WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 26, 2014 – 11:57 PM GMT

PDB ID : 3AJG
Title : Crystal structure of PcyA V225D-biliverdin IX alpha complex
Authors : Wada, K.; Hagiwara, Y.; Fukuyama, K.
Deposited on : 2010-06-05
Resolution : 1.90 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html

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The following versions of software and data (see references) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance ⓘ

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	Percentile Ranks	Value
Rfree		0.255
Clashscore		17
Ramachandran outliers		0.4%
Sidechain outliers		10.6%
RSRZ outliers		6.7%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
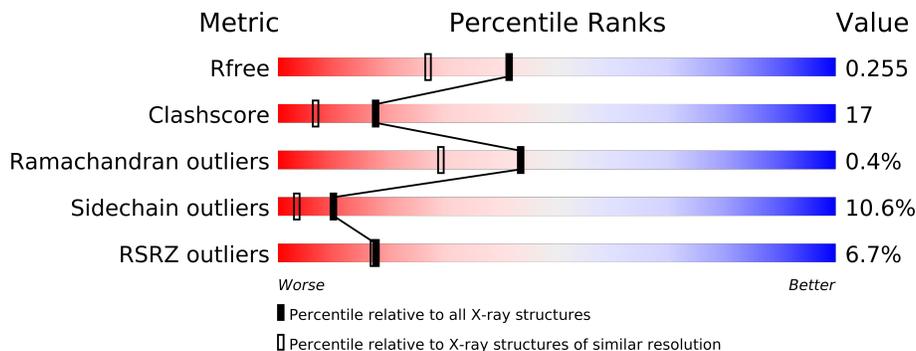
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	3684 (1.90-1.90)
Clashscore	79885	4465 (1.90-1.90)
Ramachandran outliers	78287	4413 (1.90-1.90)
Sidechain outliers	78261	4414 (1.90-1.90)
RSRZ outliers	66119	3686 (1.90-1.90)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	248	
1	B	248	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	BLA	A	1131	-	X
2	BLA	B	1130	-	X

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 4139 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Phycocyanobilin:ferredoxinoxidoreductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	238	Total 1916	C 1221	N 326	O 356	S 13	0	6	0
1	B	241	Total 1935	C 1231	N 332	O 360	S 12	0	3	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	225	ASP	VAL	ENGINEERED MUTATION	UNP Q55891
B	225	ASP	VAL	ENGINEERED MUTATION	UNP Q55891

- Molecule 2 is BILIVERDINE IX ALPHA (three-letter code: BLA) (formula: $C_{33}H_{34}N_4O_6$).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 43	C 33	N 4	O 6	0	0

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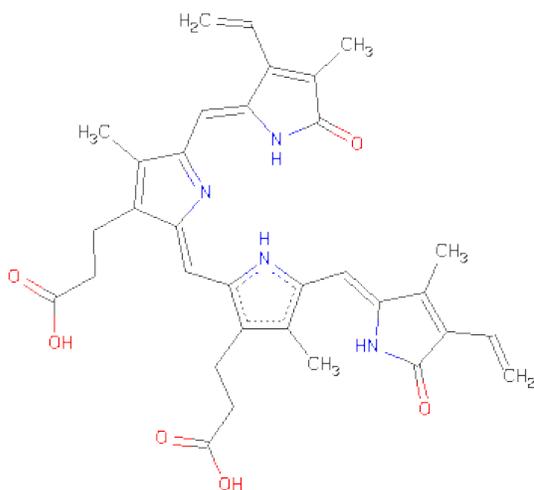
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	B	1	43	33	4	6	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	104	Total 104	O 104	0	0
3	B	98	Total 98	O 98	0	0

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 errors 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: Phycocyanobilin:ferredoxinoxidoreductase

