Full wwPDB X-ray Structure Validation Report (i)

Nov 14, 2023 – 08:16 PM JST

PDB ID	:	6AAA
Title	:	Structure of a blue-shifted Luciferase from Amydetes vivianii
Authors	:	Carrasco-Lopez, C.; Naumov, P.; Rabeh, W.
Deposited on	:	2018-07-18
Resolution	:	1.90 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 (i) 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 (1)) were used in the production of this report:

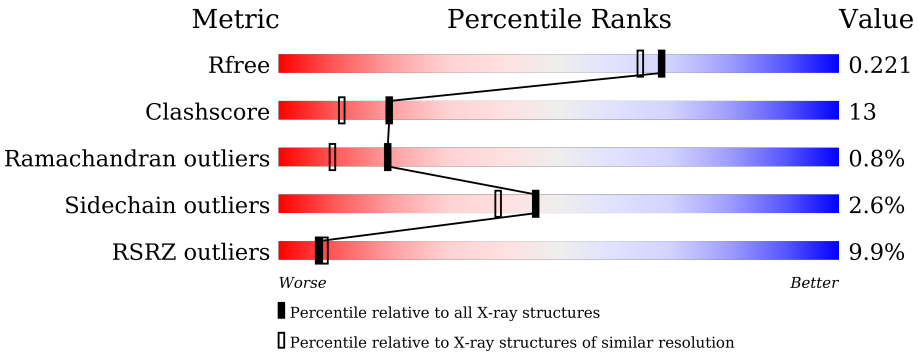
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 <=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	547	15% 78% 17%
1	B	547	5% 77% 20%

2 Entry composition

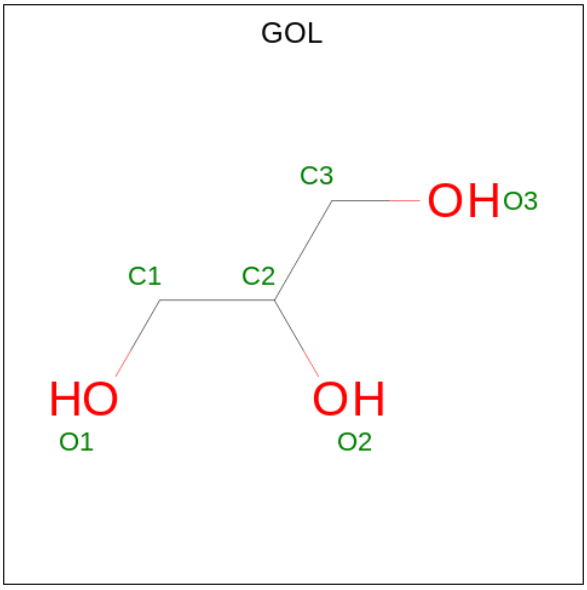
There are 3 unique types of molecules in this entry. The entry contains 9169 atoms, of which 16 are hydrogens and 0 are deuteriums.

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 Blue-shifted Luciferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	540	Total	C	N	O	S	0	0	0
			4215	2710	701	782	22			
1	B	536	Total	C	N	O	S	0	0	0
			4183	2689	694	778	22			

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	B	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 3 is water.

