Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 06:46 PM GMT

PDB ID	:	1CC0
Title	:	CRYSTAL STRUCTURE OF THE RHOA.GDP-RHOGDI COMPLEX
Authors	:	Longenecker, K.L.; Read, P.; Derewenda, U.; Dauter, Z.; Garrard, S.; Walker, L.; Somlyo, A.V.; Somlyo, A.P.; Nakamoto, R.K.; Derewenda, Z.S.
Deposited on	:	1999-03-03
Resolution	:	5.00 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

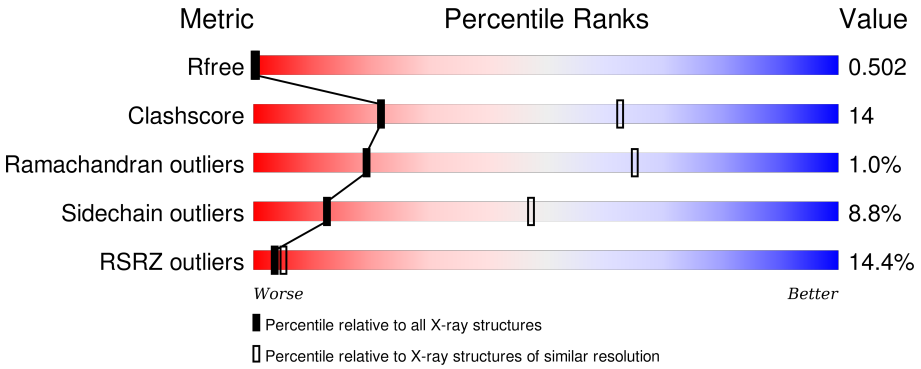
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 5.00 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}	91344	1119 (6.22-3.60)
Clashscore	102246	1019 (6.22-3.66)
Ramachandran outliers	100387	1158 (6.22-3.60)
Sidechain outliers	100360	1136 (6.22-3.60)
RSRZ outliers	91569	1122 (6.22-3.60)

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 <=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	190	6% 63% 24% 9%
1	C	190	6% 60% 27% 8%
2	E	204	21% 69% 19% 12%
2	F	204	21% 69% 19% 12%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MG	C	302	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5174 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 transforming protein rhoA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	187	Total	C	N	O	S	0	0	10
			1415	896	239	270	10			
1	C	187	Total	C	N	O	S	0	0	10
			1415	896	239	270	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	25	ASN	PHE	conflict	UNP P61586
C	25	ASN	PHE	conflict	UNP P61586

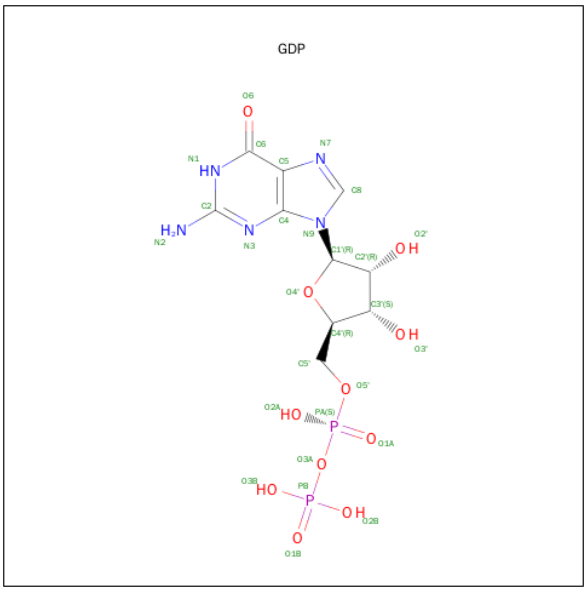
- Molecule 2 is a protein called rho GDP dissociation inhibitor alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	180	Total	C	N	O	S	0	0	44
			1143	748	183	208	4			
2	F	180	Total	C	N	O	S	0	0	44
			1143	748	183	208	4			

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



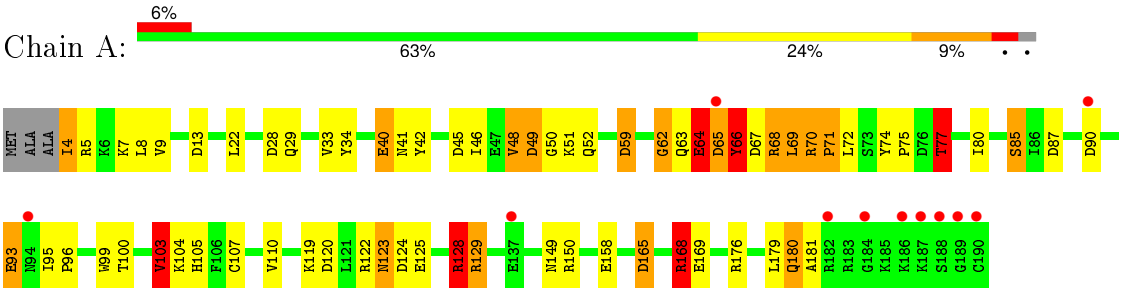
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
4	C	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

3 Residue-property plots (i)

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.

