



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2017 – 04:24 pm GMT

PDB ID : 2BRD
Title : CRYSTAL STRUCTURE OF BACTERIORHODOPSIN IN PURPLE MEMBRANE
Authors : Henderson, R.; Grigorieff, N.
Deposited on : 1995-12-27
Resolution : 3.50 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc29102

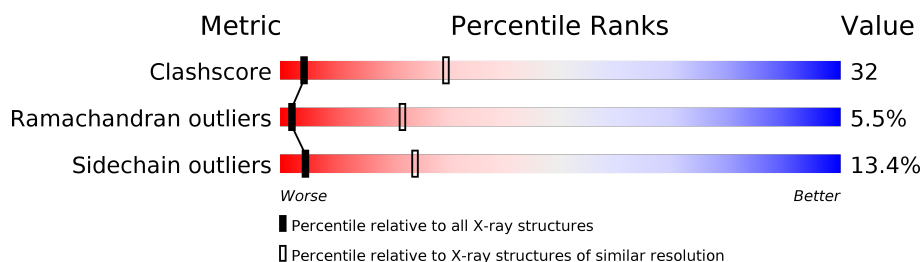
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON CRYSTALLOGRAPHY

The reported resolution of this entry is 3.50 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))
Clashscore	112137	1322 (3.60-3.40)
Ramachandran outliers	110173	1283 (3.60-3.40)
Sidechain outliers	110143	1284 (3.60-3.40)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	248	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	RET	A	271	-	-	X	-

2 Entry composition [i](#)

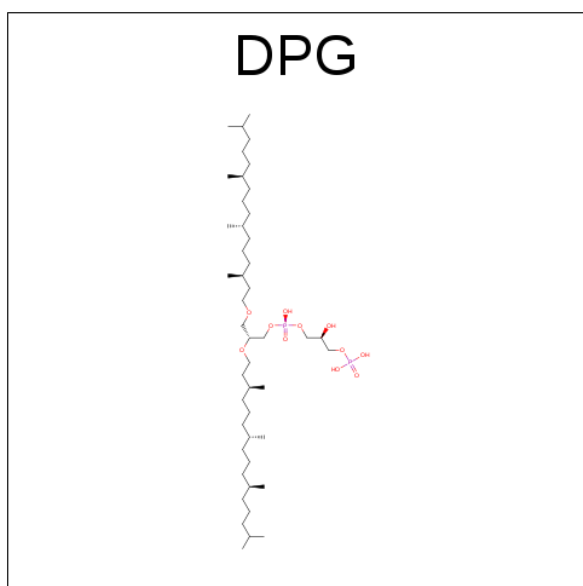
There are 3 unique types of molecules in this entry. The entry contains 2328 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 BACTERIORHODOPSIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	222	Total	C	N	O	S	0	0	1
			1718	1154	263	292	9			

- Molecule 2 is PHOSPHORIC ACID 2,3-BIS-(3,7,11,15-TETRAMETHYL-HEXADECYLOXY)-PROPYL ESTER 2-HYDROXY-3-PHOSPHONOXY-PROPYL ESTER (three-letter code: DPG) (formula: $C_{46}H_{96}O_{11}P_2$).



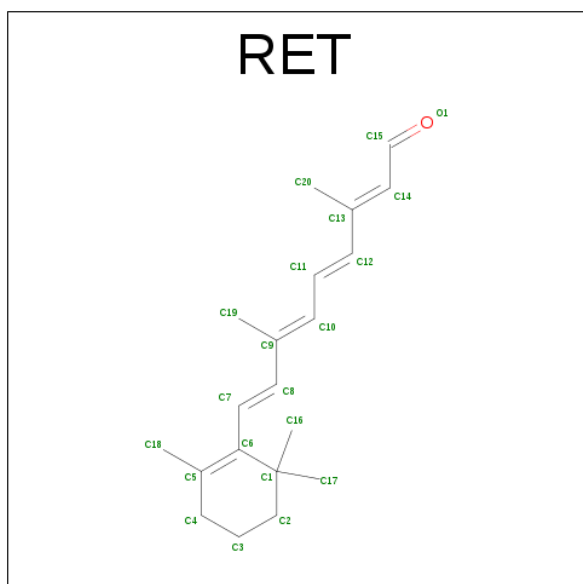
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			59	46	11	2		
2	A	1	Total	C	O	P	0	0
			59	46	11	2		
2	A	1	Total	C	O	P	0	0
			59	46	11	2		
2	A	1	Total	C	O	P	0	0
			59	46	11	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			59	46	11	2		
2	A	1	Total	C	O	P	0	0
			59	46	11	2		
2	A	1	Total	C	O	P	0	0
			59	46	11	2		
2	A	1	Total	C	O	P	0	0
			59	46	11	2		
2	A	1	Total	C	O	P	0	0
			59	46	11	2		

