



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 16, 2017 – 02:50 PM EST

PDB ID : 5W1L
Title : Echinococcus granulosus thioredoxin glutathione reductas (egTGR) with Gold
Authors : Gao, W.; Wang, Y.; Dai, S.
Deposited on : unknown
Resolution : 2.88 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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 : rb-20030345
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) : rb-20030345

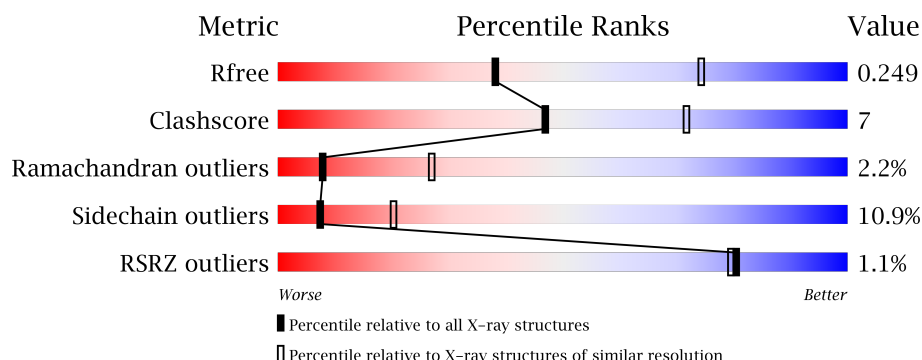
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 2.88 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	2135 (2.90-2.86)
Clashscore	112137	2400 (2.90-2.86)
Ramachandran outliers	110173	2346 (2.90-2.86)
Sidechain outliers	110143	2349 (2.90-2.86)
RSRZ outliers	101464	2149 (2.90-2.86)

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 ≥ 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	586	 77% 20% 2% 1%
2	B	584	 74% 21% 2% 1%

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 9123 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 Thioredoxin glutathione reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	584	4518	2858	766	865	29	0	1	0

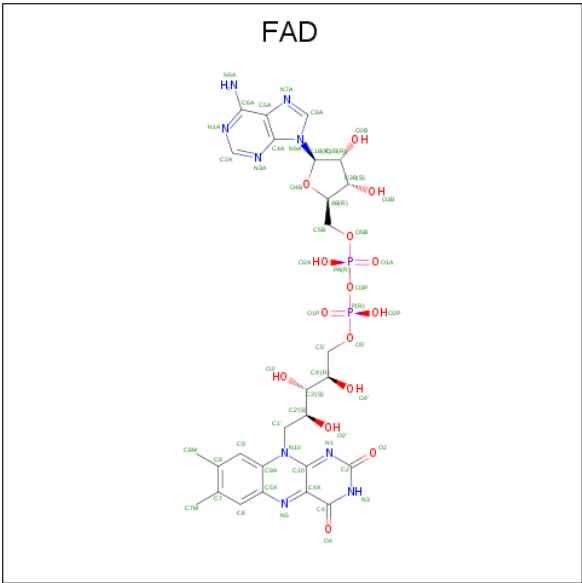
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ALA	-	expression tag	UNP Q869D7
A	3	SEC	-	expression tag	UNP Q869D7

- Molecule 2 is a protein called Thioredoxin glutathione reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	584	4497	2844	762	862	29	0	0	0

