



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 11:30 PM GMT

PDB ID : 1CC0
Title : CRYSTAL STRUCTURE OF THE RHOA.GDP-RHO GDI 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 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>

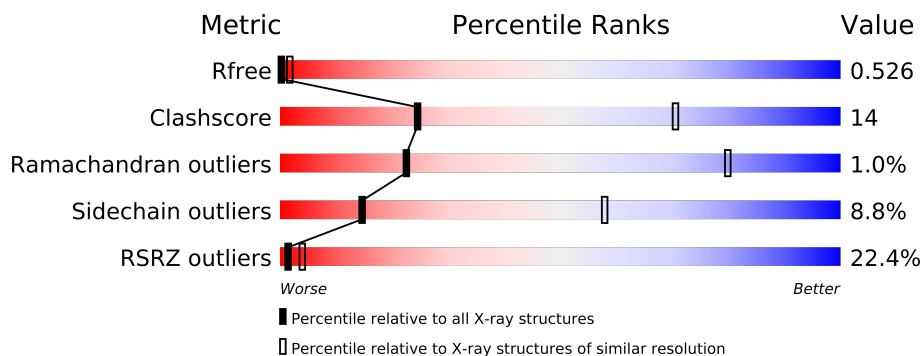
The following versions of software and data (see [references](#)) were used in the production of this report:

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 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}	66092	1052 (6.50-3.50)
Clashscore	79885	1327 (6.50-3.50)
Ramachandran outliers	78287	1242 (6.50-3.50)
Sidechain outliers	78261	1221 (6.50-3.50)
RSRZ outliers	66119	1051 (6.50-3.50)

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	190	
1	C	190	
2	E	204	
2	F	204	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5174 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 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: C₁₀H₁₅N₅O₁₁P₂).

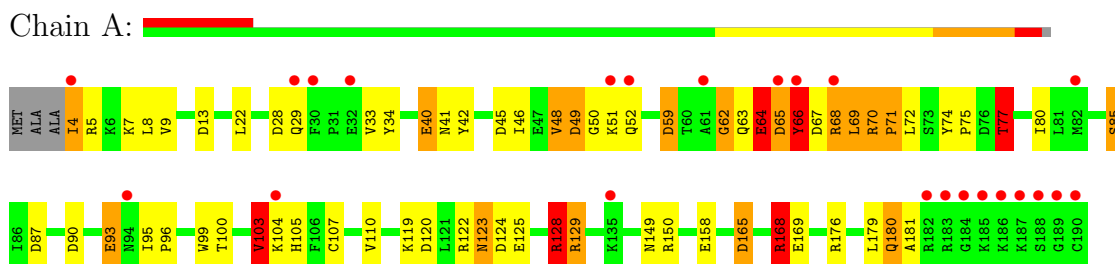


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
4	C	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

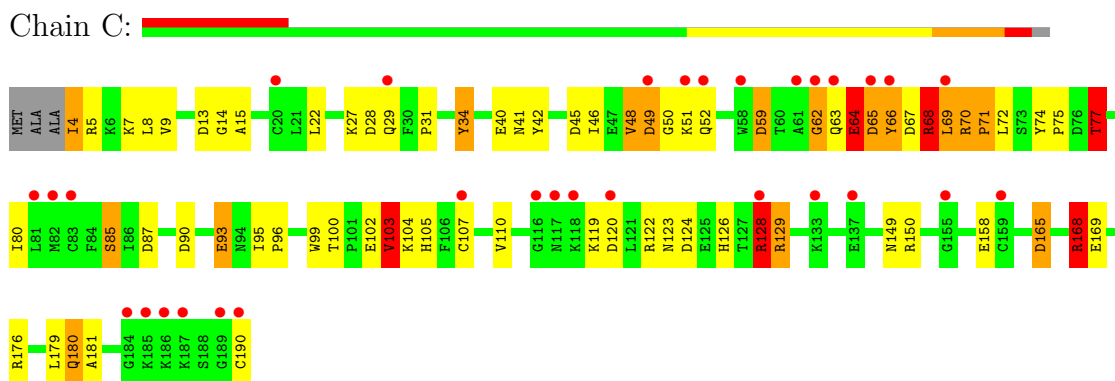
3 Residue-property plots

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.