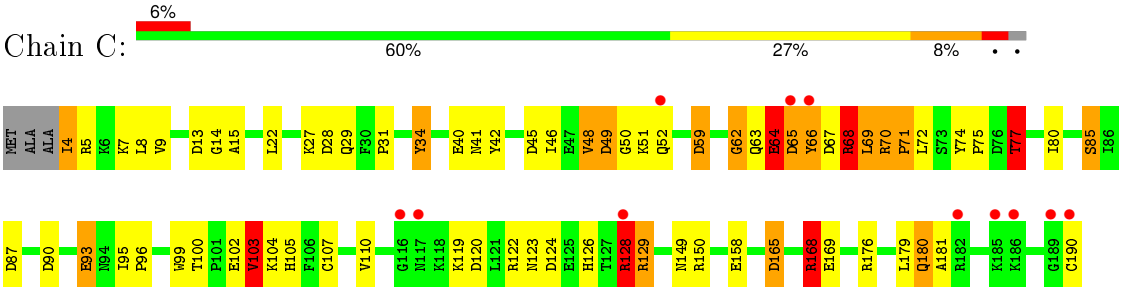
- Molecule 1: transforming protein rhoA

Chain A:



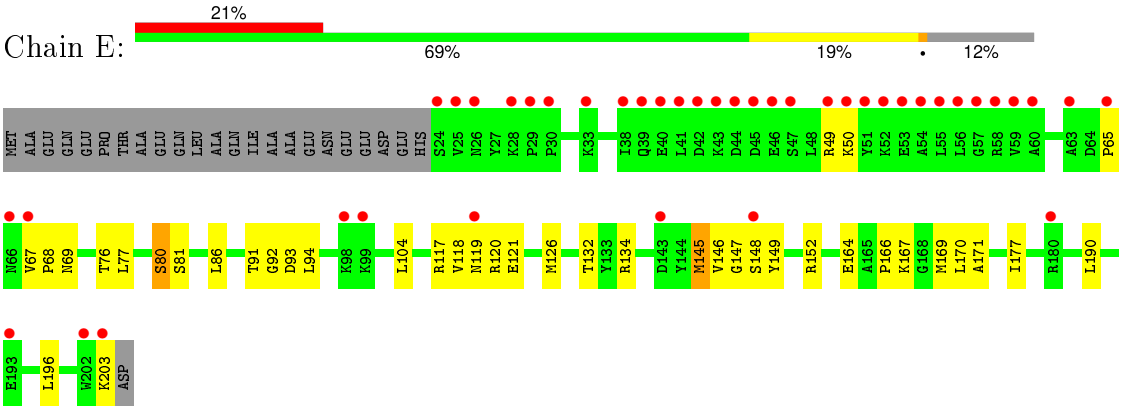
- Molecule 1: transforming protein rhoA

Chain C:



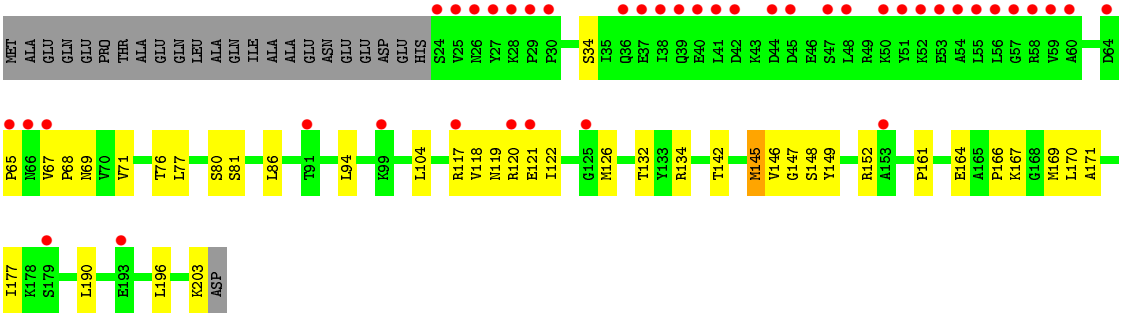
- Molecule 2: rho GDP dissociation inhibitor alpha

Chain E:



- Molecule 2: rho GDP dissociation inhibitor alpha

Chain F:


MET ALA GLU GLN GLU PRO THR ALA GLU GLN LEU ALA GLN ILE ALA ALA GLU ASN GLU GLU ASP GLU HIS S24 V25 N26 Y27 K28 P29 P30 S34 I35 Q36 E37 I38 Q39 E40 L41 D42 K43 D44 D45 E46 S47 L48 R49 K50 Y51 K52 E53 A54 L55 L56 G57 R58 V59 A60 D64
P65 N66 V67 P68 N69 V70 V71 T76 L77 S80 S81 I86 T91 L94 K99 L104 R117 V118 M119 R120 E121 I122 G125 M126 T132 Y133 R134 T142 M145 V146 G147 S148 Y149 R152 A153 P161 E164 A165 P166 K167 G168 M169 L170 A171
I177 K178 S179 L190 E193 L196 K203 ASP

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	139.30Å 139.30Å 253.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 5.00 19.97 – 4.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-5.00) 99.2 (19.97-4.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	1.66 (at 3.94Å)	Xtriage
Refinement program	O	Depositor
R, R_{free}	(Not available) , (Not available) 0.510 , 0.502	Depositor DCC
R_{free} test set	642 reflections (5.34%)	DCC
Wilson B-factor (Å^2)	138.6	Xtriage
Anisotropy	0.730	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 687.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Outliers	2 of 12673 reflections (0.016%)	Xtriage
F_o,F_c correlation	0.66	EDS
Total number of atoms	5174	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.74% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: GDP, MG

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	1.00	2/1432 (0.1%)	2.12	48/1937 (2.5%)
1	C	1.00	2/1432 (0.1%)	2.12	49/1937 (2.5%)
2	E	0.58	0/1124	0.93	1/1515 (0.1%)
2	F	0.59	0/1124	0.92	1/1515 (0.1%)
All	All	0.84	4/5112 (0.1%)	1.70	99/6904 (1.4%)

