



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 07:41 PM UTC

PDB ID : 6AAA / pdb_00006aaa
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 ⓘ 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)
Xtrriage (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

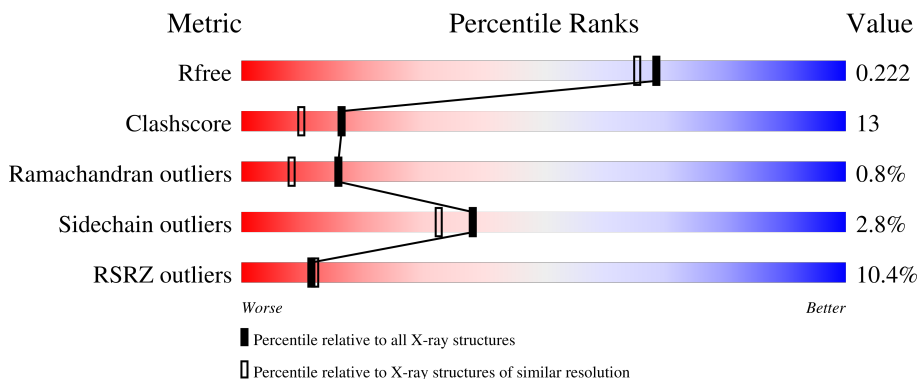
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 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}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (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 $\leq 5\%$. 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	547	
1	B	547	

2 Entry composition [i](#)

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
			Total	C	N	O	S			
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 (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
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		

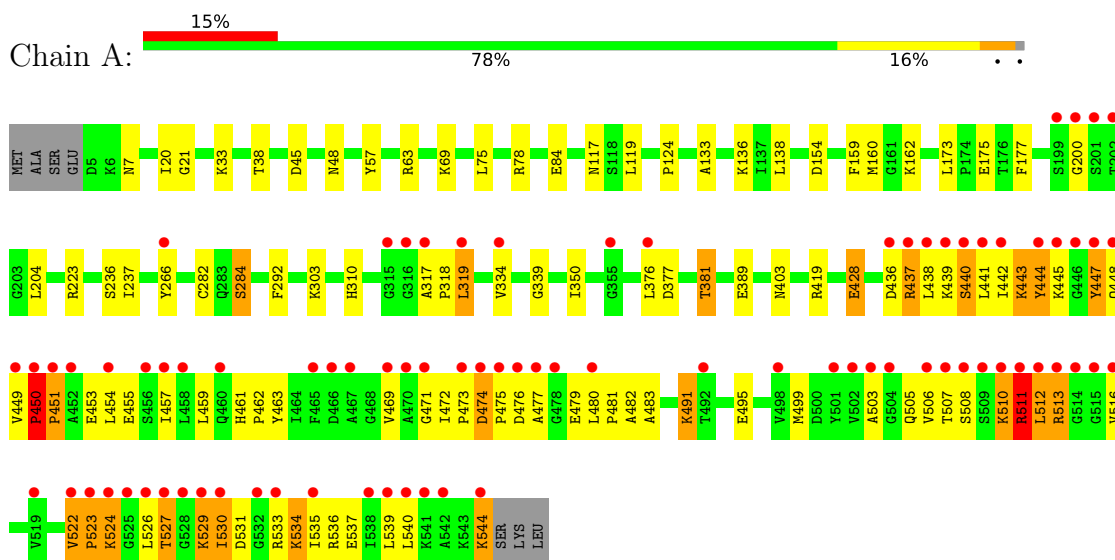
- Molecule 3 is water.