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

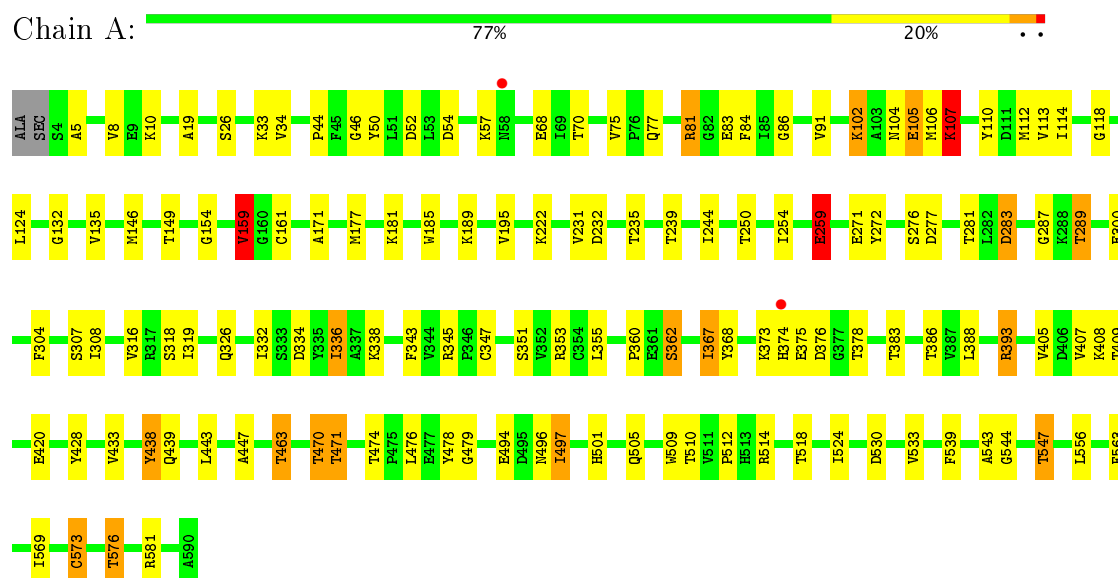
- Molecule 4 is GOLD ION (three-letter code: AU) (formula: Au).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Au	0	0
			1	1		
4	A	1	Total	Au	0	0
			1	1		

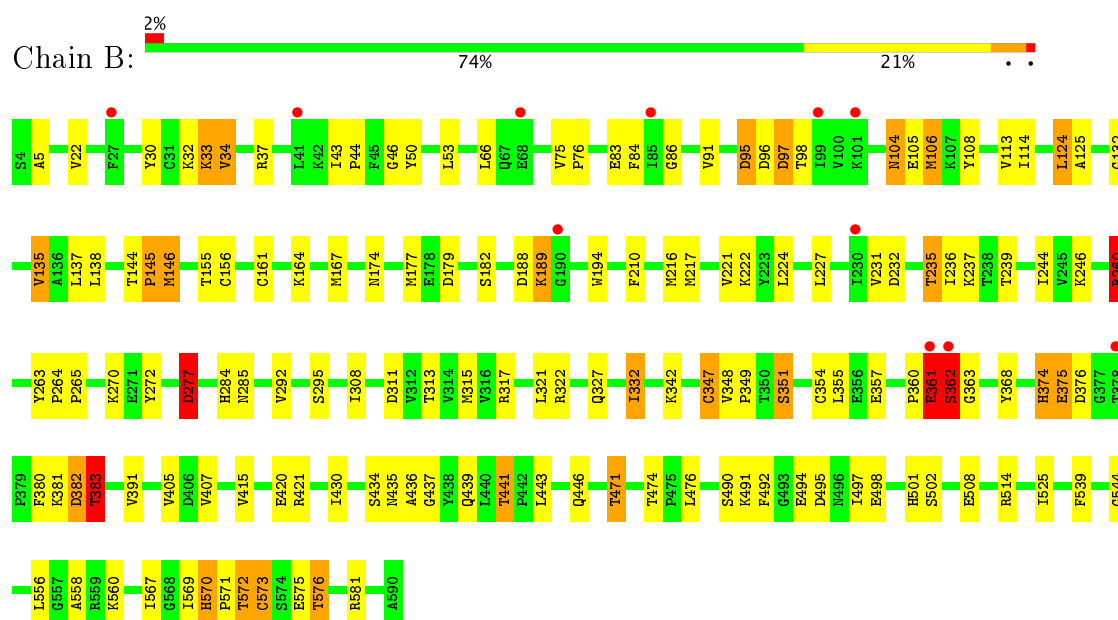
3 Residue-property plots

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: Thioredoxin glutathione reductase