Chain A:
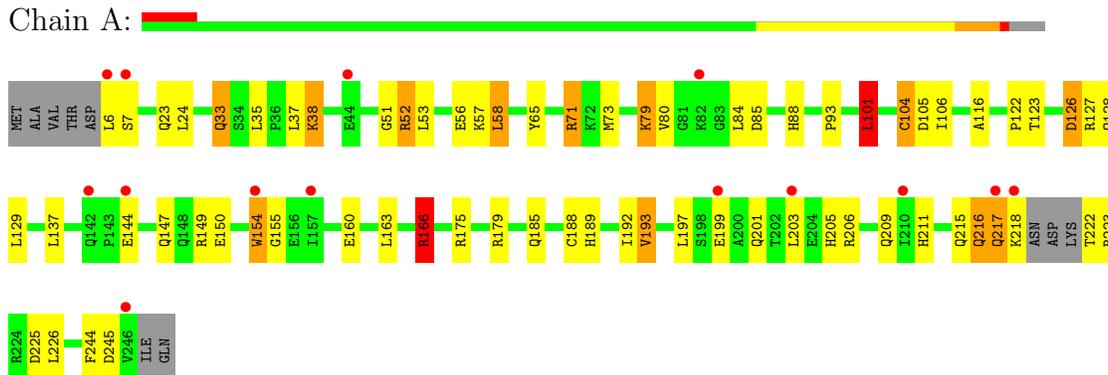
- Molecule 1: Phycocyanobilin:ferredoxinoxidoreductase

Chain B:
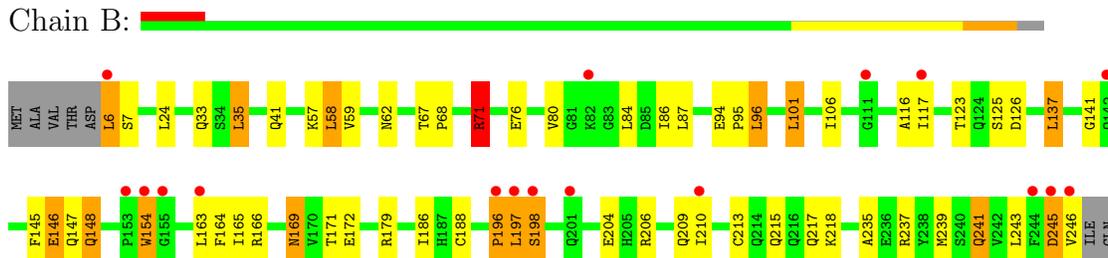
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	74.05Å 74.88Å 84.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.88 – 1.90 34.21 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.3 (32.88-1.90) 96.1 (34.21-1.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.19 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.231 , 0.295 0.224 , 0.255	Depositor DCC
R_{free} test set	1839 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	31.3	Xtriage
Anisotropy	0.289	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 37.4	EDS
Estimated twinning fraction	0.149 for k,h,-l	Xtriage
L-test for twinning	$< |L| > = 0.47, < L^2 > = 0.30$	Xtriage
Outliers	0 of 36689 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	4139	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.04% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: BLA

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	0.93	1/1986 (0.1%)	0.95	7/2694 (0.3%)
1	B	0.89	0/1994	0.91	1/2704 (0.0%)
All	All	0.91	1/3980 (0.0%)	0.93	8/5398 (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	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	188	CYS	CB-SG	-5.28	1.73	1.81

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	101	LEU	CA-CB-CG	8.10	133.93	115.30
1	A	166[A]	ARG	NE-CZ-NH1	-6.13	117.24	120.30
1	A	166[B]	ARG	NE-CZ-NH1	-6.13	117.24	120.30
1	A	79	LYS	CD-CE-NZ	-5.57	98.89	111.70
1	A	166[A]	ARG	NE-CZ-NH2	5.45	123.03	120.30
1	A	166[B]	ARG	NE-CZ-NH2	5.45	123.03	120.30
1	A	101	LEU	CB-CG-CD1	5.37	120.13	111.00
1	B	71	ARG	NE-CZ-NH2	5.21	122.91	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	154	TRP	Peptide
1	A	155	GLY	Peptide
1	B	154	TRP	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1916	0	1878	67	0
1	B	1935	0	1904	64	0
2	A	43	0	32	13	0
2	B	43	0	32	3	0
3	A	104	0	0	5	0
3	B	98	0	0	2	0
All	All	4139	0	3846	136	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 17.