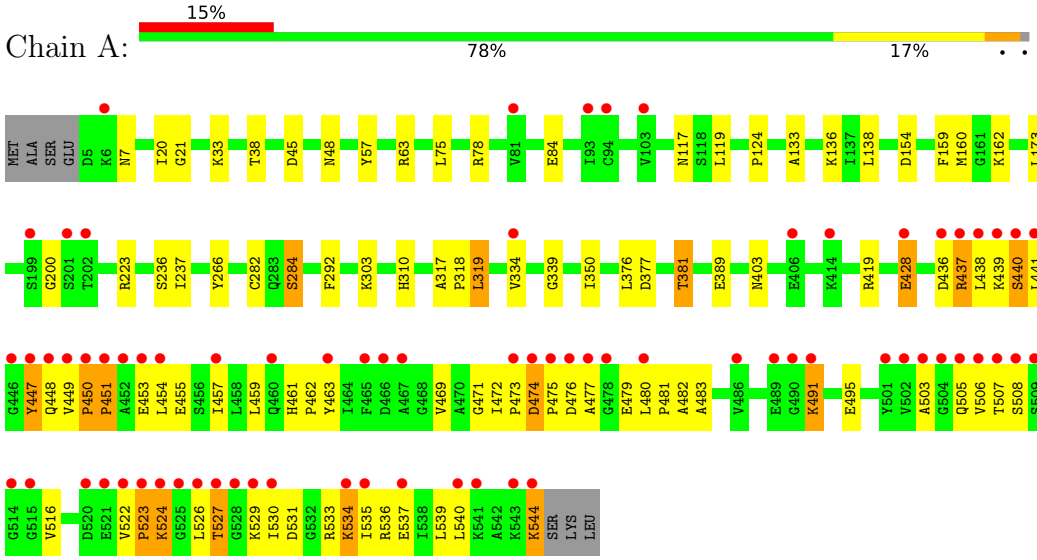
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	389	Total O 389 389	0	0
3	B	354	Total O 354 354	0	0

3 Residue-property plots (i)

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.

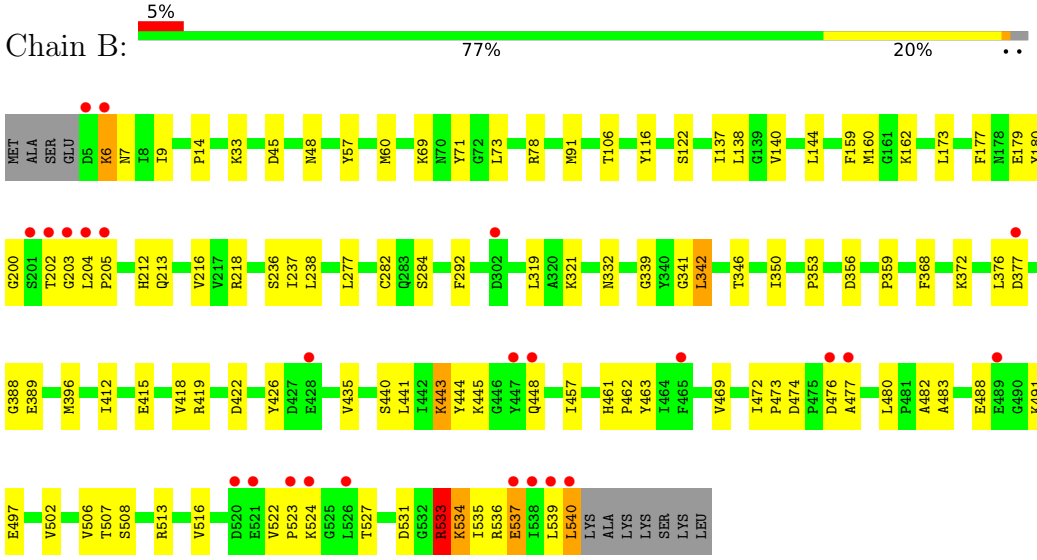
• Molecule 1: Blue-shifted Luciferase

Chain A:



• Molecule 1: Blue-shifted Luciferase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	94.28Å 110.53Å 122.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.08 – 1.90 28.08 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.5 (28.08-1.90) 89.6 (28.08-1.90)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.40 (at 1.91Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.192 , 0.219 0.198 , 0.221	Depositor DCC
R_{free} test set	7252 reflections (7.19%)	wwPDB-VP
Wilson B-factor (Å^2)	24.2	Xtriage
Anisotropy	0.167	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 50.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	9169	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: GOL

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	0.28	0/4310	0.48	0/5832
1	B	0.25	0/4278	0.43	0/5792
All	All	0.27	0/8588	0.46	0/11624

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	2
1	B	0	2
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	511	ARG	Sidechain
1	A	513	ARG	Sidechain
1	B	533	ARG	Sidechain
1	B	536	ARG	Sidechain

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	4215	0	4231	122	0
1	B	4183	0	4187	93	0
2	A	6	8	8	0	0
2	B	6	8	8	0	0
3	A	389	0	0	11	0
3	B	354	0	0	14	0
All	All	9153	16	8434	214	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 13.