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	5
1	C	0	5
All	All	0	10

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	93	GLU	CD-OE2	5.85	1.32	1.25
1	C	93	GLU	CD-OE2	5.76	1.31	1.25
1	C	93	GLU	CG-CD	5.35	1.59	1.51
1	A	93	GLU	CG-CD	5.35	1.59	1.51

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	122	ARG	NE-CZ-NH2	-16.36	112.12	120.30
1	A	122	ARG	NE-CZ-NH2	-16.21	112.20	120.30
1	A	176	ARG	NE-CZ-NH2	-15.41	112.59	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	176	ARG	NE-CZ-NH2	-15.39	112.61	120.30
1	C	150	ARG	NE-CZ-NH2	-15.31	112.64	120.30
1	A	150	ARG	NE-CZ-NH2	-15.31	112.65	120.30
1	A	168	ARG	CD-NE-CZ	15.07	144.70	123.60
1	C	168	ARG	CD-NE-CZ	15.06	144.68	123.60
1	A	5	ARG	NE-CZ-NH2	-14.77	112.92	120.30
1	C	5	ARG	NE-CZ-NH2	-14.73	112.94	120.30
1	A	5	ARG	CD-NE-CZ	14.57	144.00	123.60
1	C	5	ARG	CD-NE-CZ	14.56	143.98	123.60
1	A	5	ARG	NE-CZ-NH1	14.15	127.38	120.30
1	C	5	ARG	NE-CZ-NH1	14.01	127.30	120.30
1	C	68	ARG	NE-CZ-NH1	13.39	127.00	120.30
1	C	176	ARG	NE-CZ-NH1	13.29	126.94	120.30
1	A	176	ARG	NE-CZ-NH1	13.15	126.88	120.30
1	A	68	ARG	NE-CZ-NH1	13.05	126.83	120.30
1	A	87	ASP	CB-CG-OD2	11.21	128.38	118.30
1	C	87	ASP	CB-CG-OD2	11.11	128.30	118.30
1	A	122	ARG	NH1-CZ-NH2	9.73	130.10	119.40
1	C	122	ARG	NH1-CZ-NH2	9.73	130.10	119.40
1	C	34	TYR	CB-CG-CD1	-9.05	115.57	121.00
1	A	34	TYR	CB-CG-CD1	-8.96	115.62	121.00
1	C	124	ASP	CB-CG-OD2	8.73	126.15	118.30
1	A	124	ASP	CB-CG-OD2	8.71	126.14	118.30
1	A	40	GLU	OE1-CD-OE2	8.61	133.64	123.30
1	C	40	GLU	OE1-CD-OE2	8.59	133.61	123.30
1	C	28	ASP	CB-CG-OD1	7.79	125.31	118.30
1	A	28	ASP	CB-CG-OD1	7.77	125.29	118.30
1	A	165	ASP	CB-CG-OD2	7.65	125.19	118.30
1	C	165	ASP	CB-CG-OD2	7.62	125.16	118.30
1	A	129	ARG	NE-CZ-NH2	-7.42	116.59	120.30
1	C	129	ARG	NE-CZ-NH2	-7.31	116.64	120.30
1	C	59	ASP	CB-CG-OD1	7.00	124.60	118.30
1	A	59	ASP	CB-CG-OD1	6.99	124.59	118.30
1	C	34	TYR	CB-CG-CD2	6.97	125.19	121.00
1	A	34	TYR	CB-CG-CD2	6.85	125.11	121.00
1	C	68	ARG	NH1-CZ-NH2	-6.81	111.91	119.40
1	A	68	ARG	NH1-CZ-NH2	-6.74	111.99	119.40
1	C	129	ARG	CD-NE-CZ	6.61	132.86	123.60
1	A	129	ARG	CD-NE-CZ	6.58	132.81	123.60
1	C	42	TYR	CB-CG-CD2	-6.48	117.11	121.00
1	A	176	ARG	CD-NE-CZ	6.44	132.62	123.60
1	A	45	ASP	CB-CG-OD1	6.43	124.08	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	45	ASP	CB-CG-OD1	6.42	124.08	118.30
1	C	176	ARG	CD-NE-CZ	6.42	132.58	123.60
1	A	42	TYR	CB-CG-CD2	-6.34	117.19	121.00
1	A	103	VAL	CA-CB-CG2	6.34	120.41	110.90
1	C	103	VAL	CA-CB-CG2	6.32	120.38	110.90
1	C	59	ASP	CB-CG-OD2	-6.24	112.68	118.30
1	A	59	ASP	CB-CG-OD2	-6.17	112.75	118.30
1	A	150	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	C	150	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	C	158	GLU	OE1-CD-OE2	-5.97	116.14	123.30
1	A	158	GLU	OE1-CD-OE2	-5.95	116.16	123.30
1	C	4	ILE	N-CA-CB	5.83	124.20	110.80
1	C	90	ASP	N-CA-CB	5.81	121.06	110.60
1	A	90	ASP	N-CA-CB	5.80	121.03	110.60
1	A	4	ILE	N-CA-CB	5.79	124.11	110.80
1	A	13	ASP	CB-CG-OD1	5.64	123.38	118.30
1	C	13	ASP	CB-CG-OD1	5.63	123.37	118.30
1	A	93	GLU	OE1-CD-OE2	-5.62	116.55	123.30
1	C	49	ASP	CB-CG-OD2	-5.58	113.28	118.30
1	C	93	GLU	OE1-CD-OE2	-5.58	116.60	123.30
1	A	49	ASP	CB-CG-OD2	-5.57	113.28	118.30
1	C	66	TYR	CB-CG-CD1	5.56	124.34	121.00
1	C	65	ASP	CA-C-N	5.51	129.32	117.20
1	A	66	TYR	CB-CG-CD1	5.50	124.30	121.00
1	A	65	ASP	CA-C-N	5.50	129.30	117.20
1	A	46	ILE	CB-CG1-CD1	5.48	129.25	113.90
1	C	65	ASP	CA-C-O	-5.48	108.59	120.10
1	C	128	ARG	CD-NE-CZ	5.47	131.25	123.60
1	A	128	ARG	CD-NE-CZ	5.46	131.24	123.60
1	C	46	ILE	CB-CG1-CD1	5.46	129.18	113.90
1	A	65	ASP	CA-C-O	-5.45	108.66	120.10
1	A	77	THR	CA-CB-OG1	5.43	120.41	109.00
1	C	77	THR	CA-CB-OG1	5.42	120.38	109.00
2	E	118	VAL	N-CA-C	-5.38	96.47	111.00
1	A	70	ARG	NE-CZ-NH2	5.38	122.99	120.30
2	F	118	VAL	N-CA-C	-5.36	96.53	111.00
1	A	122	ARG	NE-CZ-NH1	-5.31	117.64	120.30
1	C	70	ARG	NE-CZ-NH2	5.31	122.95	120.30
1	A	180	GLN	CB-CA-C	-5.19	100.02	110.40
1	C	180	GLN	CB-CA-C	-5.19	100.03	110.40
1	C	122	ARG	NE-CZ-NH1	-5.17	117.72	120.30
1	C	103	VAL	CA-CB-CG1	5.15	118.62	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	103	VAL	CA-CB-CG1	5.14	118.61	110.90
1	A	85	SER	CB-CA-C	-5.12	100.37	110.10
1	C	85	SER	CB-CA-C	-5.12	100.38	110.10
1	A	120	ASP	CB-CG-OD2	5.11	122.90	118.30
1	C	120	ASP	CB-CG-OD2	5.10	122.89	118.30
1	A	65	ASP	C-N-CA	5.06	134.36	121.70
1	C	65	ASP	C-N-CA	5.05	134.34	121.70
1	A	180	GLN	N-CA-C	5.04	124.62	111.00
1	A	128	ARG	CB-CG-CD	5.04	124.70	111.60
1	C	180	GLN	N-CA-C	5.02	124.56	111.00
1	C	128	ARG	CB-CG-CD	5.01	124.62	111.60
1	C	31	PRO	O-C-N	-5.00	114.69	122.70