• Molecule 2: Thioredoxin glutathione reductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	109.35Å 109.35Å 258.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.72 – 2.88 49.61 – 2.88	Depositor EDS
% Data completeness (in resolution range)	99.0 (100.72-2.88) 99.0 (49.61-2.88)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.75 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.185 , 0.249 0.188 , 0.249	Depositor DCC
R_{free} test set	1802 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	70.9	Xtriage
Anisotropy	0.467	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 33.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9123	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% 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: AU, FAD

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	0.98	6/4613 (0.1%)	1.05	8/6255 (0.1%)
2	B	0.93	2/4592 (0.0%)	1.05	10/6231 (0.2%)
All	All	0.96	8/9205 (0.1%)	1.05	18/12486 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	5
All	All	0	6

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	259	GLU	CD-OE2	7.20	1.33	1.25
1	A	438	TYR	CG-CD2	5.92	1.46	1.39
2	B	573	CYS	CB-SG	5.73	1.92	1.82
1	A	300	GLU	CD-OE1	5.69	1.31	1.25
1	A	573	CYS	CB-SG	5.50	1.91	1.82
2	B	420	GLU	CD-OE1	5.25	1.31	1.25
1	A	420	GLU	CD-OE1	5.22	1.31	1.25
1	A	259	GLU	CG-CD	5.16	1.59	1.51

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	393	ARG	NE-CZ-NH1	6.90	123.75	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	382	ASP	N-CA-C	6.85	129.50	111.00
2	B	277	ASP	CB-CG-OD1	6.36	124.02	118.30
2	B	260	ARG	CB-CG-CD	6.21	127.74	111.60
2	B	311	ASP	CB-CG-OD1	6.17	123.85	118.30
1	A	524	ILE	CG1-CB-CG2	-6.01	98.18	111.40
2	B	570	HIS	C-N-CD	-5.96	107.48	120.60
2	B	421	ARG	NE-CZ-NH2	-5.65	117.48	120.30
2	B	332	ILE	CB-CA-C	-5.42	100.76	111.60
2	B	260	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	A	81	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	A	530	ASP	CB-CG-OD1	5.33	123.10	118.30
2	B	146	MET	CA-CB-CG	5.29	122.29	113.30
1	A	581	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	A	353	ARG	NE-CZ-NH2	5.22	122.91	120.30
2	B	295	SER	N-CA-C	-5.18	97.03	111.00
1	A	433	VAL	CB-CA-C	-5.00	101.89	111.40
1	A	514	ARG	NE-CZ-NH1	5.00	122.80	120.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	57	LYS	Peptide
2	B	104	ASN	Peptide
2	B	284	HIS	Peptide
2	B	360	PRO	Peptide
2	B	363	GLY	Peptide
2	B	434	SER	Peptide

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	4518	0	4444	64	0
2	B	4497	0	4406	70	0
3	A	53	0	31	0	0
3	B	53	0	31	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	1	0	0	0	0
4	B	1	0	0	0	0
All	All	9123	0	8912	128	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 7.