All (136) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:1131:BLA:HHA	2:A:1131:BLA:HBD2	1.31	1.09
1:B:117:ILE:HD11	1:B:164:PHE:CE2	1.87	1.08
1:B:117:ILE:CG1	1:B:164:PHE:CD2	2.43	1.02
1:A:244:PHE:HZ	2:A:1131:BLA:CMC	1.76	0.96
1:B:117:ILE:HG12	1:B:164:PHE:CD2	2.04	0.92
1:A:244:PHE:HZ	2:A:1131:BLA:HMC3	1.32	0.91
1:A:244:PHE:CZ	2:A:1131:BLA:HMC3	2.07	0.89
1:B:117:ILE:HD11	1:B:164:PHE:CD2	2.08	0.88
1:B:71:ARG:HH12	1:B:206:ARG:NH1	1.74	0.84
1:A:33:GLN:HA	1:A:33:GLN:HE21	1.43	0.84
1:B:33:GLN:HG3	3:B:274:HOH:O	1.76	0.83
2:A:1131:BLA:CBD	2:A:1131:BLA:HHA	2.10	0.82

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:6:LEU:HG	1:A:65:TYR:CZ	2.15	0.81
1:B:117:ILE:CD1	1:B:164:PHE:CD2	2.64	0.79
2:A:1131:BLA:CHA	2:A:1131:BLA:HBD2	2.12	0.79
1:B:117:ILE:CG1	1:B:164:PHE:HD2	1.90	0.79
1:B:96:LEU:HD23	1:B:96:LEU:C	2.07	0.74
1:A:71:ARG:NH1	1:A:209:GLN:OE1	2.20	0.74
1:A:105:ASP:OD2	2:A:1131:BLA:HAC	1.88	0.73
1:A:24:LEU:HD21	1:A:104[A]:CYS:SG	2.29	0.73
1:A:88:HIS:CE1	2:A:1131:BLA:HMC2	2.25	0.72
1:B:96:LEU:HD21	1:B:196:PRO:HB3	1.73	0.71
1:B:84:LEU:HD11	1:B:86:ILE:HD11	1.73	0.71
1:A:127:ARG:HG2	3:A:283:HOH:O	1.90	0.70
1:A:33:GLN:HA	1:A:33:GLN:NE2	2.10	0.66
1:A:244:PHE:CZ	2:A:1131:BLA:CMC	2.67	0.65
1:B:117:ILE:HG13	1:B:164:PHE:HD2	1.61	0.65
1:B:117:ILE:CD1	1:B:164:PHE:CE2	2.74	0.64
1:B:80:VAL:HB	1:B:84:LEU:HD23	1.79	0.63
1:A:106:ILE:HD13	1:A:116:ALA:HA	1.81	0.63
1:A:225:ASP:HB2	2:A:1131:BLA:HMB3	1.79	0.62
1:A:6:LEU:HB3	1:A:33:GLN:HE22	1.64	0.62
1:A:79:LYS:HD2	1:A:85:ASP:OD1	2.00	0.62
1:A:123:THR:HG23	1:A:205:HIS:ND1	2.14	0.61
1:B:106:ILE:HD13	1:B:116:ALA:HA	1.81	0.61
1:A:6:LEU:HD23	1:A:7:SER:N	2.16	0.61
1:A:216:GLN:HG2	1:A:244:PHE:CZ	2.37	0.60
1:B:117:ILE:HA	1:B:163:LEU:O	2.01	0.59
1:B:237:ARG:O	1:B:241:GLN:HB2	2.01	0.59
2:B:1130:BLA:HMC1	2:B:1130:BLA:HBC1	1.85	0.59
1:A:144:GLU:O	1:A:175:ARG:NH2	2.34	0.59
1:B:169:ASN:ND2	1:B:171:THR:HB	2.19	0.58
1:A:33:GLN:HE21	1:A:33:GLN:CA	2.13	0.57
1:A:53:LEU:O	1:A:56:GLU:HG2	2.04	0.57
1:B:117:ILE:HG13	1:B:164:PHE:CD2	2.34	0.57