All (214) 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:503:ALA:CA	1:A:511:ARG:HD3	1.63	1.27
1:A:503:ALA:HA	1:A:511:ARG:CD	1.63	1.26
1:B:218:ARG:HB2	1:B:396:MET:HE3	1.27	1.08
1:A:522:VAL:HG11	1:A:530:ILE:CD1	1.85	1.07
1:A:523:PRO:HG2	1:A:535:ILE:HG12	1.34	1.06
1:A:441:LEU:HD21	1:A:449:VAL:HG13	1.37	1.03
1:A:442:ILE:HG23	1:A:479:GLU:HG2	1.44	0.95
1:A:524:LYS:HE3	1:A:524:LYS:HA	1.47	0.94
1:A:448:GLN:HB3	1:A:510:LYS:HG3	1.49	0.94
1:A:522:VAL:HG11	1:A:530:ILE:HD11	1.52	0.90
1:B:377:ASP:OD1	1:B:533:ARG:NH1	2.06	0.87
1:B:396:MET:SD	3:B:965:HOH:O	2.35	0.84
1:A:503:ALA:HA	1:A:511:ARG:HD3	0.85	0.81
1:A:522:VAL:CG1	1:A:530:ILE:CD1	2.58	0.81
1:B:494:THR:HG23	1:B:497:GLU:H	1.46	0.81
1:A:523:PRO:HG2	1:A:535:ILE:CG1	2.10	0.81
1:A:447:TYR:O	1:A:448:GLN:HG3	1.81	0.80
1:A:450:PRO:HB3	1:A:510:LYS:CD	2.13	0.79
1:A:450:PRO:HB3	1:A:510:LYS:HD2	1.66	0.78
1:A:522:VAL:CG1	1:A:530:ILE:HD13	2.13	0.78
1:A:441:LEU:CD2	1:A:449:VAL:HG13	2.12	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:441:LEU:HD22	1:A:449:VAL:HA	1.65	0.77
1:A:472:ILE:HD13	1:A:482:ALA:HB3	1.67	0.76
1:A:522:VAL:HG13	1:A:523:PRO:HD2	1.68	0.76
1:B:441:LEU:HD13	1:B:448:GLN:HG2	1.69	0.74
1:A:524:LYS:HB3	1:A:531:ASP:HB2	1.69	0.74
1:A:503:ALA:CB	1:A:511:ARG:HD3	2.17	0.74
1:B:523:PRO:HB3	1:B:534:LYS:HD3	1.70	0.74
1:A:450:PRO:HB2	1:A:454:LEU:HD12	1.71	0.72
1:B:78:ARG:NH1	3:B:704:HOH:O	2.23	0.72
1:A:522:VAL:HG11	1:A:530:ILE:HD13	1.67	0.71
1:A:450:PRO:HB2	1:A:454:LEU:CD1	2.20	0.71
1:A:506:VAL:O	1:A:511:ARG:NH2	2.25	0.70
1:B:387:ARG:NH1	1:B:435:VAL:HG21	2.07	0.70
1:A:480:LEU:HD23	1:A:513:ARG:O	1.92	0.69
1:B:106:THR:O	3:B:701:HOH:O	2.10	0.69
1:A:482:ALA:CB	1:A:539:LEU:HD13	2.22	0.68
1:A:317:ALA:HB1	1:A:318:PRO:HD2	1.76	0.68
1:B:389:GLU:OE1	1:B:419:ARG:NE	2.24	0.68
1:A:440:SER:O	1:A:451:PRO:HG3	1.94	0.68
1:B:353:PRO:HG2	1:B:356:ASP:HB3	1.77	0.67
1:A:503:ALA:HA	1:A:511:ARG:NE	2.09	0.67
1:A:482:ALA:HB3	1:A:539:LEU:HD13	1.78	0.65
1:B:386:GLN:NE2	3:B:708:HOH:O	2.29	0.65
1:B:218:ARG:CB	1:B:396:MET:HE3	2.16	0.65
1:A:463:TYR:CD1	1:A:491:LYS:HD3	2.33	0.64
1:A:7:ASN:HB2	1:A:381:THR:HG23	1.80	0.63
1:B:332:ASN:HB3	3:B:724:HOH:O	1.98	0.63
1:A:7:ASN:HB2	1:A:381:THR:CG2	2.29	0.62
1:B:218:ARG:HB2	1:B:396:MET:CE	2.16	0.62
1:B:159:PHE:CE2	1:B:160:MET:HG3	2.35	0.62
1:B:203:GLY:O	1:B:205:PRO:HD3	2.00	0.61
1:B:6:LYS:HD2	1:B:381:THR:HB	1.84	0.60