- Molecule 3 is RETINAL (three-letter code: RET) (formula: $C_{20}H_{28}O$).



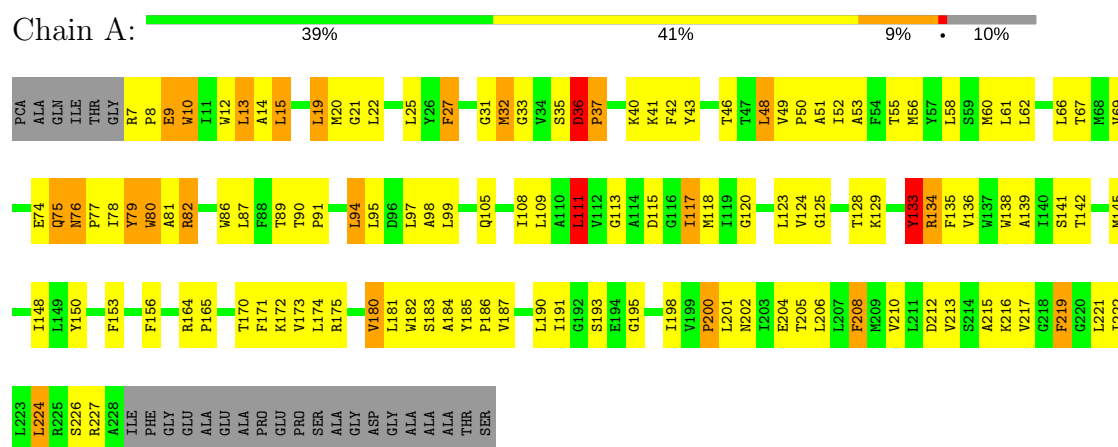
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	C	0	0
			20	20		

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.

Note EDS was not executed.

• Molecule 1: BACTERIORHODOPSIN



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, α , β , γ	62.45Å 62.45Å 100.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 3.50	Depositor
% Data completeness (in resolution range)	85.4 (30.00-3.50)	Depositor
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.280 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2328	wwPDB-VP
Average B, all atoms (Å ²)	114.0	wwPDB-VP

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: DPG, RET

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	0.67	0/1765	1.23	8/2412 (0.3%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	133	TYR	CA-CB-CG	7.68	128.00	113.40
1	A	80	TRP	CA-CB-CG	7.50	127.94	113.70
1	A	153	PHE	CA-CB-CG	5.87	128.00	113.90
1	A	111	LEU	CB-CA-C	5.47	120.58	110.20
1	A	134	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	A	10	TRP	CA-CB-CG	5.25	123.68	113.70
1	A	82	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	A	111	LEU	CA-CB-CG	5.03	126.86	115.30

There are no chirality outliers.

There are no planarity outliers.

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	1718	0	1774	118	0
2	A	590	0	930	68	0
3	A	20	0	27	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	2328	0	2731	163	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 32.