1:B:71:ARG:NH1	1:B:206:ARG:NH1	2.50	0.57
1:A:201:GLN:O	1:A:205:HIS:HD2	1.87	0.57
1:B:24:LEU:O	1:B:24:LEU:HD13	2.07	0.54
1:B:84:LEU:HD22	2:B:1130:BLA:HMD3	1.89	0.54
1:B:145:PHE:CD2	1:B:165:ILE:CD1	2.92	0.53
1:B:101:LEU:HD11	1:B:209:GLN:HG2	1.90	0.52
1:B:245:ASP:O	1:B:246:VAL:HB	2.09	0.52
1:B:24:LEU:HD13	1:B:24:LEU:C	2.31	0.50
1:B:148:GLN:HG3	3:B:297:HOH:O	2.11	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:169:ASN:ND2	1:B:172:GLU:H	2.08	0.50
1:A:6:LEU:HD12	1:A:37:LEU:HD11	1.94	0.49
1:B:101:LEU:HD12	1:B:123:THR:CG2	2.42	0.49
1:B:197:LEU:HD12	1:B:198:SER:HA	1.94	0.49
1:B:213:CYS:O	1:B:217:GLN:HG2	2.13	0.49
1:A:123:THR:HG23	1:A:205:HIS:CE1	2.48	0.49
1:A:154:TRP:CB	1:A:218:LYS:HD2	2.43	0.48
1:B:169:ASN:HD22	1:B:172:GLU:H	1.60	0.48
1:A:217:GLN:HE21	1:A:217:GLN:CA	2.26	0.48
1:B:163:LEU:HD11	1:B:179:ARG:HG2	1.95	0.48
1:A:154:TRP:HB3	1:A:218:LYS:HD2	1.94	0.48
1:A:126:ASP:HB3	1:A:128:GLN:H	1.79	0.48
2:A:1131:BLA:HBA1	2:A:1131:BLA:HMA2	1.95	0.48
1:B:84:LEU:CD2	2:B:1130:BLA:HMD3	2.44	0.47
1:B:6:LEU:CG	1:B:6:LEU:O	2.61	0.47
1:B:96:LEU:HD21	1:B:196:PRO:CB	2.43	0.47
1:A:123:THR:CG2	1:A:205:HIS:ND1	2.77	0.47
1:A:106:ILE:CD1	1:A:116:ALA:CB	2.92	0.47
1:B:217:GLN:OE1	1:B:217:GLN:HA	2.15	0.47
1:A:6:LEU:HD12	1:A:37:LEU:CD1	2.45	0.47
1:B:145:PHE:CD2	1:B:165:ILE:HD13	2.50	0.47
1:A:105:ASP:O	1:A:106:ILE:HD13	2.15	0.47
1:A:71:ARG:HG2	1:A:93:PRO:O	2.14	0.47
1:B:58:LEU:HD13	1:B:80:VAL:HA	1.96	0.47
1:A:53:LEU:O	1:A:56:GLU:CG	2.62	0.47
1:A:217:GLN:HA	1:A:217:GLN:NE2	2.30	0.46
1:B:245:ASP:OD1	1:B:246:VAL:HG23	2.16	0.46
1:B:146:GLU:HG3	1:B:147:GLN:HG3	1.97	0.46
1:A:217:GLN:HA	1:A:217:GLN:HE21	1.79	0.46
1:A:106:ILE:CD1	1:A:116:ALA:HB1	2.45	0.46
1:A:71:ARG:NH2	1:A:245:ASP:OD2	2.48	0.46
1:B:117:ILE:HG12	1:B:164:PHE:CG	2.49	0.45
1:A:147:GLN:OE1	1:A:166[A]:ARG:HD3	2.15	0.45
1:B:6:LEU:HG	1:B:6:LEU:O	2.15	0.45
1:B:148:GLN:HA	1:B:165:ILE:HG22	1.99	0.45
1:A:93:PRO:HD2	1:A:101:LEU:HD13	2.00	0.45
1:B:58:LEU:HD12	1:B:59:VAL:N	2.32	0.45
1:B:239:MET:SD	1:B:243:LEU:HD12	2.57	0.44