1:A:522:VAL:CG1	1:A:523:PRO:HD2	2.32	0.60
1:A:439:LYS:O	1:A:440:SER:HB2	2.01	0.60
1:A:450:PRO:HB3	1:A:510:LYS:HD3	1.82	0.59
1:B:457:ILE:CD1	1:B:506:VAL:CG1	2.81	0.59
1:A:503:ALA:CA	1:A:511:ARG:CD	2.47	0.59
1:B:237:ILE:CD1	1:B:284:SER:HB2	2.32	0.58
1:A:503:ALA:CB	1:A:511:ARG:CD	2.80	0.58
1:B:7:ASN:HB3	1:B:426:TYR:OH	2.04	0.58
1:A:7:ASN:CB	1:A:381:THR:HG23	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:ASP:HB2	1:A:475:PRO:HD2	1.85	0.57
1:A:38:THR:HG21	3:A:1058:HOH:O	2.05	0.57
1:A:389:GLU:OE2	1:A:419:ARG:NE	2.38	0.57
1:A:428:GLU:H	1:A:428:GLU:CD	2.08	0.57
1:B:71:TYR:HD2	1:B:73:LEU:HD13	1.71	0.56
1:B:491:LYS:NZ	3:B:706:HOH:O	2.28	0.56
1:B:502:VAL:O	1:B:506:VAL:HG22	2.05	0.56
1:B:179:GLU:HG2	1:B:180:TYR:CD1	2.41	0.56
1:A:376:LEU:HD11	1:A:438:LEU:HD13	1.88	0.55
1:B:444:TYR:O	1:B:445:LYS:HG2	2.07	0.55
1:B:69:LYS:NZ	1:B:185:ASP:OD2	2.34	0.54
1:A:442:ILE:HG23	1:A:479:GLU:CG	2.28	0.54
1:A:159:PHE:CE2	1:A:160:MET:HG3	2.42	0.54
1:B:6:LYS:HD2	1:B:381:THR:CB	2.37	0.54
1:B:33:LYS:NZ	3:B:709:HOH:O	2.30	0.54
1:A:75:LEU:HD13	3:A:1008:HOH:O	2.07	0.54
1:A:200:GLY:HA3	1:A:527:THR:HG23	1.90	0.53
1:A:236:SER:OG	1:A:282:CYS:HA	2.07	0.53
1:A:457:ILE:HD12	1:A:505:GLN:HE21	1.73	0.53
1:A:512:LEU:HD13	1:A:516:VAL:HG22	1.91	0.53
1:B:342:LEU:HD12	1:B:342:LEU:N	2.24	0.53
1:B:494:THR:HG22	1:B:497:GLU:CG	2.38	0.53
1:A:63:ARG:NE	3:A:702:HOH:O	2.22	0.52
1:B:444:TYR:CZ	1:B:445:LYS:HD3	2.44	0.52
1:A:474:ASP:OD1	1:A:476:ASP:HB2	2.10	0.52
1:A:524:LYS:HE3	1:A:524:LYS:CA	2.30	0.52
1:B:533:ARG:O	1:B:537:GLU:OE2	2.26	0.52
1:A:444:TYR:HB2	1:A:448:GLN:CD	2.30	0.52
1:B:236:SER:OG	1:B:282:CYS:HA	2.10	0.52
1:B:482:ALA:HB3	1:B:539:LEU:HD11	1.92	0.52
1:A:447:TYR:O	1:A:447:TYR:HD1	1.93	0.52
1:B:237:ILE:HD12	1:B:284:SER:HB2	1.90	0.52
1:A:495:GLU:HG3	1:A:516:VAL:HB	1.92	0.52
1:A:440:SER:O	1:A:441:LEU:HD23	2.10	0.51
1:A:524:LYS:CG	1:A:526:LEU:HB2	2.40	0.51
1:B:472:ILE:HG22	1:B:480:LEU:HB2	1.92	0.51
1:A:450:PRO:N	1:A:451:PRO:HD3	2.26	0.50
1:A:447:TYR:O	1:A:448:GLN:CG	2.55	0.50
1:A:544:LYS:HB3	1:A:544:LYS:HZ2	1.76	0.50
1:A:223:ARG:HD3	3:A:853:HOH:O	2.11	0.50
1:B:387:ARG:CZ	1:B:435:VAL:HG21	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:HIS:HB2	3:A:945:HOH:O	2.11	0.50
1:A:441:LEU:HD13	1:A:449:VAL:HG22	1.94	0.50
1:A:472:ILE:HG23	1:A:540:LEU:HD13	1.94	0.50
1:A:523:PRO:HB3	1:A:534:LYS:HB3	1.93	0.50
1:B:472:ILE:HD13	1:B:539:LEU:HD12	1.93	0.50