All (163) 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)
2:A:265:DPG:H42	2:A:265:DPG:C3	1.60	1.32
2:A:265:DPG:C4	2:A:265:DPG:H31	1.63	1.26
2:A:263:DPG:O3	2:A:263:DPG:H412	1.36	1.09
3:A:271:RET:H161	3:A:271:RET:H8	1.20	1.09
3:A:271:RET:H161	3:A:271:RET:C8	1.97	0.93
2:A:267:DPG:H471	2:A:268:DPG:H202	1.56	0.86
2:A:263:DPG:O3	2:A:263:DPG:C41	2.21	0.85
1:A:48:LEU:HD23	1:A:52:ILE:HD11	1.57	0.84
1:A:32:MET:HA	2:A:269:DPG:H172	1.65	0.79
2:A:265:DPG:H42	2:A:265:DPG:H31	0.82	0.78
3:A:271:RET:C16	3:A:271:RET:H8	2.04	0.77
1:A:115:ASP:HA	1:A:148:ILE:HD11	1.67	0.76
1:A:7:ARG:HB3	1:A:8:PRO:HD3	1.64	0.76
1:A:76:ASN:N	1:A:77:PRO:HD2	2.01	0.76
2:A:263:DPG:H242	2:A:265:DPG:H53	1.67	0.76
1:A:89:THR:HG21	3:A:271:RET:C15	2.19	0.73
1:A:164:ARG:HB3	1:A:165:PRO:HD2	1.71	0.72
2:A:267:DPG:H421	2:A:267:DPG:H142	1.72	0.72
1:A:184:ALA:HA	2:A:267:DPG:H293	1.71	0.72
1:A:15:LEU:HD21	2:A:265:DPG:H543	1.72	0.72
1:A:170:THR:HG21	1:A:226:SER:HB2	1.72	0.71
1:A:90:THR:HB	1:A:91:PRO:HD3	1.73	0.71
1:A:187:VAL:HG11	2:A:262:DPG:H243	1.71	0.71
1:A:82:ARG:HH22	1:A:204:GLU:HG3	1.55	0.70
2:A:264:DPG:H443	2:A:264:DPG:H193	1.72	0.70
2:A:261:DPG:H291	2:A:266:DPG:H602	1.75	0.68
1:A:49:VAL:HB	1:A:50:PRO:CD	2.23	0.68
1:A:94:LEU:HD13	1:A:97:LEU:HD11	1.76	0.68
2:A:262:DPG:H441	2:A:263:DPG:H442	1.76	0.68
1:A:66:LEU:HD21	2:A:261:DPG:H412	1.75	0.67
1:A:49:VAL:HB	1:A:50:PRO:HD3	1.77	0.66
1:A:173:VAL:HG21	2:A:268:DPG:H442	1.77	0.66
1:A:76:ASN:N	1:A:77:PRO:CD	2.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:267:DPG:H572	2:A:268:DPG:H592	1.79	0.64
1:A:60:MET:HG3	1:A:78:ILE:HA	1.78	0.63
3:A:271:RET:C16	3:A:271:RET:C8	2.71	0.63
2:A:266:DPG:C4	2:A:266:DPG:C3	2.77	0.63
2:A:266:DPG:C4	2:A:266:DPG:H31	2.29	0.62
1:A:76:ASN:H	1:A:77:PRO:HD2	1.62	0.62
1:A:145:MET:SD	1:A:186:PRO:HG3	2.39	0.62
1:A:76:ASN:H	1:A:77:PRO:CD	2.12	0.62
2:A:266:DPG:H41	2:A:266:DPG:C3	2.29	0.62
2:A:266:DPG:H172	2:A:266:DPG:H493	1.81	0.62
1:A:135:PHE:HA	1:A:138:TRP:HB3	1.81	0.62
1:A:40:LYS:HE3	2:A:269:DPG:H162	1.82	0.62
2:A:262:DPG:H571	2:A:268:DPG:H303	1.81	0.61
1:A:36:ASP:HB2	1:A:37:PRO:HD3	1.83	0.61
1:A:40:LYS:HG3	2:A:269:DPG:H193	1.83	0.61
1:A:75:GLN:HB3	1:A:77:PRO:HD2	1.83	0.60
1:A:67:THR:HG23	1:A:75:GLN:HG2	1.84	0.60
1:A:95:LEU:O	1:A:99:LEU:HB2	2.02	0.59
2:A:262:DPG:H593	2:A:268:DPG:H272	1.85	0.59
2:A:264:DPG:H543	2:A:264:DPG:H292	1.83	0.58
1:A:94:LEU:HD12	1:A:111:LEU:HD21	1.85	0.58
