



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:11 PM UTC

PDB ID : 1CC0 / pdb_00001cc0
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 X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

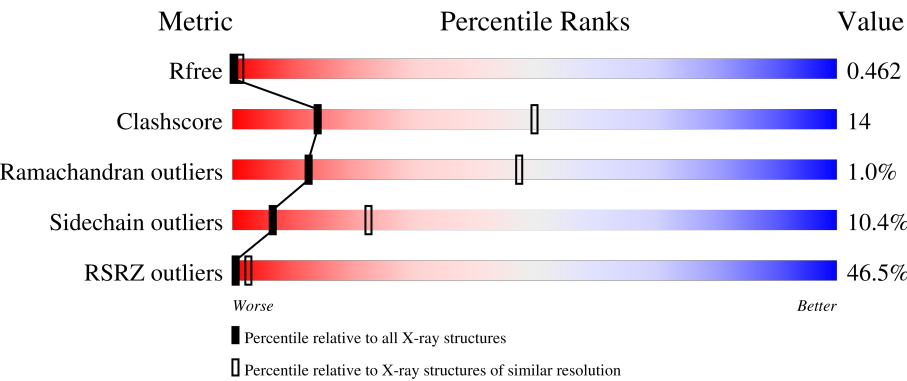
1 Overall quality at a glance i

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}	180053	1009 (6.02-3.98)
Clashscore	190562	1040 (6.00-4.00)
Ramachandran outliers	187476	1015 (6.06-3.92)
Sidechain outliers	187428	1136 (6.10-3.90)
RSRZ outliers	180081	1004 (6.02-3.98)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	190	39% 50% 33% 12% . .
1	C	190	35% 47% 37% 11% . .
2	E	204	48% 66% 20% . 12%
2	F	204	50% 66% 20% . 12%

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 (CCD ID: 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 (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).

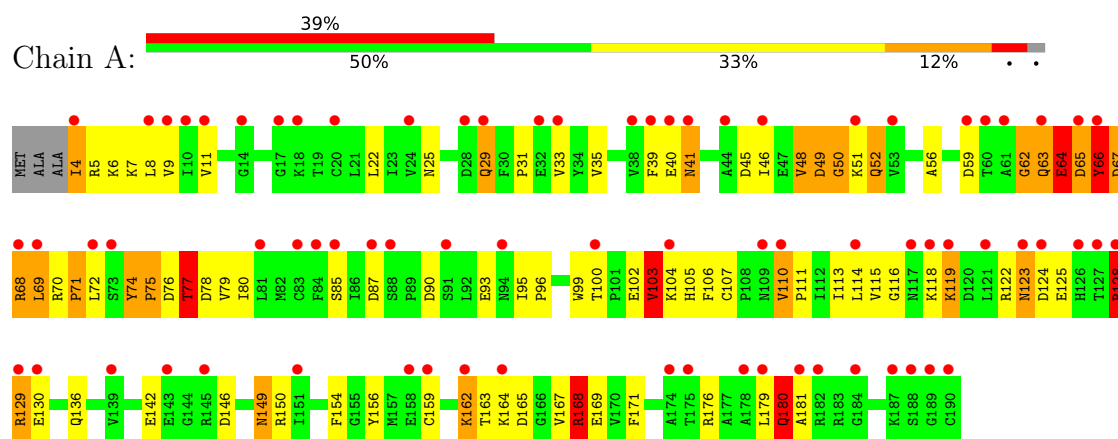


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 28	C 10	N 5	O 11	P 2	0	0
4	C	1	Total 28	C 10	N 5	O 11	P 2	0	0

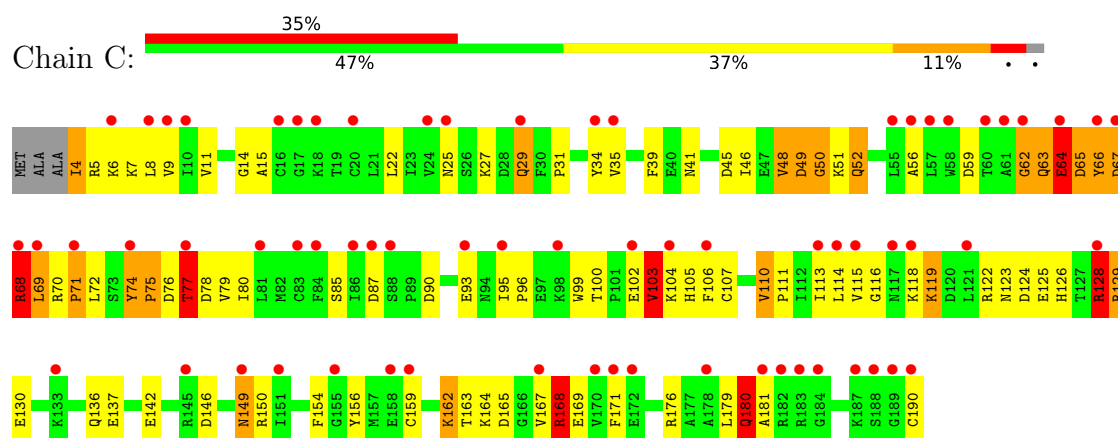
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