All (128) 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:46:GLY:C	1:A:50:TYR:N	2.14	1.01
1:A:46:GLY:O	1:A:50:TYR:N	2.09	0.86
2:B:46:GLY:O	2:B:50:TYR:N	2.10	0.85
2:B:46:GLY:C	2:B:50:TYR:N	2.33	0.82
1:A:471:THR:HG21	1:A:544:GLY:HA2	1.62	0.81
1:A:319:ILE:HG12	1:A:326:GLN:OE1	1.87	0.74
2:B:105:GLU:O	2:B:106:MET:O	2.09	0.70
1:A:476:LEU:HD23	1:A:539:PHE:CZ	2.30	0.67
2:B:232:ASP:OD1	2:B:235:THR:HG23	1.95	0.66
1:A:289:THR:HB	1:A:386:THR:HB	1.77	0.65
2:B:405:VAL:HG23	2:B:407:VAL:HG23	1.79	0.65
1:A:46:GLY:O	1:A:50:TYR:CA	2.45	0.65
1:A:447:ALA:HA	1:A:463:THR:HG21	1.80	0.64
1:A:573:CYS:O	1:A:576:THR:HG23	1.99	0.63
1:A:113:VAL:HG23	1:A:250:THR:HB	1.79	0.62
2:B:155:THR:OG1	3:B:601:FAD:O1A	2.18	0.62
2:B:138:LEU:HD11	2:B:236:ILE:HD11	1.81	0.61
2:B:347:CYS:HA	2:B:374:HIS:HB3	1.83	0.60
1:A:476:LEU:HD23	1:A:539:PHE:CE2	2.36	0.60
1:A:19:ALA:HA	1:A:81:ARG:HG2	1.84	0.60
1:A:319:ILE:CG1	1:A:326:GLN:OE1	2.50	0.60
1:A:84:PHE:CZ	1:A:86:GLY:HA2	2.38	0.59
1:A:44:PRO:HB2	1:A:132:GLY:HA2	1.86	0.58
2:B:216:MET:CE	2:B:221:VAL:HG11	2.33	0.58
2:B:34:VAL:HG23	2:B:91:VAL:HG11	1.85	0.58
1:A:46:GLY:O	1:A:50:TYR:HA	2.04	0.58
2:B:441:THR:HG22	3:B:601:FAD:H2'	1.86	0.57
2:B:315:MET:HE2	2:B:349:PRO:N	2.20	0.56
1:A:332:ILE:HD11	1:A:478:TYR:HB2	1.88	0.55
1:A:110:TYR:OH	1:A:222:LYS:HE3	2.05	0.55
2:B:315:MET:HE2	2:B:349:PRO:CA	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:505:GLN:NE2	1:A:510:THR:HG22	2.21	0.55
1:A:159:VAL:HG22	1:A:277:ASP:HA	1.89	0.55
1:A:497:ILE:HD12	1:A:497:ILE:C	2.27	0.54
2:B:144:THR:O	2:B:145:PRO:C	2.45	0.54
2:B:382:ASP:O	2:B:382:ASP:CG	2.46	0.54
1:A:287:GLY:O	1:A:289:THR:HG22	2.08	0.54
1:A:405:VAL:HG23	1:A:407:VAL:HG23	1.90	0.53
2:B:138:LEU:HD11	2:B:236:ILE:CD1	2.39	0.53
1:A:471:THR:HG23	2:B:569:ILE:HG21	1.90	0.53
1:A:113:VAL:HG23	1:A:250:THR:CB	2.39	0.53
2:B:22:VAL:O	2:B:50:TYR:HA	2.09	0.52
2:B:382:ASP:O	2:B:383:THR:HB	2.10	0.52
1:A:479:GLY:HA3	1:A:547:THR:HG21	1.92	0.51