1:A:172:LYS:HG3	1:A:175:ARG:HH21	1.69	0.58
2:A:262:DPG:H602	2:A:268:DPG:H252	1.84	0.58
1:A:156:PHE:HB2	1:A:171:PHE:HE2	1.67	0.57
2:A:263:DPG:H591	2:A:268:DPG:H541	1.87	0.56
1:A:90:THR:HG22	1:A:115:ASP:OD2	2.06	0.56
2:A:262:DPG:H121	2:A:262:DPG:H452	1.88	0.56
2:A:265:DPG:C4	2:A:265:DPG:C3	2.46	0.55
1:A:14:ALA:HA	1:A:61:LEU:HD22	1.88	0.55
1:A:183:SER:HB2	2:A:267:DPG:H242	1.89	0.55
1:A:32:MET:HG3	2:A:269:DPG:H152	1.89	0.55
1:A:22:LEU:HD12	2:A:270:DPG:H592	1.87	0.54
2:A:266:DPG:H41	2:A:266:DPG:H32	1.90	0.54
1:A:90:THR:HB	1:A:91:PRO:CD	2.37	0.54
1:A:206:LEU:O	1:A:210:VAL:HG23	2.08	0.54
2:A:263:DPG:H292	2:A:264:DPG:H302	1.89	0.54
1:A:90:THR:HG23	1:A:182:TRP:CH2	2.43	0.54
1:A:49:VAL:HG12	1:A:216:LYS:HD3	1.89	0.54
1:A:108:ILE:HA	1:A:111:LEU:HD22	1.89	0.53
1:A:20:MET:SD	1:A:53:ALA:HB1	2.49	0.53
1:A:97:LEU:HD12	1:A:98:ALA:N	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:GLY:O	1:A:128:THR:HG22	2.09	0.53
1:A:206:LEU:HD21	2:A:263:DPG:H502	1.90	0.53
2:A:263:DPG:H293	2:A:265:DPG:H603	1.89	0.53
1:A:35:SER:HB2	1:A:40:LYS:N	2.25	0.52
1:A:9:GLU:HA	1:A:12:TRP:HD1	1.74	0.52
1:A:182:TRP:HA	1:A:185:TYR:HD2	1.75	0.52
1:A:118:MET:HE1	3:A:271:RET:H192	1.91	0.52
1:A:87:LEU:HD21	2:A:261:DPG:H561	1.91	0.52
2:A:266:DPG:H31	2:A:266:DPG:H42	1.92	0.51
1:A:36:ASP:CB	1:A:37:PRO:HD3	2.40	0.51
1:A:180:VAL:HA	2:A:267:DPG:H243	1.93	0.51
1:A:86:TRP:CD1	3:A:271:RET:H14	2.47	0.50
1:A:87:LEU:O	1:A:91:PRO:HG2	2.11	0.50
1:A:13:LEU:HD13	1:A:205:THR:CG2	2.42	0.50
2:A:267:DPG:H143	2:A:267:DPG:H11	1.93	0.50
1:A:215:ALA:O	1:A:219:PHE:HB3	2.12	0.50
1:A:190:LEU:O	1:A:195:GLY:HA3	2.12	0.50
1:A:172:LYS:O	1:A:175:ARG:HG2	2.12	0.49
1:A:227:ARG:HA	1:A:227:ARG:HH11	1.76	0.49
1:A:15:LEU:HD11	2:A:265:DPG:H501	1.94	0.49
1:A:15:LEU:O	1:A:19:LEU:HB2	2.11	0.49
1:A:170:THR:O	1:A:174:LEU:HB2	2.12	0.49
1:A:118:MET:CE	3:A:271:RET:H192	2.42	0.49
2:A:263:DPG:H252	2:A:265:DPG:H522	1.95	0.49
1:A:204:GLU:O	1:A:208:PHE:HB2	2.12	0.49
2:A:267:DPG:H522	2:A:268:DPG:H242	1.93	0.49
1:A:41:LYS:NZ	1:A:99:LEU:HG	2.27	0.49
1:A:210:VAL:HG11	2:A:268:DPG:H593	1.94	0.49
1:A:141:SER:CB	3:A:271:RET:H41	2.43	0.48
1:A:170:THR:CG2	1:A:226:SER:HB2	2.43	0.48
1:A:86:TRP:CD1	3:A:271:RET:H12	2.48	0.48
1:A:31:GLY:O	1:A:32:MET:C	2.51	0.48
1:A:7:ARG:CB	1:A:8:PRO:HD3	2.38	0.48
1:A:13:LEU:HD13	1:A:205:THR:HG23	1.96	0.47
2:A:265:DPG:H572	2:A:265:DPG:H293	1.96	0.47
2:A:262:DPG:H241	2:A:267:DPG:H271	1.95	0.47