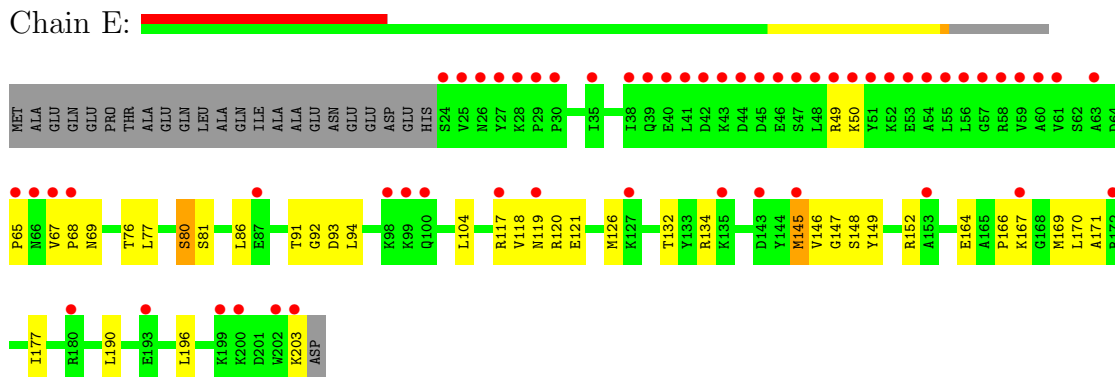
- Molecule 1: transforming protein rhoA



- Molecule 1: transforming protein rhoA

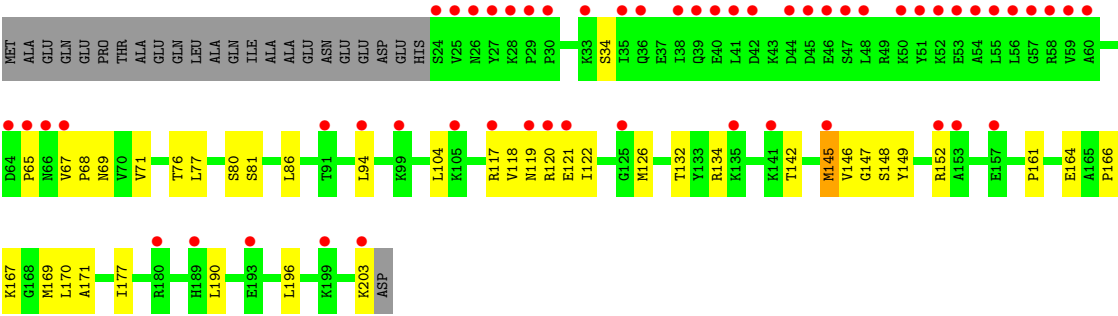


- Molecule 2: rho GDP dissociation inhibitor alpha



- Molecule 2: rho GDP dissociation inhibitor alpha





4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 3.94Å)	Xtriage
Refinement program	O	Depositor
R, R_{free}	(Not available) , (Not available) 0.545 , 0.526	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)	0.26 , -10.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	2 of 12673 reflections (0.016%)	Xtriage
F_o, F_c correlation	0.67	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.*

¹Intensities 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: 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(°)	Ideal(°)
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(°)	Ideal(°)
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(°)	Ideal(°)
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(°)	Ideal(°)
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 Close contacts ⓘ

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	1415	0	1392	56	7
1	C	1415	0	1394	61	16
2	E	1143	0	1100	34	20

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	1143	0	1100	39	6
3	A	1	0	0	0	0
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

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 14.

All (143) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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	Distance(Å)	Clash(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
2:F:69:ASN:HD22	2:F:120:ARG:H	1.56	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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	Distance(Å)	Clash(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
2:E:91:THR:O	1:C:34:TYR:CD2[6_554]	1.33	0.87
2:E:164:GLU:OE1	2:F:167:LYS:NZ[10_665]	1.35	0.85
2:E:167:LYS:NZ	2:F:164:GLU:OE1[10_665]	1.35	0.85
2:E:91:THR:C	1:C:34:TYR:CE2[6_554]	1.46	0.74

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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

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	175/190 (92%)	164 (94%)	8 (5%)	3 (2%)	14	70
1	C	175/190 (92%)	164 (94%)	8 (5%)	3 (2%)	14	70
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%)	22	80

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	C	41	ASN

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Mol	Chain	Res	Type
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%)	16	61
1	C	156/164 (95%)	143 (92%)	13 (8%)	16	61
2	E	122/180 (68%)	111 (91%)	11 (9%)	14	56
2	F	122/180 (68%)	110 (90%)	12 (10%)	12	51
All	All	556/688 (81%)	507 (91%)	49 (9%)	14	58