1:A:472:ILE:HD11	1:A:539:LEU:HD12	1.93	0.50
1:A:524:LYS:HG3	1:A:526:LEU:HB2	1.94	0.50
1:A:512:LEU:HD13	1:A:516:VAL:CG2	2.42	0.49
1:A:455:GLU:O	1:A:459:LEU:HG	2.12	0.49
1:B:137:ILE:HA	1:B:140:VAL:HG12	1.94	0.49
1:B:387:ARG:HH12	1:B:440:SER:HB3	1.77	0.49
1:B:463:TYR:CD1	1:B:491:LYS:HD3	2.47	0.49
1:B:494:THR:HG21	3:B:1025:HOH:O	2.13	0.48
1:B:474:ASP:HB3	1:B:477:ALA:O	2.13	0.48
1:A:507:THR:HA	1:A:511:ARG:NH2	2.28	0.48
1:A:512:LEU:CD1	1:A:516:VAL:CG2	2.91	0.48
1:B:173:LEU:HD21	1:B:177:PHE:CD2	2.48	0.48
1:B:213:GLN:O	1:B:216:VAL:HG22	2.13	0.48
1:A:133:ALA:O	1:A:136:LYS:HG2	2.13	0.48
1:B:292:PHE:CE1	1:B:319:LEU:HD11	2.49	0.48
1:A:507:THR:OG1	1:A:508:SER:N	2.47	0.48
1:A:482:ALA:HB1	1:A:539:LEU:HD13	1.94	0.47
1:A:38:THR:HG22	3:A:732:HOH:O	2.13	0.47
1:B:212:HIS:O	1:B:216:VAL:HG13	2.13	0.47
1:B:14:PRO:HG3	1:B:368:PHE:CZ	2.50	0.47
1:A:436:ASP:O	1:A:437:ARG:CB	2.62	0.47
1:A:522:VAL:HG12	1:A:530:ILE:HD13	1.95	0.47
1:B:339:GLY:HA2	1:B:350:ILE:O	2.15	0.47
1:B:341:GLY:C	1:B:342:LEU:HD12	2.34	0.47
1:B:116:TYR:CE1	1:B:144:LEU:HG	2.49	0.47
1:B:494:THR:HG22	1:B:497:GLU:CD	2.34	0.47
1:B:422:ASP:CG	1:B:527:THR:HG21	2.35	0.47
1:A:442:ILE:HA	1:A:479:GLU:OE2	2.15	0.47
1:B:200:GLY:HA3	3:B:861:HOH:O	2.13	0.47
1:B:138:LEU:HD21	1:B:162:LYS:HE3	1.96	0.46
1:A:175:GLU:OE2	3:A:701:HOH:O	2.20	0.46
1:B:508:SER:O	1:B:513:ARG:NH1	2.40	0.46
1:B:488:GLU:HB2	1:B:491:LYS:HD2	1.97	0.46
1:A:481:PRO:O	1:A:512:LEU:HA	2.16	0.46
1:A:138:LEU:HD21	1:A:162:LYS:HE3	1.98	0.46
1:A:173:LEU:HD21	1:A:177:PHE:CD2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:507:THR:O	1:A:508:SER:HB3	2.16	0.45
1:B:376:LEU:CD1	1:B:388:GLY:HA2	2.47	0.45
1:B:78:ARG:NH1	1:B:122:SER:O	2.42	0.45
1:B:540:LEU:HD23	1:B:540:LEU:N	2.31	0.45
1:A:510:LYS:HE3	1:A:510:LYS:HB3	1.68	0.45
1:B:461:HIS:O	3:B:702:HOH:O	2.21	0.45
1:A:457:ILE:HG23	1:A:505:GLN:HG3	1.99	0.45
1:A:524:LYS:HA	1:A:524:LYS:CE	2.34	0.45
1:A:536:ARG:NH2	1:B:476:ASP:OD1	2.50	0.45
1:B:332:ASN:CB	3:B:724:HOH:O	2.60	0.45
1:B:472:ILE:HG13	1:B:473:PRO:HD2	1.99	0.45
1:A:292:PHE:CB	1:A:319:LEU:HD21	2.47	0.44
1:A:469:VAL:HG22	1:A:483:ALA:HB2	1.99	0.44
1:A:444:TYR:CG	1:A:445:LYS:N	2.81	0.44
1:B:200:GLY:HA3	3:B:726:HOH:O	2.17	0.44
1:B:237:ILE:HD13	1:B:284:SER:HB2	1.99	0.44
1:B:441:LEU:O	1:B:443:LYS:HE2	2.17	0.44
1:B:444:TYR:C	1:B:445:LYS:HG2	2.38	0.44
1:B:457:ILE:CD1	1:B:506:VAL:HG13	2.47	0.44