1:A:185:TYR:HB2	1:A:186:PRO:CD	2.45	0.47
2:A:266:DPG:H5	2:A:266:DPG:O9	2.15	0.47
2:A:269:DPG:H32	2:A:269:DPG:H411	1.47	0.47
1:A:221:LEU:HA	1:A:224:LEU:HB3	1.96	0.46
1:A:36:ASP:H	1:A:37:PRO:HD2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:ILE:HG22	2:A:266:DPG:H601	1.96	0.46
1:A:9:GLU:HA	1:A:12:TRP:CD1	2.50	0.46
1:A:12:TRP:CE3	1:A:206:LEU:HD13	2.51	0.46
2:A:261:DPG:H58	2:A:266:DPG:H291	1.98	0.46
2:A:268:DPG:H32	2:A:268:DPG:H412	1.48	0.45
1:A:58:LEU:HD12	1:A:62:LEU:HD13	1.98	0.45
1:A:113:GLY:O	1:A:117:ILE:HG23	2.16	0.45
1:A:27:PHE:HE1	1:A:43:TYR:HD1	1.62	0.45
1:A:82:ARG:HB3	1:A:86:TRP:CZ2	2.51	0.45
1:A:185:TYR:CB	1:A:186:PRO:CD	2.95	0.45
1:A:206:LEU:HD11	2:A:263:DPG:H543	1.98	0.45
1:A:53:ALA:HB2	1:A:216:LYS:HE3	1.98	0.45
1:A:128:THR:HG23	1:A:134:ARG:HG2	1.99	0.45
1:A:164:ARG:HB3	1:A:165:PRO:CD	2.44	0.44
1:A:191:ILE:HD13	2:A:262:DPG:H171	1.98	0.44
1:A:180:VAL:HG13	2:A:267:DPG:H543	1.99	0.44
1:A:49:VAL:HG12	1:A:216:LYS:CD	2.48	0.44
1:A:53:ALA:CB	1:A:216:LYS:HE3	2.48	0.44
1:A:74:GLU:HB2	1:A:79:TYR:OH	2.18	0.43
1:A:115:ASP:O	1:A:118:MET:HB3	2.18	0.43
2:A:262:DPG:C44	2:A:263:DPG:H442	2.48	0.43
1:A:172:LYS:CG	1:A:175:ARG:HH21	2.32	0.43
1:A:198:ILE:O	2:A:262:DPG:H12	2.18	0.43
2:A:262:DPG:H552	2:A:267:DPG:H603	2.01	0.43
1:A:105:GLN:HA	2:A:266:DPG:H422	2.00	0.42
2:A:261:DPG:O5	2:A:261:DPG:H5	2.19	0.42
1:A:69:VAL:HG12	1:A:74:GLU:O	2.18	0.42
1:A:180:VAL:HG12	1:A:181:LEU:HD22	2.01	0.42
1:A:141:SER:HB3	3:A:271:RET:H41	2.02	0.42
1:A:120:GLY:O	1:A:123:LEU:HB3	2.19	0.42
1:A:21:GLY:O	1:A:25:LEU:HG	2.20	0.42
1:A:156:PHE:HB2	1:A:171:PHE:CE2	2.52	0.42
1:A:120:GLY:O	1:A:124:VAL:HG23	2.19	0.42
1:A:51:ALA:HB1	2:A:269:DPG:H302	2.01	0.42
1:A:170:THR:HG23	1:A:222:ILE:HG22	2.01	0.42
1:A:200:PRO:HB2	1:A:201:LEU:H	1.72	0.42
1:A:36:ASP:H	1:A:37:PRO:CD	2.32	0.42
2:A:264:DPG:H442	2:A:265:DPG:H43	2.03	0.41
1:A:41:LYS:HD2	1:A:99:LEU:HD21	2.00	0.41
1:A:42:PHE:O	1:A:46:THR:HG22	2.20	0.41
1:A:139:ALA:O	1:A:142:THR:HB	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:VAL:CG1	2:A:267:DPG:H292	2.50	0.41
1:A:173:VAL:HG23	2:A:268:DPG:H452	2.03	0.41
1:A:31:GLY:HA2	1:A:43:TYR:CE1	2.56	0.41
2:A:264:DPG:H412	2:A:264:DPG:H32	1.53	0.41
1:A:187:VAL:HB	2:A:267:DPG:H292	2.03	0.40
1:A:105:GLN:HB2	2:A:266:DPG:O3	2.22	0.40
1:A:56:MET:CE	1:A:81:ALA:HA	2.50	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	220/248 (89%)	168 (76%)	40 (18%)	12 (6%)	2	22

