



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:41 AM UTC

PDB ID : 3LN6 / pdb_00003ln6
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

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

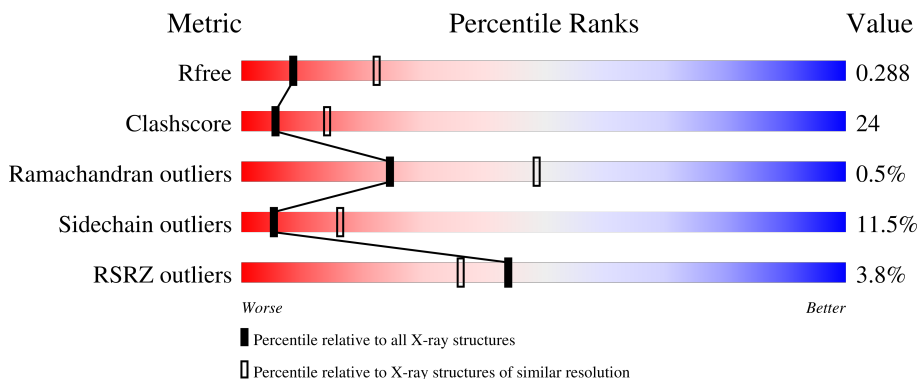
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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}	180053	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	750	4% 58% 35% 6%

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
			Total	C	N	O	S			
1	A	743	5493	3487	927	1063	16	0	5	0

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

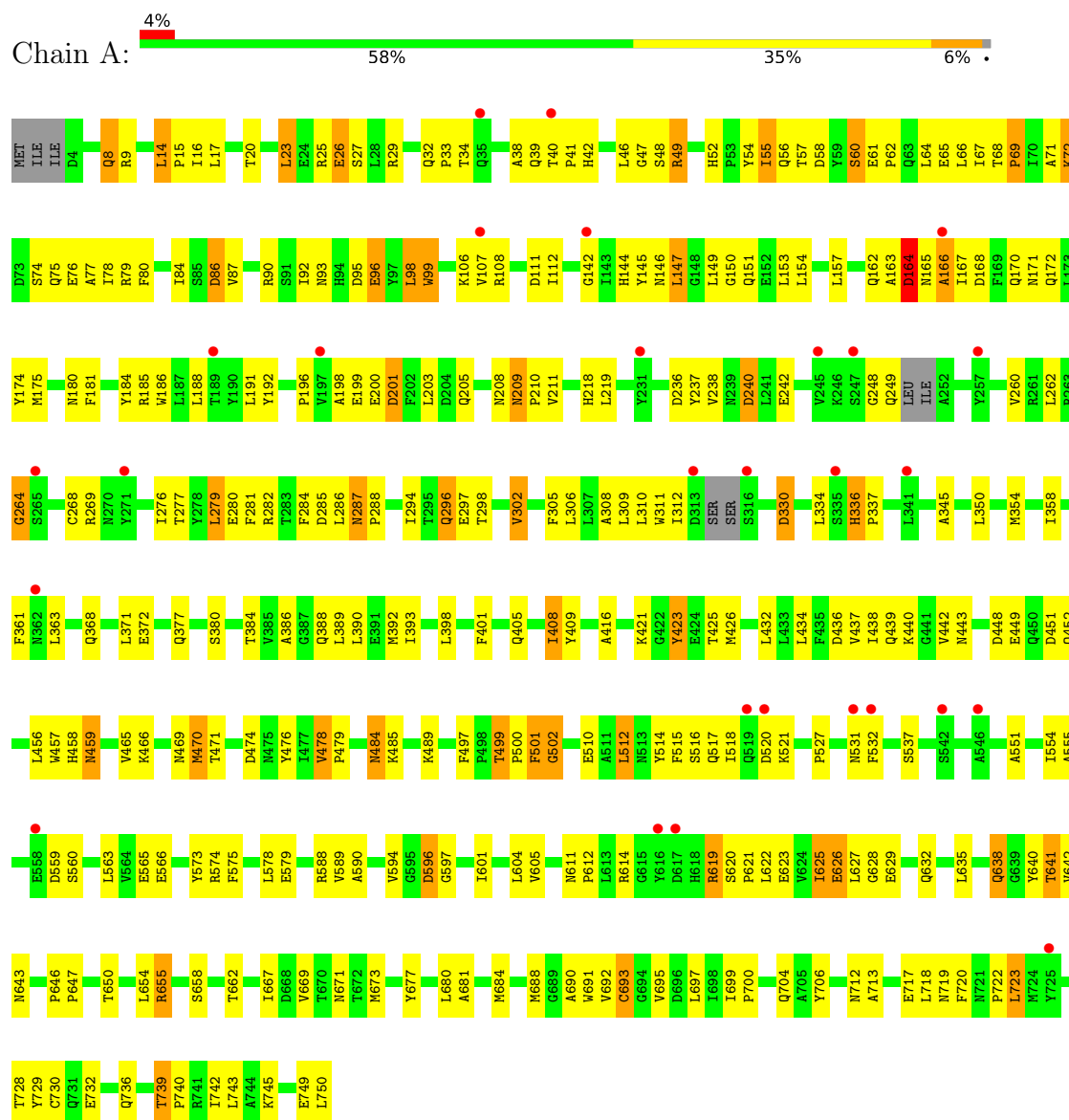
- Molecule 3 is water.