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	48	VAL	Peptide
1	A	49	ASP	Peptide
1	A	50	GLY	Peptide
1	A	62	GLY	Mainchain
1	A	64	GLU	Peptide
1	C	48	VAL	Peptide
1	C	49	ASP	Peptide
1	C	50	GLY	Peptide
1	C	62	GLY	Mainchain
1	C	64	GLU	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1415	0	1392	56	7
1	C	1415	0	1394	61	16
2	E	1143	0	1100	34	20
2	F	1143	0	1100	39	6
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1	0	0	0	0
4	A	28	0	12	0	0
4	C	28	0	12	0	0
All	All	5174	0	5010	143	26

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 14.

All (143) 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:F:67:VAL:CA	2:F:68:PRO:N	1.83	1.41
1:C:71:PRO:HB3	2:F:148:SER:OG	1.28	1.30
1:A:71:PRO:HB3	2:E:148:SER:OG	1.45	1.14
1:A:71:PRO:HB3	2:E:148:SER:CB	1.83	1.08
1:C:105:HIS:CD2	2:F:145:MET:CE	2.37	1.06
1:A:105:HIS:CD2	2:E:145:MET:CE	2.41	1.02
1:A:180:GLN:HE22	1:C:180:GLN:HE22	1.03	1.02
1:A:71:PRO:CB	2:E:148:SER:CB	2.44	0.94
1:C:105:HIS:CD2	2:F:145:MET:HE2	2.04	0.92
1:C:105:HIS:O	2:F:145:MET:HG2	1.71	0.91
1:A:105:HIS:NE2	2:E:145:MET:CE	2.35	0.89
1:A:107:CYS:HB3	1:A:110:VAL:HG13	1.56	0.88
1:C:71:PRO:CB	2:F:148:SER:OG	2.20	0.87
1:A:105:HIS:O	2:E:145:MET:HG2	1.75	0.87
1:C:107:CYS:HB3	1:C:110:VAL:HG13	1.56	0.86
1:C:71:PRO:HB3	2:F:148:SER:CB	2.06	0.85
2:F:67:VAL:CA	2:F:68:PRO:CD	2.55	0.84
1:A:105:HIS:CD2	2:E:145:MET:HE2	2.12	0.82
1:A:71:PRO:CB	2:E:148:SER:HB2	2.09	0.81
1:A:180:GLN:HE22	1:C:180:GLN:NE2	1.78	0.81
1:C:105:HIS:NE2	2:F:145:MET:CE	2.43	0.81
1:A:105:HIS:CD2	2:E:145:MET:HE1	2.15	0.80
1:A:180:GLN:NE2	1:C:180:GLN:HE22	1.79	0.80
1:C:71:PRO:CB	2:F:148:SER:CB	2.60	0.79
1:A:149:ASN:HD22	1:C:169:GLU:HG2	1.48	0.78
1:A:149:ASN:ND2	1:C:169:GLU:HG2	2.02	0.74
1:C:128:ARG:HH11	1:C:128:ARG:HG2	1.54	0.73
1:A:71:PRO:HB3	2:E:148:SER:HB2	1.68	0.72
1:A:128:ARG:HH11	1:A:128:ARG:HG2	1.54	0.71
1:A:105:HIS:NE2	2:E:145:MET:HE3	2.07	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:71:PRO:C	2:F:148:SER:HB2	2.15	0.67
1:A:71:PRO:HB2	2:E:148:SER:CB	2.25	0.67
2:E:69:ASN:ND2	2:E:120:ARG:H	1.92	0.67
2:F:69:ASN:ND2	2:F:120:ARG:H	1.92	0.66
1:C:68:ARG:NH1	2:F:34:SER:CA	2.58	0.66
1:C:72:LEU:HD21	2:F:122:ILE:HG21	1.76	0.66
1:A:4:ILE:HG22	1:A:52:GLN:O	1.96	0.66
1:A:71:PRO:CB	2:E:148:SER:OG	2.34	0.65
1:C:4:ILE:HG22	1:C:52:GLN:O	1.96	0.64
1:C:105:HIS:NE2	2:F:145:MET:HE1	2.11	0.64
1:A:119:LYS:NZ	1:A:165:ASP:OD2	2.26	0.64
1:A:107:CYS:HB3	1:A:110:VAL:CG1	2.27	0.64
1:C:107:CYS:HB3	1:C:110:VAL:CG1	2.27	0.63
1:A:105:HIS:NE2	2:E:145:MET:HE2	2.08	0.62
1:C:105:HIS:CD2	2:F:145:MET:HE3	2.33	0.62
1:C:95:ILE:HB	1:C:96:PRO:HD3	1.82	0.62
1:C:128:ARG:NH1	1:C:128:ARG:HG2	2.13	0.62
2:E:69:ASN:ND2	2:E:121:GLU:H	1.98	0.61
2:F:69:ASN:ND2	2:F:121:GLU:H	1.98	0.61
1:C:68:ARG:HH11	2:F:34:SER:CA	2.11	0.61
2:F:166:PRO:HB2	2:F:171:ALA:HB1	1.82	0.61
2:E:166:PRO:HB2	2:E:171:ALA:HB1	1.82	0.61
2:E:69:ASN:HD21	2:E:121:GLU:H	1.49	0.61
1:A:95:ILE:HB	1:A:96:PRO:HD3	1.82	0.60
1:A:128:ARG:NH1	1:A:128:ARG:HG2	2.13	0.59
1:C:105:HIS:NE2	2:F:145:MET:HE3	2.17	0.59
2:F:69:ASN:HD21	2:F:121:GLU:H	1.49	0.58
2:E:104:LEU:HD22	2:E:196:LEU:HD11	1.84	0.58
2:F:104:LEU:HD22	2:F:196:LEU:HD11	1.85	0.57
1:C:180:GLN:O	1:C:181:ALA:CA	2.53	0.57
1:A:62:GLY:C	1:A:64:GLU:N	2.57	0.57
1:A:180:GLN:O	1:A:181:ALA:CA	2.54	0.56
1:C:119:LYS:NZ	1:C:165:ASP:OD2	2.26	0.56