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
2	E	77	LEU
2	E	80	SER
2	E	81	SER
2	E	86	LEU

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

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Mol	Chain	Res	Type
2	F	119	ASN
2	F	130	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 ⓘ

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	30,30,30	1.53	5 (16%)	44,47,47	8.55	7 (15%)
4	GDP	C	202	3	30,30,30	1.53	5 (16%)	44,47,47	8.57	7 (15%)

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	-	0/16/32/32	0/1/3/3
4	GDP	C	202	3	-	0/16/32/32	0/1/3/3

All (10) 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	-2.82	1.31	1.35
4	C	202	GDP	C4-N3	-2.81	1.31	1.35
4	C	202	GDP	C8-N9	2.63	1.40	1.36
4	A	201	GDP	C8-N9	2.58	1.40	1.36
4	A	201	GDP	PB-O3A	2.24	1.64	1.60
4	C	202	GDP	PB-O3A	2.18	1.64	1.60
4	A	201	GDP	C2-N1	2.11	1.40	1.36
4	C	202	GDP	C2-N1	2.05	1.40	1.36

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	202	GDP	C6-C5-N7	-55.86	126.62	134.14
4	A	201	GDP	C6-C5-N7	-55.72	126.64	134.14
4	C	202	GDP	C4-C5-N7	4.48	113.36	109.52
4	A	201	GDP	C4-C5-N7	4.44	113.32	109.52
4	A	201	GDP	O2'-C2'-C1'	-4.09	98.85	111.23
4	C	202	GDP	O2'-C2'-C1'	-4.08	98.89	111.23
4	A	201	GDP	O3B-PB-O2B	3.69	121.96	107.61
4	C	202	GDP	O3B-PB-O2B	3.67	121.92	107.61
4	A	201	GDP	O4'-C1'-C2'	-2.99	102.19	106.77
4	C	202	GDP	O4'-C1'-C2'	-2.98	102.21	106.77
4	C	202	GDP	C4'-O4'-C1'	2.83	112.83	109.75
4	A	201	GDP	C4'-O4'-C1'	2.83	112.82	109.75
4	A	201	GDP	O3A-PB-O1B	-2.18	96.09	111.00
4	C	202	GDP	O3A-PB-O1B	-2.18	96.12	111.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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, 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	187/190 (98%)	1.04	23 (12%) 5 10	35, 35, 35, 35	0
1	C	187/190 (98%)	1.18	31 (16%) 2 6	35, 35, 35, 35	0
2	E	180/204 (88%)	1.87	56 (31%) 1 3	35, 35, 35, 35	0
2	F	180/204 (88%)	2.05	55 (30%) 1 3	35, 35, 35, 35	0
All	All	734/788 (93%)	1.53	165 (22%) 1 4	35, 35, 35, 35	0

All (165) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	186	LYS	17.4
2	F	36	GLN	13.0
1	A	186	LYS	12.0
2	E	57	GLY	11.6
2	F	39	GLN	11.4
1	A	187	LYS	11.2
2	E	60	ALA	9.6
2	F	65	PRO	9.4
1	A	190	CYS	9.4
1	A	183	ARG	9.2
2	F	26	ASN	9.1
2	F	55	LEU	8.8
1	C	185	LYS	8.8
2	E	56	LEU	8.6
2	E	45	ASP	8.4
2	E	65	PRO	8.4
2	F	51	TYR	8.2
2	E	67	VAL	8.1
2	E	99	LYS	8.0
2	F	52	LYS	7.9
2	F	42	ASP	7.7

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Mol	Chain	Res	Type	RSRZ
2	E	25	VAL	7.7
2	F	40	GLU	7.6
2	E	66	ASN	7.4
2	F	54	ALA	7.0
2	F	27	TYR	7.0
1	C	190	CYS	6.8
2	F	58	ARG	6.7
2	F	53	GLU	6.6
2	F	117	ARG	6.2
2	F	28	LYS	6.2
2	E	58	ARG	6.2
1	A	189	GLY	6.0
2	F	60	ALA	5.9
2	E	26	ASN	5.8
2	F	59	VAL	5.6
1	C	189	GLY	5.6
2	E	51	TYR	5.5
2	F	57	GLY	5.5
2	E	59	VAL	5.5
2	F	29	PRO	5.4
2	F	38	ILE	5.3
2	E	55	LEU	5.3
2	E	53	GLU	5.3
2	E	28	LYS	5.2
2	F	56	LEU	5.2
1	A	188	SER	5.2
2	F	66	ASN	5.2
2	E	50	LYS	5.0
2	F	47	SER	4.9
1	A	184	GLY	4.9
2	E	63	ALA	4.9
2	E	29	PRO	4.8
2	E	49	ARG	4.8
2	F	30	PRO	4.6
2	E	98	LYS	4.6
2	F	25	VAL	4.5
2	E	54	ALA	4.5
2	E	42	ASP	4.4
2	E	41	LEU	4.3
2	E	48	LEU	4.3
1	C	66	TYR	4.3
2	E	46	GLU	4.2