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

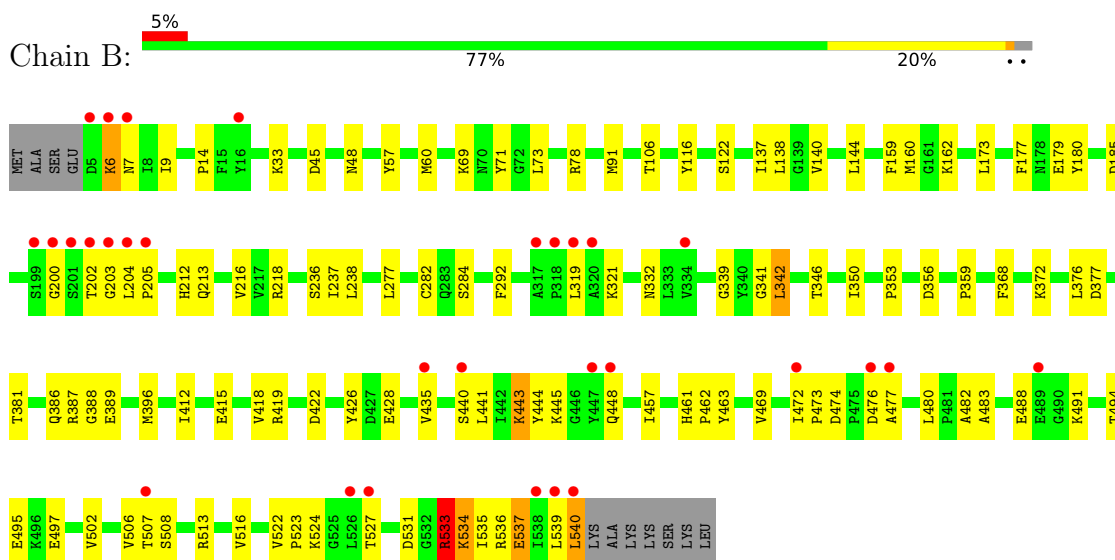
3 Residue-property plots i

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



• Molecule 1: Blue-shifted Luciferase



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 1.91Å)	Xtrriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.192 , 0.219 0.198 , 0.222	Depositor DCC
R_{free} test set	7252 reflections (7.19%)	wwPDB-VP
Wilson B-factor (Å ²)	24.2	Xtrriage
Anisotropy	0.167	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 51.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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.*

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 [i](#)

5.1 Standard geometry [i](#)

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	0.38	0/4310	0.83	9/5832 (0.2%)
1	B	0.33	0/4278	0.74	0/5792
All	All	0.36	0/8588	0.78	9/11624 (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	2
1	B	0	2
All	All	0	4

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	522	VAL	CA-C-N	7.26	128.91	119.84
1	A	522	VAL	C-N-CA	7.26	128.91	119.84
1	A	529	LYS	CA-C-N	6.86	129.75	120.63
1	A	529	LYS	C-N-CA	6.86	129.75	120.63
1	A	204	LEU	CA-C-N	6.83	126.81	119.78
1	A	204	LEU	C-N-CA	6.83	126.81	119.78
1	A	530	ILE	N-CA-C	5.22	116.42	109.37
1	A	510	LYS	N-CA-C	-5.21	106.68	112.57
1	A	450	PRO	N-CA-C	5.14	116.97	110.70

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	123	0
1	B	4183	0	4187	95	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	217	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 (217) 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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:441:LEU:HD22	1:A:449:VAL:HA	1.65	0.77
1:B:218:ARG:HB2	1:B:396:MET:HE3	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:218:ARG:HB2	1:B:396:MET:CE	2.16	0.75
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:B:346:THR:HB	1:B:396:MET:HE2	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:346:THR:CG2	1:B:396:MET:HE2	2.22	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:346:THR:CB	1:B:396:MET:HE2	2.27	0.65
1:B:386:GLN:NE2	3:B:708:HOH:O	2.29	0.65
1:B:33:LYS:NZ	3:B:709:HOH:O	2.30	0.64
1:A:463:TYR:CD1	1:A:491:LYS:HD3	2.33	0.64
1:B:491:LYS:NZ	3:B:706:HOH:O	2.28	0.63
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:159:PHE:CE2	1:B:160:MET:HG3	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:428:GLU:H	1:A:428:GLU:CD	2.08	0.61
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:B:69:LYS:NZ	1:B:185:ASP:OD2	2.34	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:A:544:LYS:HZ2	1:A:544:LYS:HB3	1.67	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
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:444:TYR:HB2	1:A:448:GLN:CD	2.30	0.56
1:B:71:TYR:HD2	1:B:73:LEU:HD13	1.71	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: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: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:218:ARG:HB2	1:B:396:MET:HE1	1.91	0.52
1:B:494:THR:HG22	1:B:497:GLU:CD	2.34	0.52
1:B:533:ARG:O	1:B:537:GLU:OE2	2.26	0.52
1:B:236:SER:OG	1:B:282:CYS:HA	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:341:GLY:C	1:B:342:LEU:HD12	2.34	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:B:422:ASP:CG	1:B:527:THR:HG21	2.35	0.51
1:A:499:MET:HE3	1:A:512:LEU:O	2.09	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: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
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:444:TYR:C	1:B:445:LYS:HG2	2.38	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:B:346:THR:HG21	1:B:396:MET:HE2	1.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:116:TYR:CE1	1:B:144:LEU:HG	2.49	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
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:N	1:B:540:LEU:HD23	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:412:ILE:HG12	1:B:418:VAL:HG22	2.00	0.43
1:B:377:ASP:CG	1:B:533:ARG:NH1	2.77	0.42
1:B:531:ASP:O	1:B:535:ILE:HG13	2.19	0.42
1:A:447:TYR:C	1:A:448:GLN:HG3	2.44	0.42
1:A:544:LYS:HB3	1:A:544:LYS:NZ	2.33	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:60:MET:HG2	1:B:91:MET:SD	2.60	0.42
1:B:372:LYS:NZ	3:B:736:HOH:O	2.51	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: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:507:THR:HG22	1:B:508:SER:H	1.84	0.41
1:A:303:LYS:HG3	1:A:303:LYS:O	2.19	0.40
1:A:442:ILE:HG12	1:A:471:GLY:HA3	2.02	0.40
1:B:472:ILE:CG2	1:B:480:LEU:HB2	2.51	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%)	7	2
1	B	534/547 (98%)	518 (97%)	16 (3%)	0	100	100
All	All	1072/1094 (98%)	1028 (96%)	35 (3%)	9 (1%)	16	8