1:A:360:PRO:O	1:A:362:SER:HA	2.11	0.51
2:B:125:ALA:HB3	2:B:216:MET:HE1	1.92	0.51
1:A:443:LEU:HD13	2:B:567:ILE:HG13	1.92	0.51
1:A:355:LEU:HD12	1:A:367:ILE:HD11	1.93	0.51
1:A:259:GLU:OE2	1:A:393:ARG:HD3	2.11	0.50
1:A:171:ALA:HB1	1:A:307:SER:HB2	1.94	0.50
1:A:543:ALA:O	1:A:547:THR:HG23	2.11	0.50
2:B:313:THR:HA	2:B:342:LYS:O	2.12	0.50
1:A:470:THR:O	1:A:471:THR:HG22	2.12	0.49
2:B:260:ARG:NH1	2:B:277:ASP:OD2	2.35	0.49
1:A:185:TRP:CZ2	2:B:174:ASN:HB2	2.48	0.49
2:B:216:MET:HE2	2:B:221:VAL:HG11	1.93	0.49
2:B:476:LEU:HD23	2:B:539:PHE:CZ	2.47	0.49
2:B:113:VAL:HG11	2:B:236:ILE:HG12	1.93	0.49
2:B:361:GLU:O	2:B:362:SER:HB2	2.13	0.49
2:B:44:PRO:HB2	2:B:132:GLY:HA2	1.94	0.48
2:B:135:VAL:HG22	2:B:221:VAL:HG13	1.95	0.48
2:B:260:ARG:CG	2:B:260:ARG:HH11	2.26	0.48
2:B:441:THR:CG2	3:B:601:FAD:H2'	2.43	0.48
1:A:83:GLU:OE1	1:A:102:LYS:NZ	2.29	0.48
2:B:114:ILE:HD12	2:B:124:LEU:HD13	1.94	0.48
1:A:316:VAL:HG11	1:A:345:ARG:HD2	1.96	0.48
1:A:8:VAL:HG21	1:A:68:GLU:OE2	2.14	0.48
2:B:347:CYS:HA	2:B:374:HIS:CB	2.44	0.48
2:B:260:ARG:HH11	2:B:260:ARG:HG2	1.79	0.47
2:B:137:LEU:HD22	2:B:216:MET:HE1	1.97	0.47
2:B:471:THR:HG21	2:B:544:GLY:HA2	1.97	0.47
1:A:471:THR:HG21	1:A:544:GLY:CA	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:354:CYS:SG	2:B:355:LEU:N	2.88	0.47
1:A:569:ILE:HG21	2:B:471:THR:HG23	1.96	0.47
2:B:476:LEU:HD23	2:B:539:PHE:CE2	2.49	0.47
1:A:177:MET:HG2	2:B:177:MET:HG2	1.97	0.47
2:B:491:LYS:HE2	2:B:492:PHE:CZ	2.50	0.46
2:B:375:GLU:OE2	2:B:375:GLU:N	2.49	0.46
2:B:114:ILE:HB	2:B:137:LEU:HD12	1.96	0.46
2:B:30:TYR:O	2:B:34:VAL:HG12	2.16	0.46
2:B:497:ILE:HA	2:B:525:ILE:O	2.16	0.46
1:A:104:ASN:O	1:A:105:GLU:C	2.54	0.45
1:A:272:TYR:HB3	1:A:368:TYR:CE2	2.51	0.45
1:A:543:ALA:O	1:A:547:THR:CG2	2.64	0.45
1:A:509:TRP:C	1:A:512:PRO:HD2	2.37	0.45
1:A:114:ILE:HD12	1:A:124:LEU:HD23	1.97	0.45
1:A:124:LEU:HD21	1:A:254:ILE:HG12	1.98	0.45
2:B:179:ASP:OD2	2:B:514:ARG:NH1	2.50	0.45