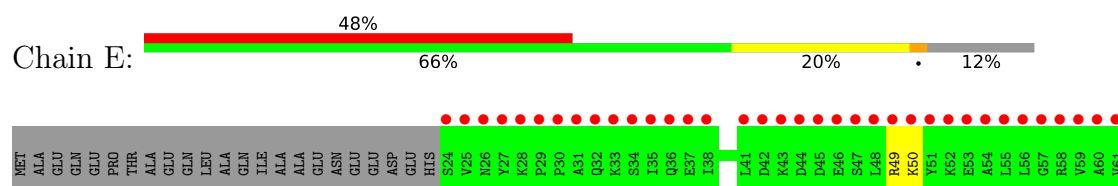
- Molecule 1: transforming protein rhoA

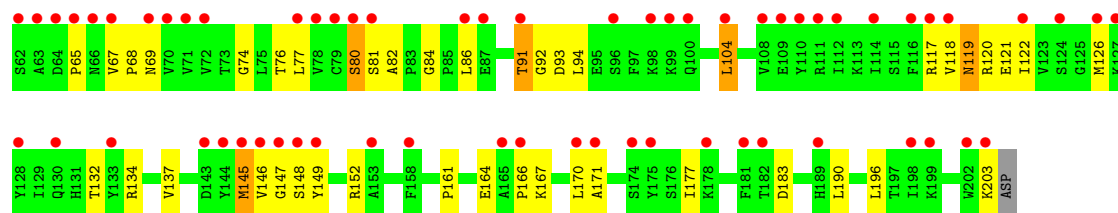


- Molecule 1: transforming protein rhoA

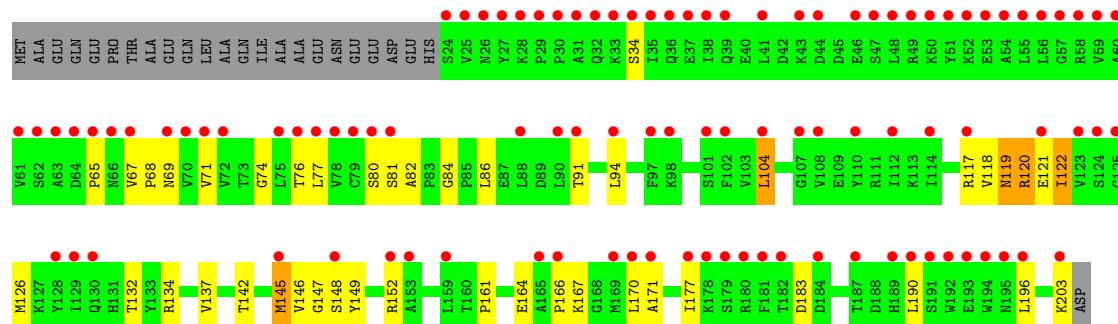


- Molecule 2: rho GDP dissociation inhibitor alpha





● 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) – 5.00 120.64 – 5.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-5.00) 96.7 (120.64-5.00)	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		Depositor
R, R_{free}	(Not available) , (Not available) 0.480 , 0.462	Depositor DCC
R_{free} test set	642 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	138.6	Xtriage
Anisotropy	0.730	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 56.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.63	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.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	1.27	1/1432 (0.1%)	2.42	93/1937 (4.8%)
1	C	1.27	1/1432 (0.1%)	2.42	95/1937 (4.9%)
2	E	0.73	1/1124 (0.1%)	1.21	10/1515 (0.7%)
2	F	0.74	1/1124 (0.1%)	1.21	11/1515 (0.7%)
All	All	1.06	4/5112 (0.1%)	1.98	209/6904 (3.0%)

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	116	GLY	N-CA	5.51	1.52	1.44
1	C	116	GLY	N-CA	5.50	1.52	1.44
2	F	122	ILE	CA-CB	5.31	1.60	1.54
2	E	122	ILE	CA-CB	5.16	1.60	1.54