1:A:20:ILE:HG22	1:A:21:GLY:N	2.33	0.44
1:B:482:ALA:CB	1:B:539:LEU:HD11	2.48	0.44
1:A:436:ASP:O	1:A:437:ARG:HB2	2.18	0.44
1:A:443:LYS:HE3	1:A:443:LYS:HB3	1.78	0.44
1:A:474:ASP:CB	1:A:475:PRO:HD2	2.48	0.44
1:B:238:LEU:HD23	1:B:277:LEU:HD13	1.99	0.44
1:B:469:VAL:HG22	1:B:483:ALA:HB2	2.00	0.44
1:A:461:HIS:HA	1:A:462:PRO:HD3	1.88	0.44
1:A:544:LYS:HB3	1:A:544:LYS:NZ	2.33	0.44
1:A:339:GLY:HA2	1:A:350:ILE:O	2.18	0.43
1:A:526:LEU:HD12	1:A:526:LEU:HA	1.82	0.43
1:A:403:ASN:ND2	3:A:730:HOH:O	2.50	0.43
1:B:202:THR:HB	1:B:204:LEU:HD13	2.00	0.43
1:B:457:ILE:HD13	1:B:506:VAL:HG13	1.99	0.43
1:A:84:GLU:HG3	1:A:266:TYR:HD2	1.82	0.43
1:A:237:ILE:HD12	1:A:284:SER:HB2	2.00	0.43
1:A:453:GLU:O	1:A:457:ILE:HG12	2.18	0.43
1:B:7:ASN:O	1:B:9:ILE:CD1	2.66	0.43
1:A:511:ARG:O	1:A:512:LEU:O	2.36	0.43
1:A:33:LYS:NZ	3:A:715:HOH:O	2.41	0.43
1:A:78:ARG:NH2	3:A:734:HOH:O	2.52	0.43
1:A:508:SER:O	1:A:508:SER:OG	2.29	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:412:ILE:HG12	1:B:418:VAL:HG22	2.00	0.43
1:B:531:ASP:O	1:B:535:ILE:HG13	2.19	0.42
1:B:495:GLU:HG3	1:B:516:VAL:HB	2.00	0.42
1:A:45:ASP:HB3	1:A:48:ASN:OD1	2.19	0.42
1:A:442:ILE:HD13	1:A:481:PRO:HA	2.01	0.42
1:B:6:LYS:HB2	1:B:6:LYS:HE3	1.79	0.42
1:B:346:THR:HG21	1:B:396:MET:HE2	2.02	0.42
1:B:60:MET:HG2	1:B:91:MET:SD	2.60	0.42
1:A:533:ARG:O	1:A:537:GLU:HG2	2.20	0.42
1:B:6:LYS:HD2	1:B:381:THR:OG1	2.19	0.42
1:B:321:LYS:NZ	1:B:359:PRO:HB2	2.35	0.42
1:A:119:LEU:HD22	1:A:124:PRO:HG3	2.02	0.41
1:B:415:GLU:OE2	3:B:703:HOH:O	2.22	0.41
1:B:346:THR:CG2	1:B:396:MET:CE	2.98	0.41
1:A:529:LYS:HB3	1:A:530:ILE:H	1.58	0.41
1:B:45:ASP:HB3	1:B:48:ASN:OD1	2.20	0.41
1:B:522:VAL:O	1:B:524:LYS:HG3	2.20	0.41
1:A:117:ASN:HB2	3:A:990:HOH:O	2.20	0.41
1:A:154:ASP:OD1	1:A:154:ASP:N	2.54	0.41
1:A:506:VAL:O	1:A:511:ARG:CZ	2.69	0.41
1:B:372:LYS:NZ	3:B:736:HOH:O	2.51	0.41
1:B:507:THR:HG22	1:B:508:SER:H	1.84	0.41
1:A:303:LYS:O	1:A:303:LYS:HG3	2.19	0.40
1:A:442:ILE:HG12	1:A:471:GLY:HA3	2.02	0.40
1:B:346:THR:CG2	1:B:396:MET:HE1	2.51	0.40
1:B:472:ILE:CG2	1:B:480:LEU:HB2	2.51	0.40
1:A:236:SER:HG	1:A:282:CYS:HA	1.86	0.40
1:B:461:HIS:HA	1:B:462:PRO:HD3	1.89	0.40
1:A:472:ILE:HD11	1:A:539:LEU:HB2	2.02	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	538/547 (98%)	510 (95%)	19 (4%)	9 (2%)	9 2
1	B	534/547 (98%)	518 (97%)	16 (3%)	0	100 100
All	All	1072/1094 (98%)	1028 (96%)	35 (3%)	9 (1%)	19 9