1:A:51:GLY:O	1:A:52:ARG:HD2	2.18	0.44
1:A:6:LEU:CD2	1:A:6:LEU:C	2.86	0.44
1:A:6:LEU:HD23	1:A:6:LEU:C	2.38	0.44
1:B:35:LEU:HD11	1:B:188:CYS:SG	2.57	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:222:THR:HG23	2:A:1131:BLA:C3B	2.47	0.44
1:B:94:GLU:OE2	1:B:95:PRO:HD2	2.18	0.44
1:B:197:LEU:HG	1:B:198:SER:OG	2.18	0.44
1:A:58:LEU:HD13	1:A:80:VAL:HA	2.00	0.43
1:A:57:LYS:HB3	1:A:57:LYS:HE2	1.82	0.43
1:A:122:PRO:HD3	1:A:129:LEU:HD11	2.00	0.43
1:B:145:PHE:CG	1:B:165:ILE:HD13	2.53	0.43
1:B:235:ALA:O	1:B:239:MET:HG2	2.19	0.43
1:B:67:THR:HB	1:B:68:PRO:HD2	1.99	0.43
1:A:6:LEU:HB3	1:A:33:GLN:NE2	2.31	0.43
1:B:6:LEU:HD12	1:B:6:LEU:C	2.39	0.43
1:B:137:LEU:HD13	1:B:186:ILE:HD13	2.01	0.43
1:B:206:ARG:O	1:B:210:ILE:HG13	2.19	0.42
1:A:80:VAL:HB	1:A:84:LEU:HD23	2.01	0.42
1:B:169:ASN:C	1:B:169:ASN:HD22	2.23	0.42
1:B:101:LEU:HD12	1:B:123:THR:HG22	2.01	0.42
1:B:154:TRP:HA	1:B:215:GLN:NE2	2.34	0.42
1:A:223:ARG:O	1:A:226:LEU:N	2.53	0.42
1:A:6:LEU:HG	1:A:65:TYR:CE2	2.55	0.41
1:B:147:GLN:HB2	1:B:166:ARG:O	2.20	0.41
1:A:123:THR:HG21	3:A:325:HOH:O	2.20	0.41
1:A:201:GLN:NE2	3:A:304:HOH:O	2.53	0.41
1:A:147:GLN:OE1	1:A:166[B]:ARG:CZ	2.68	0.41
1:A:211:HIS:HD2	3:A:296:HOH:O	2.03	0.41
1:A:201:GLN:O	1:A:205:HIS:CD2	2.72	0.41
1:B:246:VAL:O	1:B:246:VAL:HG12	2.20	0.41
1:A:38:LYS:HB2	1:A:38:LYS:HE3	1.92	0.41
1:A:217:GLN:CA	1:A:217:GLN:NE2	2.83	0.41
1:B:67:THR:HB	1:B:68:PRO:CD	2.51	0.41
1:B:62:ASN:HD21	1:B:76:GLU:HG3	1.85	0.41
1:A:215:GLN:NE2	1:A:215:GLN:HA	2.36	0.41
1:A:189:HIS:O	1:A:193:VAL:HG13	2.20	0.41
1:B:87:LEU:C	1:B:87:LEU:HD23	2.42	0.41
1:A:244:PHE:HZ	2:A:1131:BLA:HMC2	1.72	0.40
1:A:185:GLN:NE2	3:A:324:HOH:O	2.47	0.40
1:B:117:ILE:HG12	1:B:164:PHE:HD2	1.58	0.40
1:A:163:LEU:HD11	1:A:179:ARG:HG2	2.04	0.40
1:A:52:ARG:HD2	1:A:52:ARG:HA	1.95	0.40
1:A:154:TRP:HB3	1:A:218:LYS:CD	2.52	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	240/248 (97%)	233 (97%)	7 (3%)	0	100	100
1	B	242/248 (98%)	234 (97%)	6 (2%)	2 (1%)	27	12
All	All	482/496 (97%)	467 (97%)	13 (3%)	2 (0%)	43	29