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, 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: 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, α , β , γ	143.02Å 143.02Å 211.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.95 20.00 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.9 (20.00-2.95) 99.4 (20.00-2.95)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 2.90Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.253 , 0.286 0.253 , 0.288	Depositor DCC
R_{free} test set	1246 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	76.2	Xtriage
Anisotropy	0.013	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 92.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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	0.93	EDS
Total number of atoms	5533	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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

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	0.88	3/5627 (0.1%)	1.12	29/7696 (0.4%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	478	VAL	CA-CB	8.44	1.58	1.54
1	A	416	ALA	CA-CB	-5.59	1.45	1.53
1	A	625	ILE	CA-CB	5.51	1.60	1.54

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	287	ASN	CA-C-N	9.08	128.82	119.56
1	A	287	ASN	C-N-CA	9.08	128.82	119.56
1	A	416	ALA	CA-C-N	7.89	127.96	119.28
1	A	416	ALA	C-N-CA	7.89	127.96	119.28
1	A	380	SER	CA-C-N	7.37	127.08	119.56
1	A	380	SER	C-N-CA	7.37	127.08	119.56
1	A	166	ALA	N-CA-C	-7.26	103.30	111.07
1	A	502	GLY	N-CA-C	7.12	121.23	111.54
1	A	459	ASN	CB-CA-C	-6.95	108.57	116.63
1	A	336	HIS	CA-C-N	6.25	125.74	119.24
1	A	336	HIS	C-N-CA	6.25	125.74	119.24
1	A	484	ASN	N-CA-C	6.09	117.61	110.97
1	A	164	ASP	N-CA-C	6.05	117.54	111.07
1	A	499	THR	CA-C-N	5.86	126.32	120.52
1	A	499	THR	C-N-CA	5.86	126.32	120.52
1	A	8	GLN	N-CA-C	-5.83	105.01	111.71
1	A	72	LYS	N-CA-C	5.70	117.50	111.28
1	A	423	TYR	N-CA-C	5.59	118.05	110.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	388	GLN	N-CA-C	-5.57	105.21	111.28
1	A	99	TRP	CA-C-N	5.54	124.89	118.85
1	A	99	TRP	C-N-CA	5.54	124.89	118.85
1	A	646	PRO	CA-C-N	5.26	125.17	119.85
1	A	646	PRO	C-N-CA	5.26	125.17	119.85
1	A	172	GLN	N-CA-C	-5.23	105.47	111.07
1	A	596	ASP	N-CA-C	-5.20	100.43	108.90
1	A	302	VAL	N-CA-C	-5.16	105.35	110.62
1	A	629	GLU	N-CA-C	-5.08	105.83	111.36
1	A	264	GLY	N-CA-C	-5.07	108.32	115.32
1	A	55	ILE	N-CA-C	5.04	115.17	108.11