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Mol	Chain	Res	Type	RSRZ
2	F	48	LEU	4.1
1	A	185	LYS	4.0
1	C	83	CYS	3.9
1	C	187	LYS	3.9
1	C	159	CYS	3.9
2	F	35	ILE	3.8
2	E	44	ASP	3.8
1	C	128	ARG	3.8
2	F	145	MET	3.7
2	E	199	LYS	3.7
1	C	52	GLN	3.7
2	F	44	ASP	3.6
2	E	87	GLU	3.6
2	F	67	VAL	3.6
1	C	82	MET	3.6
2	E	47	SER	3.5
2	E	145	MET	3.5
2	F	50	LYS	3.5
2	E	52	LYS	3.5
1	C	62	GLY	3.4
1	C	155	GLY	3.4
2	F	153	ALA	3.3
1	C	65	ASP	3.3
1	C	61	ALA	3.3
2	E	43	LYS	3.3
2	F	119	ASN	3.2
1	A	82	MET	3.2
2	E	167	LYS	3.2
1	C	49	ASP	3.2
2	E	135	LYS	3.1
1	C	69	LEU	3.1
2	F	193	GLU	3.0
2	E	100	GLN	3.0
1	C	63	GLN	3.0
2	E	202	TRP	3.0
2	E	39	GLN	2.9
2	E	38	ILE	2.9
2	F	99	LYS	2.9
2	E	143	ASP	2.9
1	C	29	GLN	2.9
2	F	203	LYS	2.9
2	E	203	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
2	E	30	PRO	2.8
2	E	180	ARG	2.8
2	E	193	GLU	2.8
1	C	133	LYS	2.8
1	A	66	TYR	2.8
2	E	119	ASN	2.8
2	F	121	GLU	2.7
1	A	32	GLU	2.7
1	A	65	ASP	2.7
2	E	117	ARG	2.6
1	C	117	ASN	2.6
2	F	180	ARG	2.6
2	F	135	LYS	2.6
2	F	120	ARG	2.5
1	C	184	GLY	2.5
1	C	51	LYS	2.5
2	E	172	ARG	2.5
1	A	30	PHE	2.5
1	A	4	ILE	2.4
1	A	51	LYS	2.4
1	C	120	ASP	2.4
2	F	152	ARG	2.4
1	A	135	LYS	2.4
2	E	35	ILE	2.4
1	A	104	LYS	2.3
2	E	153	ALA	2.3
2	F	64	ASP	2.3
1	C	107	CYS	2.3
2	F	45	ASP	2.3
2	E	27	TYR	2.3
2	F	189	HIS	2.3
2	F	105	LYS	2.3
1	A	61	ALA	2.3
2	F	24	SER	2.3
1	C	81	LEU	2.3
1	C	118	LYS	2.2
2	F	157	GLU	2.2
2	F	41	LEU	2.2
2	E	68	PRO	2.2
1	A	68	ARG	2.2
2	E	40	GLU	2.2
2	F	199	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
2	F	141	LYS	2.2
1	C	58	TRP	2.2
2	E	200	LYS	2.1
1	C	137	GLU	2.1
2	F	94	LEU	2.1
1	C	116	GLY	2.1
2	F	33	LYS	2.1
1	A	94	ASN	2.1
2	F	125	GLY	2.1
2	F	46	GLU	2.1
2	F	91	THR	2.1
2	E	61	VAL	2.1
1	A	182	ARG	2.0
1	A	29	GLN	2.0
2	E	127	LYS	2.0
1	C	20	CYS	2.0
1	A	52	GLN	2.0
2	E	24	SER	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
4	GDP	C	202	28/28	0.38	-	35,35,35,35	0
3	MG	C	302	1/1	0.48	-	35,35,35,35	0
3	MG	A	301	1/1	0.36	-	35,35,35,35	0
4	GDP	A	201	28/28	0.32	-	35,35,35,35	0

6.5 Other polymers ⓘ

There are no such residues in this entry.