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	141	GLY
1	B	196	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	211/216 (98%)	186 (88%)	25 (12%)	8	2
1	B	212/216 (98%)	191 (90%)	21 (10%)	11	4
All	All	423/432 (98%)	377 (89%)	46 (11%)	10	3

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	33	GLN
1	A	35	LEU
1	A	38	LYS
1	A	52	ARG
1	A	58	LEU
1	A	71	ARG

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Mol	Chain	Res	Type
1	A	101	LEU
1	A	104[A]	CYS
1	A	104[B]	CYS
1	A	126	ASP
1	A	137	LEU
1	A	149	ARG
1	A	150	GLU
1	A	160	GLU
1	A	166[A]	ARG
1	A	166[B]	ARG
1	A	192	ILE
1	A	193	VAL
1	A	197	LEU
1	A	199	GLU
1	A	203	LEU
1	A	206	ARG
1	A	216	GLN
1	A	217	GLN
1	B	6	LEU
1	B	7	SER
1	B	35	LEU
1	B	41	GLN
1	B	57	LYS
1	B	58	LEU
1	B	71	ARG
1	B	96	LEU
1	B	101	LEU
1	B	125	SER
1	B	126	ASP
1	B	137	LEU
1	B	146	GLU
1	B	148	GLN
1	B	169	ASN
1	B	197	LEU
1	B	198	SER
1	B	204	GLU
1	B	218	LYS
1	B	241	GLN
1	B	245	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	23	GLN
1	A	33	GLN
1	A	62	ASN
1	A	134	GLN
1	A	211	HIS
1	A	215	GLN
1	A	217	GLN
1	B	33	GLN
1	B	62	ASN
1	B	66	GLN
1	B	134	GLN
1	B	169	ASN
1	B	209	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	BLA	A	1131	-	46,46,46	3.80	14 (30%)	65,67,67	2.56	25 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z|$ > 2	Counts	RMSZ	#$|Z|$ > 2
2	BLA	B	1130	-	46,46,46	3.51	14 (30%)	65,67,67	2.81	33 (50%)

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	BLA	A	1131	-	-	0/26/74/74	0/4/4/4
2	BLA	B	1130	-	-	0/26/74/74	0/4/4/4