1:C:7:LYS:HE2	1:C:77:THR:HG22	1.88	0.56
1:A:7:LYS:HE2	1:A:77:THR:HG22	1.88	0.56
1:C:62:GLY:C	1:C:64:GLU:N	2.57	0.55
1:C:63:GLN:O	1:C:64:GLU:HB2	2.07	0.55
1:A:63:GLN:O	1:A:64:GLU:HB2	2.07	0.54
1:A:72:LEU:HD22	1:A:72:LEU:H	1.72	0.54
1:C:72:LEU:HD22	1:C:72:LEU:H	1.72	0.54
2:E:69:ASN:HD22	2:E:120:ARG:H	1.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:69:ASN:HD22	2:F:120:ARG:H	1.56	0.54
1:C:105:HIS:CD2	2:F:145:MET:HE1	2.36	0.53
1:A:71:PRO:HB3	2:E:148:SER:HG	1.64	0.53
1:C:74:TYR:N	1:C:75:PRO:CD	2.72	0.53
1:A:149:ASN:ND2	1:C:169:GLU:CG	2.71	0.52
1:A:74:TYR:N	1:A:75:PRO:CD	2.72	0.52
1:A:65:ASP:C	1:A:67:ASP:H	2.13	0.52
2:F:117:ARG:HG2	2:F:119:ASN:HD21	1.75	0.52
2:E:117:ARG:HG2	2:E:119:ASN:HD21	1.75	0.52
1:C:105:HIS:O	2:F:145:MET:CG	2.53	0.51
2:F:146:VAL:HG12	2:F:149:TYR:CE1	2.46	0.50
2:F:126:MET:HB2	2:F:147:GLY:O	2.11	0.50
2:E:146:VAL:HG12	2:E:149:TYR:CE1	2.46	0.50
2:E:126:MET:HB2	2:E:147:GLY:O	2.11	0.50
1:C:65:ASP:C	1:C:67:ASP:H	2.13	0.49
1:A:40:GLU:OE1	2:E:49:ARG:CA	2.61	0.49
2:E:134:ARG:HH11	2:E:134:ARG:HG2	1.77	0.49
1:C:71:PRO:HB2	2:F:148:SER:CB	2.43	0.49
1:A:100:THR:O	1:A:104:LYS:HG2	2.13	0.48
2:F:134:ARG:HG2	2:F:134:ARG:HH11	1.77	0.48
2:F:126:MET:HB3	2:F:146:VAL:HB	1.96	0.48
1:C:72:LEU:HD11	2:F:122:ILE:HG23	1.95	0.48
1:C:100:THR:O	1:C:104:LYS:HG2	2.13	0.48
1:A:168:ARG:HE	1:A:168:ARG:CA	2.27	0.48
2:E:126:MET:HB3	2:E:146:VAL:HB	1.96	0.47
1:C:168:ARG:HE	1:C:168:ARG:CA	2.27	0.47
1:C:169:GLU:N	1:C:169:GLU:OE1	2.45	0.47
1:A:93:GLU:O	1:A:96:PRO:HD2	2.15	0.47
1:C:93:GLU:O	1:C:96:PRO:HD2	2.14	0.47
1:C:9:VAL:HB	1:C:80:ILE:HD13	1.97	0.47
1:A:22:LEU:CD1	1:A:59:ASP:HB2	2.46	0.46
1:A:9:VAL:HB	1:A:80:ILE:HD13	1.97	0.46
2:E:117:ARG:HG2	2:E:119:ASN:ND2	2.31	0.46
1:A:169:GLU:N	1:A:169:GLU:OE1	2.45	0.46
1:A:99:TRP:O	1:A:103:VAL:HG13	2.16	0.45
1:C:190:CYS:CA	2:F:142:THR:HG23	2.47	0.45
1:C:22:LEU:CD1	1:C:59:ASP:HB2	2.46	0.45
2:F:117:ARG:HG2	2:F:119:ASN:ND2	2.31	0.45
1:C:65:ASP:C	1:C:67:ASP:N	2.71	0.45
2:F:134:ARG:HG2	2:F:134:ARG:NH1	2.32	0.45
2:E:134:ARG:NH1	2:E:134:ARG:HG2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:99:TRP:O	1:C:103:VAL:HG13	2.16	0.44
1:A:66:TYR:OH	2:E:50:LYS:CA	2.66	0.44
1:A:65:ASP:C	1:A:67:ASP:N	2.71	0.44
2:E:132:THR:HG23	2:E:177:ILE:HG13	2.01	0.43
1:A:71:PRO:HB2	2:E:148:SER:HB3	2.01	0.43
1:A:74:TYR:O	1:A:77:THR:HG23	2.19	0.43
1:C:70:ARG:HB3	1:C:71:PRO:HD3	2.00	0.43
1:A:95:ILE:HB	1:A:96:PRO:CD	2.49	0.42
1:A:69:LEU:HA	1:A:72:LEU:HD23	2.01	0.42
1:C:74:TYR:O	1:C:77:THR:HG23	2.19	0.42
2:E:146:VAL:HG12	2:E:149:TYR:HE1	1.85	0.42
2:F:65:PRO:CA	2:F:120:ARG:NH2	2.82	0.42
1:A:169:GLU:HG2	1:C:149:ASN:HD22	1.84	0.42
1:C:9:VAL:HG21	1:C:77:THR:HG21	2.02	0.42
2:F:132:THR:HG23	2:F:177:ILE:HG13	2.00	0.42
1:C:69:LEU:HA	1:C:72:LEU:HD23	2.01	0.42
1:A:51:LYS:CG	1:A:52:GLN:H	2.33	0.42
1:C:51:LYS:HG3	1:C:52:GLN:H	1.85	0.42
1:A:9:VAL:HG21	1:A:77:THR:HG21	2.02	0.42
1:C:74:TYR:OH	1:C:102:GLU:OE2	2.31	0.41
1:A:51:LYS:HG3	1:A:52:GLN:H	1.85	0.41
1:A:70:ARG:HB3	1:A:71:PRO:HD3	2.01	0.41
1:C:72:LEU:HD21	2:F:122:ILE:CG2	2.46	0.41
1:C:105:HIS:CE1	2:F:145:MET:HE3	2.56	0.41
1:C:51:LYS:CG	1:C:52:GLN:H	2.33	0.41
1:C:14:GLY:O	1:C:15:ALA:HB3	2.21	0.41
1:C:8:LEU:HD23	1:C:8:LEU:C	2.41	0.41
2:E:67:VAL:CA	2:E:68:PRO:N	2.84	0.41
1:A:8:LEU:HD23	1:A:8:LEU:C	2.41	0.41
1:C:95:ILE:HB	1:C:96:PRO:CD	2.49	0.41
1:A:74:TYR:O	1:A:75:PRO:C	2.59	0.41