2:B:573:CYS:O	2:B:576:THR:HG23	2.16	0.45
2:B:138:LEU:HD23	2:B:224:LEU:HB2	1.99	0.44
1:A:496:ASN:OD1	1:A:496:ASN:N	2.50	0.44
2:B:236:ILE:HD12	2:B:236:ILE:C	2.38	0.44
1:A:232:ASP:OD1	1:A:232:ASP:C	2.56	0.44
2:B:263:TYR:CE2	2:B:270:LYS:HA	2.53	0.44
2:B:332:ILE:HG21	2:B:474:THR:HG21	1.99	0.43
1:A:70:THR:HG21	1:A:77:GLN:OE1	2.18	0.43
2:B:125:ALA:HB3	2:B:216:MET:CE	2.48	0.43
1:A:106:MET:O	1:A:107:LYS:CB	2.66	0.43
1:A:336:ILE:HG21	1:A:343:PHE:HZ	1.83	0.43
2:B:415:VAL:HA	2:B:435:ASN:HB2	2.00	0.43
2:B:84:PHE:CZ	2:B:86:GLY:HA2	2.53	0.43
2:B:156:CYS:HB2	2:B:441:THR:HG21	1.99	0.43
1:A:34:VAL:HG22	1:A:91:VAL:HG11	2.01	0.43
2:B:216:MET:HE3	2:B:221:VAL:HG11	2.00	0.43
1:A:304:PHE:O	1:A:308:ILE:HG12	2.20	0.42
2:B:188:ASP:OD1	2:B:189:LYS:N	2.51	0.42
1:A:46:GLY:CA	1:A:50:TYR:N	2.80	0.42
1:A:159:VAL:O	1:A:159:VAL:HG13	2.20	0.42
2:B:572:THR:HG22	2:B:575:GLU:HG2	2.02	0.42
2:B:33:LYS:O	2:B:33:LYS:HG2	2.18	0.42
2:B:315:MET:HE2	2:B:349:PRO:CB	2.50	0.42
1:A:254:ILE:HG13	1:A:428:TYR:HB2	2.01	0.41
2:B:264:PRO:HA	2:B:265:PRO:HD3	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:556:LEU:HD11	2:B:558:ALA:HB2	2.02	0.41
1:A:195:VAL:HG22	1:A:283:ASP:O	2.20	0.41
1:A:112:MET:HG3	1:A:254:ILE:HD13	2.02	0.41
1:A:318:SER:OG	1:A:319:ILE:N	2.52	0.41
1:A:52:ASP:OD1	1:A:54:ASP:HB2	2.20	0.41
2:B:167:MET:HE3	2:B:194:TRP:CH2	2.55	0.41
2:B:315:MET:HE2	2:B:349:PRO:HB3	2.01	0.41
2:B:75:VAL:HG22	2:B:76:PRO:HA	2.03	0.41
2:B:95:ASP:OD1	2:B:95:ASP:N	2.51	0.41
2:B:272:TYR:HB3	2:B:368:TYR:CD2	2.55	0.41
1:A:533:VAL:HG21	1:A:563:PHE:CE1	2.56	0.40
1:A:118:GLY:HA2	1:A:154:GLY:HA3	2.03	0.40
2:B:570:HIS:HA	2:B:571:PRO:HA	1.84	0.40
1:A:181:LYS:HA	1:A:185:TRP:O	2.21	0.40
2:B:321:LEU:O	2:B:322:ARG:C	2.59	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	581/586 (99%)	534 (92%)	39 (7%)	8 (1%)	13	40
2	B	580/584 (99%)	510 (88%)	52 (9%)	18 (3%)	5	18
All	All	1161/1170 (99%)	1044 (90%)	91 (8%)	26 (2%)	8	27

