER	3.7
1	A	166	ALA	3.6
1	A	534	LEU	3.5
1	A	102	SER	3.3
1	A	252	ALA	3.1
1	A	616	TYR	3.0
1	A	271	TYR	2.9
1	A	607	LEU	2.8
1	A	257	TYR	2.8
1	A	531	ASN	2.7
1	A	285	ASP	2.6
1	A	244	ALA	2.5
1	A	107	VAL	2.4
1	A	542	SER	2.3
1	A	618	HIS	2.3
1	A	216	ASN	2.3
1	A	265	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	507	ASP	2.2
1	A	11	HIS	2.2
1	A	116	GLN	2.2
1	A	226	ASP	2.2
1	A	248	GLY	2.1
1	A	554	ILE	2.1
1	A	309	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
2	SO4	A	751	5/5	0.98	0.11	-1.54	73,77,82,91	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.