All (26) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:91:THR:O	1:C:34:TYR:CE2[6_554]	0.52	1.68
2:E:91:THR:O	1:C:34:TYR:CZ[6_554]	1.09	1.11
1:A:123:ASN:OD1	1:C:129:ARG:NH1[7_555]	1.17	1.03
2:E:80:SER:OG	2:E:80:SER:OG[10_665]	1.20	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:91:THR:O	1:C:34:TYR:CD2[6_554]	1.33	0.87
2:E:167:LYS:NZ	2:F:164:GLU:OE1[10_665]	1.35	0.85
2:E:164:GLU:OE1	2:F:167:LYS:NZ[10_665]	1.35	0.85
2:E:91:THR:C	1:C:34:TYR:CE2[6_554]	1.46	0.74
2:E:91:THR:C	1:C:34:TYR:CZ[6_554]	1.75	0.45
2:E:91:THR:CB	1:C:34:TYR:CE1[6_554]	1.84	0.36
2:E:91:THR:C	1:C:34:TYR:CD2[6_554]	1.87	0.33
1:A:4:ILE:N	2:E:203:LYS:CG[10_665]	1.90	0.30
1:C:4:ILE:N	2:F:203:LYS:CD[10_665]	1.91	0.29
2:E:91:THR:O	1:C:34:TYR:CE1[6_554]	1.93	0.27
1:A:129:ARG:NH2	2:E:65:PRO:CA[11_555]	1.98	0.22
2:E:93:ASP:OD1	1:C:27:LYS:NZ[6_554]	1.98	0.22
2:E:167:LYS:CE	2:F:164:GLU:OE1[10_665]	2.04	0.16
2:E:91:THR:O	1:C:34:TYR:CG[6_554]	2.07	0.13
2:E:80:SER:N	2:E:80:SER:OG[10_665]	2.13	0.07
1:A:33:VAL:CG1	2:F:71:VAL:CG1[5_565]	2.14	0.06
2:E:164:GLU:OE1	2:F:167:LYS:CE[10_665]	2.15	0.05
1:A:123:ASN:OD1	1:C:129:ARG:CZ[7_555]	2.18	0.02
1:A:125:GLU:OE1	1:C:126:HIS:CD2[7_555]	2.18	0.02
2:E:92:GLY:N	1:C:34:TYR:CE2[6_554]	2.18	0.02
1:A:123:ASN:O	1:C:129:ARG:NH2[7_555]	2.19	0.01
2:E:80:SER:CB	2:E:80:SER:OG[10_665]	2.19	0.01