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	32	MET
1	A	193	SER
1	A	200	PRO
1	A	9	GLU
1	A	33	GLY
1	A	37	PRO
1	A	133	TYR
1	A	36	ASP
1	A	75	GLN
1	A	212	ASP
1	A	76	ASN
1	A	180	VAL

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	179/193 (93%)	155 (87%)	24 (13%)	4 24

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

Mol	Chain	Res	Type
1	A	10	TRP
1	A	13	LEU
1	A	15	LEU
1	A	19	LEU
1	A	27	PHE
1	A	36	ASP
1	A	48	LEU
1	A	55	THR
1	A	79	TYR
1	A	80	TRP
1	A	94	LEU
1	A	109	LEU
1	A	111	LEU
1	A	117	ILE
1	A	129	LYS
1	A	133	TYR
1	A	136	VAL
1	A	150	TYR
1	A	202	ASN
1	A	208	PHE
1	A	213	VAL
1	A	217	VAL
1	A	219	PHE
1	A	224	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

11 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	DPG	A	261	-	58,58,58	0.86	1 (1%)	64,73,73	1.00	3 (4%)
2	DPG	A	262	-	58,58,58	0.86	1 (1%)	64,73,73	0.99	4 (6%)
2	DPG	A	263	-	58,58,58	0.87	1 (1%)	64,73,73	1.00	4 (6%)
2	DPG	A	264	-	58,58,58	0.86	1 (1%)	64,73,73	1.01	1 (1%)
2	DPG	A	265	-	58,58,58	0.87	1 (1%)	64,73,73	0.99	3 (4%)
2	DPG	A	266	-	58,58,58	0.86	1 (1%)	64,73,73	0.94	1 (1%)
2	DPG	A	267	-	58,58,58	0.87	1 (1%)	64,73,73	1.06	4 (6%)
2	DPG	A	268	-	58,58,58	0.87	1 (1%)	64,73,73	1.06	5 (7%)
2	DPG	A	269	-	58,58,58	0.87	1 (1%)	64,73,73	0.94	4 (6%)
2	DPG	A	270	-	58,58,58	0.87	1 (1%)	64,73,73	1.02	3 (4%)
3	RET	A	271	1	19,20,21	0.98	2 (10%)	27,27,28	0.82	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	DPG	A	261	-	-	1/67/67/67	0/0/0/0
2	DPG	A	262	-	-	0/67/67/67	0/0/0/0
2	DPG	A	263	-	-	0/67/67/67	0/0/0/0
2	DPG	A	264	-	-	0/67/67/67	0/0/0/0
2	DPG	A	265	-	-	0/67/67/67	0/0/0/0
2	DPG	A	266	-	-	0/67/67/67	0/0/0/0
2	DPG	A	267	-	-	0/67/67/67	0/0/0/0
2	DPG	A	268	-	-	0/67/67/67	0/0/0/0
2	DPG	A	269	-	-	0/67/67/67	0/0/0/0
2	DPG	A	270	-	-	0/67/67/67	0/0/0/0
3	RET	A	271	1	-	0/13/30/31	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	271	RET	C2-C3	-2.75	1.45	1.52
3	A	271	RET	C15-C14	-2.44	1.39	1.49
2	A	266	DPG	C4-C5	2.06	1.59	1.51
2	A	269	DPG	C4-C5	2.07	1.59	1.51
2	A	265	DPG	C4-C5	2.08	1.59	1.51
2	A	261	DPG	C4-C5	2.09	1.59	1.51
2	A	267	DPG	C4-C5	2.09	1.59	1.51
2	A	264	DPG	C4-C5	2.10	1.59	1.51
2	A	268	DPG	C4-C5	2.10	1.59	1.51
2	A	263	DPG	C4-C5	2.11	1.59	1.51
2	A	270	DPG	C4-C5	2.11	1.59	1.51
2	A	262	DPG	C4-C5	2.12	1.59	1.51