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%)	443 (96%)	17 (4%)	30	22
1	B	457/466 (98%)	448 (98%)	9 (2%)	48	46
All	All	917/932 (98%)	891 (97%)	26 (3%)	38	32

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	TYR
1	A	69	LYS
1	A	284	SER
1	A	319	LEU
1	A	334	VAL
1	A	377	ASP
1	A	381	THR
1	A	428	GLU
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	428	GLU
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 (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	HIS
1	A	66	GLN
1	A	117	ASN
1	A	135	GLN
1	A	213	GLN
1	A	460	GLN
1	A	505	GLN
1	B	66	GLN
1	B	230	GLN
1	B	431	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	0.76	0	5,5,5	0.77	0
2	GOL	B	601	-	5,5,5	0.14	0	5,5,5	0.73	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, 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	540/547 (98%)	0.48	82 (15%) 5 5	18, 32, 114, 169	0
1	B	536/547 (97%)	0.23	30 (5%) 30 32	19, 37, 73, 112	0
All	All	1076/1094 (98%)	0.36	112 (10%) 11 12	18, 35, 99, 169	0

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	511	ARG	7.9
1	A	448	GLN	7.3
1	A	450	PRO	7.2
1	A	526	LEU	6.8
1	A	506	VAL	6.5
1	A	449	VAL	5.9
1	A	515	GLY	5.8
1	A	510	LYS	5.7
1	A	438	LEU	5.7
1	B	540	LEU	5.6
1	A	446	GLY	5.6
1	A	523	PRO	5.4
1	A	476	ASP	5.2
1	A	477	ALA	5.0
1	A	502	VAL	4.9
1	A	266	TYR	4.9
1	B	539	LEU	4.7
1	A	512	LEU	4.7
1	A	475	PRO	4.6
1	B	6	LYS	4.6
1	A	507	THR	4.5
1	A	451	PRO	4.4
1	A	315	GLY	4.4
1	A	514	GLY	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	503	ALA	4.1
1	B	203	GLY	4.0
1	B	201	SER	3.9
1	A	444	TYR	3.8
1	A	447	TYR	3.7
1	A	457	ILE	3.7
1	A	439	LYS	3.7
1	B	202	THR	3.7
1	A	480	LEU	3.7
1	B	448	GLN	3.7
1	A	508	SER	3.6
1	B	205	PRO	3.6
1	A	436	ASP	3.6
1	B	526	LEU	3.6
1	B	5	ASP	3.6
1	A	513	ARG	3.6
1	A	465	PHE	3.5
1	B	200	GLY	3.5
1	A	527	THR	3.5
1	A	469	VAL	3.5
1	A	540	LEU	3.5
1	A	544	LYS	3.4
1	A	202	THR	3.4
1	A	509	SER	3.3
1	A	452	ALA	3.2
1	A	474	ASP	3.2
1	A	522	VAL	3.2
1	B	472	ILE	3.1
1	A	501	TYR	3.1
1	A	437	ARG	3.1
1	B	204	LEU	3.1
1	A	441	LEU	3.1
1	B	489	GLU	3.1
1	A	319	LEU	3.0
1	A	532	GLY	3.0
1	A	470	ALA	3.0
1	A	445	LYS	3.0
1	A	442	ILE	3.0
1	A	334	VAL	2.9
1	B	334	VAL	2.9
1	A	478	GLY	2.9
1	B	477	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	528	GLY	2.9
1	B	318	PRO	2.8
1	A	530	ILE	2.8
1	A	199	SER	2.8
1	B	199	SER	2.7
1	A	538	ILE	2.7
1	B	435	VAL	2.7
1	A	316	GLY	2.6
1	A	535	ILE	2.6
1	A	467	ALA	2.6
1	B	447	TYR	2.5
1	A	541	LYS	2.5
1	A	440	SER	2.5
1	A	524	LYS	2.5
1	A	504	GLY	2.5
1	B	7	ASN	2.5
1	A	516	VAL	2.4
1	A	454	LEU	2.4
1	A	539	LEU	2.4
1	B	319	LEU	2.4
1	A	529	LYS	2.4
1	A	460	GLN	2.4
1	B	476	ASP	2.3
1	A	473	PRO	2.3
1	A	498	VAL	2.3
1	A	376	LEU	2.3
1	B	317	ALA	2.3
1	B	320	ALA	2.3
1	A	466	ASP	2.3
1	A	519	VAL	2.3
1	B	527	THR	2.3
1	B	538	ILE	2.2
1	A	458	LEU	2.2
1	A	525	GLY	2.2
1	A	317	ALA	2.2
1	B	507	THR	2.2
1	A	201	SER	2.2
1	A	200	GLY	2.2
1	A	542	ALA	2.2
1	B	16	TYR	2.1
1	A	492	THR	2.1
1	B	440	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	533	ARG	2.1
1	A	471	GLY	2.0
1	A	456	SER	2.0
1	A	355	GLY	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(Å ²)	Q < 0.9
2	GOL	B	601	6/6	0.85	0.17	73,88,92,93	0
2	GOL	A	601	6/6	0.86	0.20	72,86,91,92	0

6.5 Other polymers [i](#)

There are no such residues in this entry.