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	175/190 (92%)	164 (94%)	8 (5%)	3 (2%)	11 56
1	C	175/190 (92%)	164 (94%)	8 (5%)	3 (2%)	11 56
2	E	134/204 (66%)	132 (98%)	2 (2%)	0	100 100
2	F	134/204 (66%)	132 (98%)	2 (2%)	0	100 100
All	All	618/788 (78%)	592 (96%)	20 (3%)	6 (1%)	19 65

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	C	41	ASN
1	A	64	GLU
1	A	66	TYR
1	C	64	GLU
1	C	66	TYR

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	156/164 (95%)	143 (92%)	13 (8%)	14	51
1	C	156/164 (95%)	143 (92%)	13 (8%)	14	51
2	E	122/180 (68%)	111 (91%)	11 (9%)	12	46
2	F	122/180 (68%)	110 (90%)	12 (10%)	10	42
All	All	556/688 (81%)	507 (91%)	49 (9%)	12	47

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	48	VAL
1	A	64	GLU
1	A	68	ARG
1	A	69	LEU
1	A	71	PRO
1	A	77	THR
1	A	85	SER
1	A	103	VAL
1	A	123	ASN
1	A	128	ARG
1	A	168	ARG
1	A	179	LEU
2	E	76	THR

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Mol	Chain	Res	Type
2	E	77	LEU
2	E	80	SER
2	E	81	SER
2	E	86	LEU
2	E	94	LEU
2	E	145	MET
2	E	152	ARG
2	E	169	MET
2	E	170	LEU
2	E	190	LEU
1	C	29	GLN
1	C	48	VAL
1	C	64	GLU
1	C	68	ARG
1	C	69	LEU
1	C	71	PRO
1	C	77	THR
1	C	85	SER
1	C	103	VAL
1	C	123	ASN
1	C	128	ARG
1	C	168	ARG
1	C	179	LEU
2	F	76	THR
2	F	77	LEU
2	F	80	SER
2	F	81	SER
2	F	86	LEU
2	F	94	LEU
2	F	145	MET
2	F	152	ARG
2	F	161	PRO
2	F	169	MET
2	F	170	LEU
2	F	190	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
2	E	69	ASN
2	E	100	GLN
2	E	119	ASN

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Mol	Chain	Res	Type
2	E	130	GLN
1	C	180	GLN
2	F	69	ASN
2	F	100	GLN
2	F	119	ASN
2	F	130	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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	GDP	A	201	3	23,30,30	1.63	4 (17%)	30,47,47	2.32	7 (23%)
4	GDP	C	202	3	23,30,30	1.63	4 (17%)	30,47,47	2.32	8 (26%)

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
4	GDP	A	201	3	-	0/12/32/32	0/3/3/3
4	GDP	C	202	3	-	0/12/32/32	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	202	GDP	C5-C4	-4.63	1.30	1.40
4	A	201	GDP	C5-C4	-4.59	1.30	1.40
4	A	201	GDP	C4-N3	-2.99	1.31	1.35
4	C	202	GDP	C4-N3	-2.97	1.31	1.35
4	A	201	GDP	C6-N1	2.17	1.37	1.33
4	C	202	GDP	C6-N1	2.19	1.37	1.33
4	C	202	GDP	C2-N1	2.60	1.40	1.35
4	A	201	GDP	C2-N1	2.66	1.40	1.35