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	5493	0	4883	242	0
2	A	5	0	0	0	0
3	A	35	0	0	5	0
All	All	5533	0	4883	242	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 (242) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:423:TYR:HD2	1:A:426:MET:HE3	1.68	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:285:ASP:O	1:A:286:LEU:C	2.46	0.58
1:A:218:HIS:CG	1:A:219:LEU:N	2.71	0.58
1:A:619:ARG:HA	1:A:619:ARG:NE	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:501:PHE:C	1:A:501:PHE:CD2	2.83	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
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:HG12	1:A:669:VAL:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:66:LEU:N	1:A:66:LEU:HD12	2.23	0.54
1:A:611:ASN:CG	1:A:612:PRO:HD2	2.33	0.54
1:A:611:ASN:HB3	1:A:614:ARG:HG3	1.88	0.54
1:A:501:PHE:C	1:A:501:PHE:HD2	2.15	0.53
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: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: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:54:TYR:HB3	1:A:84:ILE:HD12	1.90	0.53
1:A:484:ASN:O	1:A:485:LYS:CB	2.57	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:HD12	1:A:66:LEU:H	1.74	0.52
1:A:32:GLN:HB3	1:A:33:PRO:HD3	1.92	0.52
1:A:336:HIS:CD2	1:A:337:PRO:HD2	2.44	0.52
1:A:86:ASP:OD1	1:A:421:LYS:HG3	2.10	0.52
1:A:248:GLY:O	1:A:249:GLN:O	2.28	0.52
1:A:551:ALA:O	1:A:554:ILE:HG22	2.10	0.52
1:A:87:VAL:HG21	1:A:438:ILE:HB	1.91	0.51
1:A:284:PHE:CE2	1:A:302:VAL:HG21	2.44	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:HG22	1:A:34:THR:O	2.10	0.51
1:A:268:CYS:O	1:A:269:ARG:CB	2.57	0.51
1:A:29:ARG:HG3	1:A:62:PRO:O	2.10	0.51
1:A:514:TYR:O	1:A:517:GLN:N	2.44	0.51
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:66:LEU:HB3	1:A:84:ILE:HG21	1.94	0.49
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:667:ILE:HA	1:A:732:GLU:O	2.12	0.49
1:A:423:TYR:CD2	1:A:426:MET:HE3	2.48	0.49
1:A:25:ARG:O	1:A:65:GLU:HA	2.12	0.49
1:A:655:ARG:HG3	1:A:662:THR:HB	1.95	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:99:TRP:HD1	3:A:754:HOH:O	1.96	0.48
1:A:655:ARG:HH21	1:A:655:ARG:CG	2.27	0.48
1:A:287:ASN:HA	1:A:288:PRO:HD3	1.65	0.48
1:A:589:VAL:C	1:A:658:SER:HB2	2.39	0.48
1:A:86:ASP:CG	1:A:421:LYS:HG3	2.38	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:86:ASP:CG	1:A:421:LYS:CG	2.87	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:54:TYR:O	1:A:66:LEU:HA	2.14	0.47
1:A:297:GLU:CD	1:A:297:GLU:H	2.22	0.47
1:A:465:VAL:HG12	1:A:471:THR:HG22	1.96	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:501:PHE:CG	1:A:566:GLU:HB2	2.50	0.47
1:A:739:THR:OG1	1:A:740:PRO:HD3	2.14	0.47
1:A:58:ASP:OD1	1:A:58:ASP:C	2.57	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:237:TYR:C	1:A:237:TYR:CD2	2.93	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:CD1	1:A:284:PHE:N	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:CD2	1:A:575:PHE:N	2.83	0.45
1:A:700:PRO:HD2	1:A:712:ASN:O	2.16	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: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:673:MET:HE1	1:A:699:ILE:HD13	1.98	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:60:SER:HB3	1:A:112:ILE:HG23	1.99	0.45
1:A:144:HIS:CE1	1:A:282:ARG:HD2	2.52	0.45
1:A:218:HIS:CD2	1:A:219:LEU:N	2.85	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:185:ARG:O	1:A:186:TRP:C	2.59	0.44
1:A:466:LYS:O	1:A:470:MET:HB2	2.16	0.44
1:A:559:ASP:CG	1:A:560:SER:N	2.74	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:680:LEU:HG	1:A:684:MET:HE2	1.99	0.44
1:A:14:LEU:CD2	1:A:361:PHE:CE1	3.00	0.44
1:A:54:TYR:CE1	1:A:69:PRO:HD3	2.53	0.44
1:A:521:LYS:H	1:A:521:LYS:HG2	1.49	0.44
1:A:188:LEU:HG	1:A:305:PHE:CE2	2.52	0.44
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:HD13	1:A:334:LEU:HA	1.76	0.44
1:A:54:TYR:HA	1:A:67:ILE:O	2.17	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:596:ASP:O	1:A:597:GLY:C	2.61	0.44
1:A:620:SER:HB2	1:A:621:PRO:CD	2.48	0.44
1:A:654:LEU:HD22	1:A:654:LEU:N	2.32	0.44
1:A:628:GLY:O	1:A:632:GLN:HG3	2.18	0.44
1:A:684:MET:HE1	1:A:697:LEU:HD21	1.99	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: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:432:LEU:CB	1:A:739:THR:HG21	2.48	0.43
1:A:66:LEU:HB3	1:A:84:ILE:CG2	2.48	0.43
1:A:181:PHE:CD2	1:A:260:VAL:HB	2.53	0.43
1:A:191:LEU:HD23	1:A:191:LEU:HA	1.72	0.43
1:A:469:ASN:HB2	1:A:692:VAL:HG11	2.01	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: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:47:GLY:O	1:A:48:SER:C	2.63	0.42
1:A:588:ARG:HG3	3:A:775:HOH:O	2.19	0.42
1:A:434:LEU:HD12	1:A:434:LEU:HA	1.71	0.42
1:A:641:THR:O	1:A:642:VAL:C	2.61	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:573:TYR:CD2	1:A:699:ILE:HD12	2.55	0.41
1:A:49[B]:ARG:HH12	1:A:57:THR:HG21	1.85	0.41
1:A:181:PHE:CZ	1:A:281:PHE:HD1	2.38	0.41
1:A:150:GLY:O	1:A:151:GLN:C	2.63	0.41
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:HD23	1:A:635:LEU:HA	1.82	0.41
1:A:38:ALA:O	1:A:39:GLN:HB2	2.21	0.41
1:A:205:GLN:HB3	1:A:208:ASN:HB3	2.03	0.41
1:A:248:GLY:C	1:A:249:GLN:O	2.62	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:218:HIS:HB3	1:A:330:ASP:CG	2.45	0.41
1:A:512:LEU:O	1:A:512:LEU:HG	2.21	0.41
1:A:501:PHE:CZ	1:A:566:GLU:HB2	2.56	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:578:LEU:O	1:A:579:GLU:C	2.63	0.41
1:A:681:ALA:O	1:A:695:VAL:HG21	2.21	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: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: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:389:LEU:HD12	1:A:389:LEU:HA	1.84	0.40
1:A:594:VAL:O	1:A:594:VAL:HG23	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%)	24	49