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	437	ARG
1	A	440	SER
1	A	444	TYR
1	A	450	PRO
1	A	523	PRO
1	A	451	PRO
1	A	512	LEU
1	A	477	ALA
1	A	473	PRO

5.3.2 Protein sidechains (i)

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	460/466 (99%)	444 (96%)	16 (4%)	36 27
1	B	457/466 (98%)	449 (98%)	8 (2%)	59 55
All	All	917/932 (98%)	893 (97%)	24 (3%)	46 39

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	TYR
1	A	284	SER
1	A	319	LEU
1	A	334	VAL
1	A	377	ASP
1	A	381	THR
1	A	428	GLU

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Mol	Chain	Res	Type
1	A	443	LYS
1	A	447	TYR
1	A	474	ASP
1	A	491	LYS
1	A	511	ARG
1	A	524	LYS
1	A	527	THR
1	A	534	LYS
1	A	544	LYS
1	B	6	LYS
1	B	57	TYR
1	B	342	LEU
1	B	443	LYS
1	B	533	ARG
1	B	534	LYS
1	B	537	GLU
1	B	540	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	GLN
1	A	213	GLN
1	A	505	GLN
1	B	36	GLN
1	B	230	GLN
1	B	431	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

2 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	GOL	A	601	-	5,5,5	0.73	0	5,5,5	0.70	0
2	GOL	B	601	-	5,5,5	0.13	0	5,5,5	0.68	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	GOL	A	601	-	-	2/4/4/4	-
2	GOL	B	601	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	601	GOL	O1-C1-C2-C3
2	B	601	GOL	C1-C2-C3-O3
2	B	601	GOL	O2-C2-C3-O3
2	B	601	GOL	O1-C1-C2-O2
2	A	601	GOL	O2-C2-C3-O3
2	A	601	GOL	C1-C2-C3-O3

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^{th} 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	540/547 (98%)	0.74	81 (15%) 2 2	18, 32, 114, 169	0
1	B	536/547 (97%)	0.11	26 (4%) 29 33	19, 37, 73, 112	0
All	All	1076/1094 (98%)	0.42	107 (9%) 7 8	18, 35, 99, 169	0