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	202	GDP	C5-C6-N1	-7.40	113.47	123.59
4	A	201	GDP	C5-C6-N1	-7.40	113.47	123.59
4	A	201	GDP	N3-C2-N1	-4.06	121.27	127.44
4	C	202	GDP	N3-C2-N1	-4.04	121.29	127.44
4	C	202	GDP	C1'-N9-C4	2.02	129.99	126.94
4	C	202	GDP	N2-C2-N3	2.39	122.39	117.80
4	A	201	GDP	N2-C2-N3	2.42	122.45	117.80
4	A	201	GDP	C4'-O4'-C1'	2.82	112.82	109.72
4	C	202	GDP	C4'-O4'-C1'	2.83	112.83	109.72
4	C	202	GDP	O3B-PB-O2B	3.82	121.92	107.38
4	A	201	GDP	O3B-PB-O2B	3.83	121.96	107.38
4	A	201	GDP	C4-C5-N7	4.18	113.32	109.48
4	C	202	GDP	C4-C5-N7	4.22	113.36	109.48
4	A	201	GDP	C6-N1-C2	4.42	122.07	115.94
4	C	202	GDP	C6-N1-C2	4.42	122.08	115.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

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, 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	187/190 (98%)	0.39	11 (5%) 26 20	35, 35, 35, 35	0
1	C	187/190 (98%)	0.57	11 (5%) 26 20	35, 35, 35, 35	0
2	E	180/204 (88%)	1.39	42 (23%) 1 3	35, 35, 35, 35	0
2	F	180/204 (88%)	1.58	42 (23%) 1 3	35, 35, 35, 35	0
All	All	734/788 (93%)	0.97	106 (14%) 3 5	35, 35, 35, 35	0

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	186	LYS	18.2
2	E	58	ARG	15.7
2	F	36	GLN	13.5
2	E	57	GLY	12.5
2	F	28	LYS	12.0
2	F	39	GLN	11.0
2	E	59	VAL	10.8
2	F	29	PRO	10.7
2	F	51	TYR	10.5
1	A	186	LYS	9.1
2	E	45	ASP	8.9
2	E	60	ALA	7.9
2	F	65	PRO	7.5
2	E	25	VAL	7.3
2	F	52	LYS	6.9
2	E	65	PRO	6.9
1	A	190	CYS	6.8
1	C	189	GLY	6.7
2	E	56	LEU	6.6
2	E	42	ASP	6.3
1	C	185	LYS	6.1

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Mol	Chain	Res	Type	RSRZ
2	F	38	ILE	6.1
1	A	187	LYS	6.1
2	F	47	SER	5.7
1	C	190	CYS	5.5
2	F	57	GLY	5.5
2	F	54	ALA	5.5
2	F	25	VAL	5.5
1	A	188	SER	5.3
2	F	40	GLU	5.2
2	F	53	GLU	5.2
2	E	99	LYS	5.0
2	F	26	ASN	5.0
2	F	60	ALA	4.9
2	E	66	ASN	4.9
2	F	58	ARG	4.9
2	F	59	VAL	4.8
2	E	53	GLU	4.6
2	E	47	SER	4.5
2	F	27	TYR	4.5
1	A	184	GLY	4.4
2	F	56	LEU	4.3
2	F	117	ARG	4.3
2	E	55	LEU	4.2
2	F	44	ASP	4.2
2	E	54	ALA	4.1
2	F	42	ASP	4.1
2	E	51	TYR	4.1
2	E	50	LYS	4.0
2	E	41	LEU	4.0
2	E	28	LYS	3.9
2	E	29	PRO	3.9
2	F	45	ASP	3.8
2	F	55	LEU	3.6
2	F	50	LYS	3.6
2	E	119	ASN	3.6
2	E	67	VAL	3.4
1	A	182	ARG	3.3
2	E	46	GLU	3.3
2	F	24	SER	3.3
2	E	39	GLN	3.2
2	E	52	LYS	3.1
2	E	98	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
2	F	67	VAL	3.0
2	E	49	ARG	3.0
1	C	66	TYR	3.0
2	E	180	ARG	3.0
1	A	189	GLY	3.0
1	C	52	GLN	2.8
2	F	193	GLU	2.8
2	F	66	ASN	2.8
1	A	94	ASN	2.8
2	F	30	PRO	2.8
2	E	40	GLU	2.7
1	C	182	ARG	2.6
2	E	148	SER	2.6
2	F	153	ALA	2.6
2	F	121	GLU	2.6
1	C	116	GLY	2.6
2	F	48	LEU	2.6
2	E	193	GLU	2.6
2	E	203	LYS	2.5
2	F	64	ASP	2.5
1	A	65	ASP	2.5
2	E	43	LYS	2.5
2	E	30	PRO	2.4
2	F	41	LEU	2.4
2	F	179	SER	2.4
2	E	143	ASP	2.4
1	C	128	ARG	2.4
2	F	120	ARG	2.3
2	E	202	TRP	2.3
2	E	38	ILE	2.3
2	F	99	LYS	2.3
1	A	137	GLU	2.2
2	E	63	ALA	2.2
2	F	37	GLU	2.2
2	E	24	SER	2.2
2	F	91	THR	2.2
2	F	125	GLY	2.2
1	A	90	ASP	2.1
2	E	26	ASN	2.1
1	C	117	ASN	2.1
2	E	44	ASP	2.1
2	E	33	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	65	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 carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å^2)	Q<0.9
4	GDP	C	202	28/28	0.70	0.34	-0.57	35,35,35,35	0
4	GDP	A	201	28/28	0.80	0.25	-0.71	35,35,35,35	0
3	MG	C	302	1/1	0.51	0.41	-0.75	35,35,35,35	0
3	MG	A	301	1/1	0.92	0.29	-0.79	35,35,35,35	0

6.5 Other polymers (i)

There are no such residues in this entry.