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1131	BLA	CHA-C4D	20.48	1.49	1.35
2	B	1130	BLA	CHA-C4D	19.06	1.48	1.35
2	A	1131	BLA	CHB-C1B	6.37	1.49	1.34
2	B	1130	BLA	C3C-C2C	6.02	1.48	1.36
2	A	1131	BLA	C3B-C2B	5.90	1.48	1.36
2	A	1131	BLA	C3C-C2C	5.33	1.47	1.36
2	B	1130	BLA	CHB-C1B	5.31	1.46	1.34
2	A	1131	BLA	C3D-C2D	5.10	1.47	1.36
2	B	1130	BLA	C3B-C2B	5.03	1.46	1.36
2	B	1130	BLA	C3D-C2D	4.44	1.46	1.36
2	A	1131	BLA	CHD-C4C	4.17	1.47	1.37
2	A	1131	BLA	C2A-C3A	3.74	1.48	1.37
2	B	1130	BLA	CHD-C4C	3.56	1.46	1.37
2	A	1131	BLA	C4A-C3A	3.28	1.50	1.42
2	A	1131	BLA	OC-C1C	3.18	1.29	1.23
2	A	1131	BLA	CHD-C1D	3.15	1.48	1.40
2	A	1131	BLA	C1A-C2A	3.11	1.49	1.42
2	B	1130	BLA	CHD-C1D	3.01	1.47	1.40
2	A	1131	BLA	C1B-C2B	2.96	1.50	1.45
2	B	1130	BLA	OB-C4B	2.95	1.29	1.23
2	A	1131	BLA	C4D-C3D	2.80	1.50	1.45
2	A	1131	BLA	OB-C4B	2.73	1.28	1.23
2	B	1130	BLA	C2A-C3A	2.67	1.45	1.37
2	B	1130	BLA	C4C-NC	-2.53	1.33	1.37
2	B	1130	BLA	C1A-C2A	2.49	1.48	1.42
2	B	1130	BLA	C4D-C3D	2.48	1.49	1.45
2	B	1130	BLA	C1A-NA	2.23	1.38	1.36
2	B	1130	BLA	OC-C1C	2.23	1.27	1.23

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1131	BLA	C3B-C4B-NB	8.63	114.46	106.66
2	B	1130	BLA	C3B-C4B-NB	8.10	113.98	106.66
2	B	1130	BLA	C2B-C1B-NB	6.21	116.97	107.14
2	B	1130	BLA	C4A-C3A-C2A	-5.72	103.14	107.04
2	B	1130	BLA	C3B-C2B-C1B	-5.01	100.72	107.14
2	B	1130	BLA	C1B-NB-C4B	-4.89	103.83	110.74
2	A	1131	BLA	C2A-C1A-NA	4.83	114.75	106.79
2	A	1131	BLA	C4A-C3A-C2A	-4.72	103.82	107.04
2	B	1130	BLA	C4C-NC-C1C	-4.66	104.15	110.74
2	A	1131	BLA	C4C-NC-C1C	-4.59	104.26	110.74
2	A	1131	BLA	CMB-C2B-C1B	4.56	130.45	124.23
2	A	1131	BLA	C2B-C1B-NB	4.49	114.24	107.14
2	A	1131	BLA	C1A-C2A-C3A	-4.35	102.42	106.92
2	B	1130	BLA	C2A-C1A-NA	4.28	113.85	106.79
2	B	1130	BLA	CAD-C3D-C4D	4.12	132.48	124.85
2	B	1130	BLA	C3A-C4A-NA	4.02	115.97	108.16
2	B	1130	BLA	CMC-C2C-C1C	3.95	131.81	121.59
2	A	1131	BLA	C3B-C2B-C1B	-3.90	102.14	107.14
2	A	1131	BLA	CMC-C2C-C1C	3.90	131.69	121.59
2	A	1131	BLA	C1A-CHA-C4D	3.88	137.49	129.92
2	B	1130	BLA	C2C-C1C-NC	3.83	117.30	106.27
2	A	1131	BLA	C1B-NB-C4B	-3.76	105.43	110.74
2	B	1130	BLA	C3A-C4A-CHB	-3.72	115.18	125.72
2	B	1130	BLA	CHA-C4D-ND	-3.64	121.87	128.59
2	A	1131	BLA	C3C-C4C-NC	3.61	113.86	106.59
2	B	1130	BLA	C3C-C4C-NC	3.56	113.75	106.59
2	B	1130	BLA	CMB-C2B-C1B	3.51	129.02	124.23
2	B	1130	BLA	C1D-C2D-C3D	-3.34	102.50	106.64
2	A	1131	BLA	C4B-C3B-C2B	-3.31	103.73	107.97
2	A	1131	BLA	CAD-C3D-C4D	3.24	130.85	124.85
2	B	1130	BLA	C2A-C1A-CHA	-3.24	116.54	125.72
2	B	1130	BLA	CHB-C1B-NB	-3.18	118.96	130.23
2	B	1130	BLA	C3D-C4D-ND	3.14	114.76	109.79
2	A	1131	BLA	C2C-C1C-NC	3.14	115.30	106.27
2	A	1131	BLA	CAD-CBD-CGD	-3.07	107.83	113.53
2	A	1131	BLA	C1D-C2D-C3D	-3.07	102.84	106.64
2	B	1130	BLA	C4D-C3D-C2D	-3.05	103.31	106.86
2	A	1131	BLA	OB-C4B-C3B	-3.03	122.14	130.22
2	A	1131	BLA	CHB-C1B-NB	-2.97	119.70	130.23
2	B	1130	BLA	C2D-C1D-ND	2.74	116.84	110.31
2	B	1130	BLA	C4B-C3B-C2B	-2.71	104.50	107.97
2	A	1131	BLA	C3A-C4A-NA	2.69	113.40	108.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1130	BLA	C4A-NA-C1A	-2.66	102.62	108.72
2	A	1131	BLA	CHD-C1D-C2D	-2.64	118.52	125.10
2	A	1131	BLA	C4D-C3D-C2D	-2.62	103.81	106.86
2	B	1130	BLA	C1A-C2A-C3A	-2.60	104.23	106.92
2	B	1130	BLA	CAD-CBD-CGD	-2.57	108.77	113.53
2	A	1131	BLA	C3D-C4D-ND	2.55	113.83	109.79
2	B	1130	BLA	C4C-CHD-C1D	-2.43	122.09	128.13
2	B	1130	BLA	OC-C1C-NC	-2.29	119.13	125.12
2	B	1130	BLA	CHD-C1D-C2D	-2.29	119.39	125.10
2	B	1130	BLA	O1A-CGA-CBA	-2.25	115.30	123.03
2	A	1131	BLA	C2D-C1D-ND	2.19	115.55	110.31
2	B	1130	BLA	CAD-C3D-C2D	-2.13	124.19	128.00
2	B	1130	BLA	CMD-C2D-C1D	2.11	128.50	125.02
2	B	1130	BLA	C1A-CHA-C4D	2.10	134.02	129.92
2	B	1130	BLA	C4D-ND-C1D	-2.05	102.57	106.55
2	A	1131	BLA	CHA-C4D-ND	-2.01	124.88	128.59