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%)	443 (88%)	59 (12%)	5	15

All (59) 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	72	LYS
1	A	74	SER
1	A	76	GLU
1	A	86	ASP
1	A	92	ILE
1	A	95	ASP
1	A	96	GLU
1	A	98	LEU
1	A	147	LEU

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Mol	Chain	Res	Type
1	A	157	LEU
1	A	164	ASP
1	A	175	MET
1	A	201	ASP
1	A	203	LEU
1	A	240	ASP
1	A	262	LEU
1	A	279	LEU
1	A	294	ILE
1	A	296	GLN
1	A	330	ASP
1	A	371	LEU
1	A	377	GLN
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	626[A]	GLU
1	A	626[B]	GLU
1	A	638	GLN
1	A	641	THR
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	730	CYS
1	A	736	GLN
1	A	739	THR
1	A	742	ILE
1	A	745	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
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	162	GLN
1	A	208	ASN
1	A	209	ASN
1	A	216	ASN
1	A	336	HIS
1	A	344	GLN
1	A	368	GLN
1	A	403	GLN
1	A	405	GLN
1	A	458	HIS
1	A	610	GLN
1	A	657	ASN
1	A	671	ASN
1	A	679	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 oligosaccharides 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	0.35	0	6,6,6	0.41	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, 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	743/750 (99%)	0.17	28 (3%) 44 36	29, 91, 158, 211	5 (0%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	531	ASN	4.6
1	A	231	TYR	3.7
1	A	519	GLN	3.4
1	A	362	ASN	3.3
1	A	189	THR	3.3
1	A	316	SER	3.2
1	A	341	LEU	3.2
1	A	257	TYR	3.0
1	A	247	SER	3.0
1	A	546	ALA	2.8
1	A	40	THR	2.7
1	A	142	GLY	2.7
1	A	265	SER	2.7
1	A	542	SER	2.7
1	A	271	TYR	2.6
1	A	313	ASP	2.6
1	A	107	VAL	2.5
1	A	532	PHE	2.5
1	A	520	ASP	2.5
1	A	616	TYR	2.4
1	A	197	VAL	2.4
1	A	558	GLU	2.3
1	A	35	GLN	2.3
1	A	335	SER	2.3
1	A	166	ALA	2.2
1	A	245	VAL	2.1
1	A	725	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	617	ASP	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
2	SO4	A	751	5/5	0.96	0.08	73,77,82,91	0

6.5 Other polymers [i](#)

There are no such residues in this entry.