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	265	DPG	C21-C20-C18	-2.35	108.03	115.73
2	A	268	DPG	C21-C20-C18	-2.19	108.55	115.73
2	A	262	DPG	C56-C57-C58	-2.19	105.53	115.96
2	A	267	DPG	C21-C20-C18	-2.18	108.57	115.73
2	A	269	DPG	C56-C57-C58	-2.16	105.65	115.96
2	A	261	DPG	C56-C57-C58	-2.16	105.67	115.96
2	A	268	DPG	C56-C57-C58	-2.15	105.71	115.96
2	A	270	DPG	C21-C20-C18	-2.13	108.74	115.73
2	A	263	DPG	C21-C20-C18	-2.10	108.83	115.73
2	A	262	DPG	C21-C20-C18	-2.09	108.88	115.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	263	DPG	C56-C57-C58	-2.04	106.22	115.96
2	A	269	DPG	C21-C20-C18	-2.04	109.04	115.73
2	A	265	DPG	C21-C22-C23	2.00	122.31	115.73
2	A	269	DPG	C54-C53-C52	2.00	118.67	111.36
2	A	268	DPG	C54-C53-C52	2.01	118.68	111.36
2	A	269	DPG	C21-C22-C23	2.01	122.33	115.73
2	A	261	DPG	C54-C53-C52	2.03	118.75	111.36
2	A	262	DPG	C54-C53-C52	2.06	118.89	111.36
2	A	265	DPG	C54-C53-C52	2.08	118.94	111.36
2	A	263	DPG	C54-C53-C52	2.09	118.97	111.36
2	A	268	DPG	C46-C45-C43	2.14	122.76	115.73
2	A	266	DPG	C16-C17-C18	2.20	122.94	115.73
2	A	267	DPG	C21-C22-C23	2.24	123.08	115.73
2	A	270	DPG	C16-C17-C18	2.31	123.30	115.73
2	A	263	DPG	C21-C22-C23	2.33	123.39	115.73
2	A	267	DPG	C46-C47-C48	2.40	123.60	115.73
2	A	267	DPG	C46-C45-C43	2.53	124.02	115.73
2	A	268	DPG	C16-C17-C18	2.60	124.26	115.73
2	A	262	DPG	C21-C22-C23	2.73	124.68	115.73
2	A	270	DPG	C21-C22-C23	2.89	125.23	115.73
2	A	264	DPG	C21-C22-C23	3.40	126.90	115.73
2	A	261	DPG	C21-C22-C23	3.43	126.98	115.73

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	261	DPG	P1-O6-C4-C5

There are no ring outliers.

11 monomers are involved in 79 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	261	DPG	5	0
2	A	262	DPG	11	0
2	A	263	DPG	11	0
2	A	264	DPG	5	0
2	A	265	DPG	11	0
2	A	266	DPG	12	0
2	A	267	DPG	13	0
2	A	268	DPG	11	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	269	DPG	6	0
2	A	270	DPG	1	0
3	A	271	RET	11	0

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.