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

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	238/248 (95%)	0.67	14 (5%)	22	22	19, 34, 50, 58	1 (0%)
1	B	241/248 (97%)	0.72	17 (7%)	16	15	21, 35, 50, 58	0
All	All	479/496 (96%)	0.69	31 (6%)	17	18	19, 35, 50, 58	1 (0%)

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	155	GLY	7.5
1	B	197	LEU	6.6
1	A	154	TRP	5.8
1	A	142	GLN	4.5
1	A	144	GLU	4.3
1	A	44	GLU	4.2
1	A	218	LYS	4.1
1	B	210	ILE	3.9
1	A	203	LEU	3.8
1	A	6	LEU	3.8
1	B	246	VAL	3.7
1	B	201	GLN	3.4
1	B	82	LYS	3.3
1	B	244	PHE	3.3
1	B	6	LEU	3.2
1	B	117	ILE	3.1
1	B	154	TRP	3.0
1	B	245	ASP	2.9
1	A	217	GLN	2.9
1	A	82	LYS	2.8
1	A	157	ILE	2.8
1	B	111	GLY	2.7
1	A	246	VAL	2.6
1	B	198	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	7	SER	2.2
1	A	210	ILE	2.2
1	B	196	PRO	2.2
1	B	142	GLN	2.2
1	A	199	GLU	2.1
1	B	163	LEU	2.1
1	B	153	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	BLA	A	1131	43/43	0.37	7.56	63,70,75,76	0
2	BLA	B	1130	43/43	0.22	2.23	33,43,48,50	0

6.5 Other polymers ⓘ

There are no such residues in this entry.