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	ALA
1	A	375	GLU
2	B	5	ALA

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Mol	Chain	Res	Type
2	B	34	VAL
2	B	106	MET
2	B	361	GLU
2	B	362	SER
2	B	374	HIS
2	B	436	ALA
1	A	334	ASP
1	A	336	ILE
2	B	189	LYS
2	B	437	GLY
1	A	26	SER
1	A	189	LYS
2	B	277	ASP
2	B	351	SER
2	B	391	VAL
1	A	107	LYS
2	B	96	ASP
2	B	97	ASP
1	A	159	VAL
2	B	145	PRO
2	B	244	ILE
2	B	383	THR
2	B	285	ASN

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	493/493 (100%)	446 (90%)	47 (10%)	10	27
2	B	489/493 (99%)	428 (88%)	61 (12%)	5	14
All	All	982/986 (100%)	874 (89%)	108 (11%)	7	20

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LYS
1	A	33	LYS
1	A	75	VAL
1	A	102	LYS
1	A	105	GLU
1	A	107	LYS
1	A	135	VAL
1	A	146	MET
1	A	149	THR
1	A	159	VAL
1	A	161	CYS
1	A	231	VAL
1	A	235	THR
1	A	239	THR
1	A	244	ILE
1	A	259	GLU
1	A	271	GLU
1	A	276	SER
1	A	281	THR
1	A	283	ASP
1	A	289	THR
1	A	338[A]	LYS
1	A	338[B]	LYS
1	A	347	CYS
1	A	351	SER
1	A	362	SER
1	A	367	ILE
1	A	373	LYS
1	A	374	HIS
1	A	376	ASP
1	A	378	THR
1	A	383	THR
1	A	388	LEU
1	A	408	LYS
1	A	409	THR
1	A	438	TYR
1	A	439	GLN
1	A	463	THR
1	A	470	THR
1	A	471	THR
1	A	474	THR
1	A	494	GLU
1	A	497	ILE

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Mol	Chain	Res	Type
1	A	501	HIS
1	A	518	THR
1	A	547	THR
1	A	576	THR
2	B	32	LYS
2	B	33	LYS
2	B	37	ARG
2	B	43	ILE
2	B	53	LEU
2	B	66	LEU
2	B	83	GLU
2	B	95	ASP
2	B	97	ASP
2	B	98	THR
2	B	104	ASN
2	B	108	TYR
2	B	124	LEU
2	B	135	VAL
2	B	146	MET
2	B	161	CYS
2	B	164	LYS
2	B	182	SER
2	B	210	PHE
2	B	217	MET
2	B	222	LYS
2	B	227	LEU
2	B	231	VAL
2	B	235	THR
2	B	237	LYS
2	B	239	THR
2	B	246	LYS
2	B	260	ARG
2	B	292	VAL
2	B	308	ILE
2	B	317	ARG
2	B	327	GLN
2	B	347	CYS
2	B	348	VAL
2	B	351	SER
2	B	357	GLU
2	B	361	GLU
2	B	362	SER

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Mol	Chain	Res	Type
2	B	375	GLU
2	B	376	ASP
2	B	380	PHE
2	B	381	LYS
2	B	383	THR
2	B	430	ILE
2	B	439	GLN
2	B	441	THR
2	B	443	LEU
2	B	446	GLN
2	B	471	THR
2	B	490	SER
2	B	494	GLU
2	B	495	ASP
2	B	498	GLU
2	B	501	HIS
2	B	502	SER
2	B	508	GLU
2	B	556	LEU
2	B	560	LYS
2	B	572	THR
2	B	576	THR
2	B	581	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	505	GLN
1	A	517	ASN
2	B	446	GLN

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	$\# Z > 2$
3	FAD	A	601	-	51,58,58	1.36	10 (19%)	54,89,89	2.37	11 (20%)
3	FAD	B	601	-	51,58,58	1.45	6 (11%)	54,89,89	2.25	13 (24%)

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	FAD	A	601	-	-	0/28/50/50	0/6/6/6
3	FAD	B	601	-	-	0/28/50/50	0/6/6/6

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	FAD	C4X-N5	-3.06	1.28	1.33
3	B	601	FAD	C1'-N10	-2.92	1.45	1.48
3	A	601	FAD	C2-N3	-2.66	1.32	1.38
3	A	601	FAD	C2B-C1B	-2.31	1.50	1.53
3	A	601	FAD	C2-N1	-2.22	1.33	1.38
3	A	601	FAD	C5X-N5	-2.21	1.31	1.35
3	A	601	FAD	C2A-N1A	2.08	1.37	1.33
3	B	601	FAD	C10-N1	2.12	1.36	1.33
3	A	601	FAD	C8-C7	2.17	1.46	1.41
3	A	601	FAD	C2A-N3A	2.18	1.35	1.32
3	B	601	FAD	C8-C7	2.27	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	FAD	C9A-C5X	2.38	1.47	1.42
3	B	601	FAD	C5A-C4A	2.86	1.47	1.40
3	A	601	FAD	C5A-C4A	3.47	1.48	1.40
3	B	601	FAD	C9A-C5X	4.09	1.51	1.42
3	B	601	FAD	C4X-C10	4.63	1.49	1.41