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	476	ASP	15.8
1	A	447	TYR	15.3
1	A	449	VAL	14.7
1	A	446	GLY	12.0
1	A	510	LYS	11.4
1	A	448	GLN	11.1
1	A	475	PRO	10.4
1	A	511	ARG	9.9
1	A	450	PRO	9.5
1	A	508	SER	9.4
1	A	444	TYR	8.9
1	A	474	ASP	8.6
1	A	445	LYS	8.4
1	A	438	LEU	8.3
1	A	523	PRO	8.3
1	A	506	VAL	8.1
1	A	507	THR	7.7
1	B	201	SER	6.9
1	A	465	PHE	6.4
1	A	513	ARG	6.3
1	A	528	GLY	6.0
1	A	480	LEU	5.8
1	A	443	LYS	5.8
1	A	201	SER	5.7

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Mol	Chain	Res	Type	RSRZ
1	A	477	ALA	5.6
1	A	442	ILE	5.5
1	A	541	LYS	5.4
1	A	441	LEU	5.3
1	A	439	LYS	5.2
1	A	515	GLY	5.0
1	B	203	GLY	4.9
1	A	436	ASP	4.8
1	A	202	THR	4.7
1	A	437	ARG	4.7
1	A	514	GLY	4.6
1	A	544	LYS	4.6
1	A	502	VAL	4.6
1	A	524	LYS	4.5
1	A	529	LYS	4.4
1	A	527	THR	4.2
1	A	540	LEU	4.2
1	A	509	SER	4.1
1	B	448	GLN	4.1
1	A	526	LEU	4.0
1	B	199	SER	4.0
1	B	537	GLU	3.9
1	A	440	SER	3.9
1	A	522	VAL	3.8
1	B	540	LEU	3.8
1	A	512	LEU	3.8
1	B	6	LYS	3.8
1	A	453	GLU	3.6
1	A	525	GLY	3.4
1	A	473	PRO	3.4
1	A	6	LYS	3.3
1	A	490	GLY	3.3
1	A	489	GLU	3.3
1	A	466	ASP	3.2
1	B	520	ASP	3.2
1	A	530	ILE	3.2
1	A	537	GLU	3.1
1	A	505	GLN	3.1
1	B	538	ILE	3.0
1	B	5	ASP	3.0
1	A	452	ALA	2.9
1	B	477	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	467	ALA	2.9
1	B	489	GLU	2.8
1	A	521	GLU	2.8
1	A	503	ALA	2.8
1	A	451	PRO	2.8
1	A	460	GLN	2.7
1	A	504	GLY	2.7
1	A	463	TYR	2.7
1	A	486	VAL	2.7
1	A	478	GLY	2.6
1	A	414	LYS	2.6
1	A	457	ILE	2.6
1	B	202	THR	2.6
1	A	501	TYR	2.5
1	B	205	PRO	2.4
1	B	447	TYR	2.3
1	B	526	LEU	2.3
1	A	491	LYS	2.3
1	B	523	PRO	2.3
1	B	302	ASP	2.3
1	A	520	ASP	2.3
1	B	476	ASP	2.2
1	A	535	ILE	2.2
1	A	428	GLU	2.2
1	B	539	LEU	2.2
1	A	199	SER	2.2
1	A	103	VAL	2.2
1	B	524	LYS	2.2
1	B	204	LEU	2.2
1	A	543	LYS	2.2
1	B	428	GLU	2.1
1	A	534	LYS	2.1
1	B	465	PHE	2.1
1	A	94	CYS	2.1
1	A	454	LEU	2.1
1	A	81	VAL	2.1
1	B	521	GLU	2.0
1	A	334	VAL	2.0
1	A	93	ILE	2.0
1	A	406	GLU	2.0
1	B	377	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 monosaccharides 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, 95^{th} 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(Å^2)	Q<0.9
2	GOL	B	601	6/6	0.89	0.14	73,88,92,93	0
2	GOL	A	601	6/6	0.92	0.26	72,86,91,92	0

6.5 Other polymers (i)

There are no such residues in this entry.