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	601	FAD	N3A-C2A-N1A	-7.39	122.42	128.86
3	A	601	FAD	N3A-C2A-N1A	-4.13	125.26	128.86
3	A	601	FAD	C4-C4X-C10	-4.09	116.66	119.96
3	B	601	FAD	C4A-C5A-N7A	-3.75	105.79	109.41
3	B	601	FAD	C4-C4X-C10	-3.59	117.06	119.96
3	B	601	FAD	C4X-C10-N10	-3.30	118.23	120.52
3	A	601	FAD	C4X-C4-N3	-3.21	118.91	123.48
3	B	601	FAD	C4X-C4-N3	-2.81	119.48	123.48
3	B	601	FAD	C4B-O4B-C1B	-2.64	106.95	109.77
3	B	601	FAD	O4'-C4'-C5'	-2.49	104.46	110.00
3	A	601	FAD	O2'-C2'-C1'	-2.36	104.34	109.79
3	A	601	FAD	O4'-C4'-C5'	-2.24	105.01	110.00
3	B	601	FAD	C9-C8-C7	2.03	123.57	119.95
3	A	601	FAD	N6A-C6A-N1A	2.44	123.60	118.77
3	A	601	FAD	C4B-O4B-C1B	2.53	112.47	109.77
3	B	601	FAD	C5X-C9A-N10	2.55	119.56	117.66
3	B	601	FAD	C2A-N1A-C6A	2.61	123.33	118.77
3	B	601	FAD	C10-C4X-N5	3.31	124.39	120.59
3	A	601	FAD	C4-C4X-N5	3.52	122.53	118.68
3	B	601	FAD	C1'-N10-C9A	5.61	123.49	118.35
3	A	601	FAD	C4X-N5-C5X	5.95	123.05	116.76
3	A	601	FAD	C1'-N10-C9A	6.77	124.55	118.35
3	B	601	FAD	C4-N3-C2	7.81	121.99	115.16
3	A	601	FAD	C4-N3-C2	10.63	124.45	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	601	FAD	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	1
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	46:GLY	C	50:TYR	N	2.33
1	A	46:GLY	C	50:TYR	N	2.14

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	584/586 (99%)	-0.04	2 (0%) 93 93	46, 69, 109, 142	0
2	B	584/584 (100%)	0.09	11 (1%) 67 65	47, 78, 123, 150	0
All	All	1168/1170 (99%)	0.02	13 (1%) 80 79	46, 72, 118, 150	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	362	SER	3.4
2	B	378	THR	3.0
2	B	99	ILE	2.8
2	B	190	GLY	2.6
1	A	58	ASN	2.6
2	B	41	LEU	2.6
2	B	101	LYS	2.5
2	B	68	GLU	2.5
2	B	85	ILE	2.2
2	B	27	PHE	2.2
2	B	361	GLU	2.1
2	B	230	ILE	2.1
1	A	374	HIS	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, 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	LLDF	B-factors(Å ²)	Q<0.9
3	FAD	B	601	53/53	0.97	0.18	0.26	54,60,69,71	0
3	FAD	A	601	53/53	0.97	0.19	0.05	49,54,59,60	0
4	AU	B	602	1/1	0.96	0.15	-0.85	126,126,126,126	0
4	AU	A	602	1/1	0.97	0.06	-4.47	116,116,116,116	0

6.5 Other polymers [i](#)

There are no such residues in this entry.