All (209) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	168	ARG	CD-NE-CZ	14.50	144.70	124.40
1	C	168	ARG	CD-NE-CZ	14.49	144.68	124.40
1	A	5	ARG	CD-NE-CZ	14.00	144.00	124.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	5	ARG	CD-NE-CZ	13.99	143.98	124.40
1	C	65	ASP	CA-C-O	-10.36	108.59	120.20
1	A	65	ASP	CA-C-O	-10.31	108.66	120.20
1	A	49	ASP	CA-CB-CG	-9.34	103.26	112.60
1	A	65	ASP	CA-CB-CG	-9.32	103.28	112.60
1	C	65	ASP	CA-CB-CG	-9.32	103.28	112.60
1	C	49	ASP	CA-CB-CG	-9.31	103.29	112.60
1	C	78	ASP	CA-CB-CG	-8.52	104.08	112.60
1	A	11	VAL	CA-C-O	-8.51	112.74	121.67
1	C	11	VAL	CA-C-O	-8.47	112.77	121.67
1	A	78	ASP	CA-CB-CG	-8.42	104.18	112.60
1	A	122	ARG	NH1-CZ-NH2	8.31	130.10	119.30
1	C	122	ARG	NH1-CZ-NH2	8.31	130.10	119.30
1	C	106	PHE	CA-C-N	8.15	132.02	122.89
1	C	106	PHE	C-N-CA	8.15	132.02	122.89
1	A	106	PHE	CA-C-N	8.11	131.97	122.89
1	A	106	PHE	C-N-CA	8.11	131.97	122.89
1	C	35	VAL	CA-C-O	7.89	124.05	119.94
1	C	122	ARG	NE-CZ-NH2	-7.87	112.12	119.20
1	A	122	ARG	NE-CZ-NH2	-7.78	112.20	119.20
1	C	25	ASN	CA-CB-CG	-7.72	104.88	112.60
1	A	35	VAL	CA-C-O	7.70	123.94	119.94
1	A	156	TYR	CA-C-O	-7.70	112.05	120.36
1	C	156	TYR	CA-C-O	-7.65	112.09	120.36
1	A	25	ASN	CA-CB-CG	-7.64	104.96	112.60
1	C	90	ASP	N-CA-CB	7.62	121.06	110.01
1	A	90	ASP	N-CA-CB	7.60	121.03	110.01
1	C	4	ILE	N-CA-CB	7.47	124.20	111.50
1	A	4	ILE	N-CA-CB	7.42	124.11	111.50
2	E	118	VAL	N-CA-C	-7.37	96.47	107.37
1	A	46	ILE	CB-CG1-CD1	7.36	129.25	113.80
1	A	176	ARG	NE-CZ-NH2	-7.34	112.59	119.20
1	C	176	ARG	NE-CZ-NH2	-7.33	112.61	119.20
2	F	118	VAL	N-CA-C	-7.33	96.53	107.37
1	C	46	ILE	CB-CG1-CD1	7.32	129.18	113.80
1	A	150	ARG	NE-CZ-NH2	-7.28	112.65	119.20
1	C	150	ARG	NE-CZ-NH2	-7.28	112.64	119.20
1	A	77	THR	CA-CB-OG1	7.21	120.41	109.60
1	C	77	THR	CA-CB-OG1	7.19	120.38	109.60
1	A	129	ARG	N-CA-C	7.13	119.72	111.02
1	C	39	PHE	CA-CB-CG	7.12	120.92	113.80
1	C	129	ARG	N-CA-C	7.09	119.67	111.02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	39	PHE	CA-CB-CG	7.08	120.88	113.80
1	A	5	ARG	NE-CZ-NH2	-6.98	112.92	119.20
1	A	149	ASN	CA-CB-CG	-6.96	105.64	112.60
1	C	29	GLN	OE1-CD-NE2	6.96	129.56	122.60
1	C	149	ASN	CA-CB-CG	-6.96	105.64	112.60
1	C	5	ARG	NE-CZ-NH2	-6.96	112.94	119.20
1	A	154	PHE	CA-CB-CG	6.95	120.75	113.80
1	A	29	GLN	OE1-CD-NE2	6.93	129.53	122.60
1	C	154	PHE	CA-CB-CG	6.92	120.72	113.80
1	C	130	GLU	CA-C-O	-6.87	113.60	120.82
1	A	130	GLU	CA-C-O	-6.87	113.61	120.82
1	C	56	ALA	CA-C-N	-6.85	113.38	123.11
1	C	56	ALA	C-N-CA	-6.85	113.38	123.11
1	A	56	ALA	CA-C-N	-6.83	113.42	123.11
1	A	56	ALA	C-N-CA	-6.83	113.42	123.11
1	C	63	GLN	N-CA-C	-6.81	104.03	112.47
1	A	63	GLN	N-CA-C	-6.79	104.05	112.47
1	A	52	GLN	OE1-CD-NE2	-6.74	115.86	122.60
2	E	91	THR	N-CA-C	-6.74	105.09	113.38
1	A	113	ILE	N-CA-CB	6.72	119.07	111.21
1	A	65	ASP	CA-C-N	6.71	134.36	121.54
1	A	65	ASP	C-N-CA	6.71	134.36	121.54
1	C	65	ASP	CA-C-N	6.70	134.34	121.54
1	C	65	ASP	C-N-CA	6.70	134.34	121.54
2	F	91	THR	N-CA-C	-6.69	105.15	113.38
1	C	52	GLN	OE1-CD-NE2	-6.65	115.95	122.60
1	A	65	ASP	N-CA-C	6.63	120.24	111.75
1	C	113	ILE	N-CA-CB	6.63	118.97	111.21
1	C	65	ASP	N-CA-C	6.62	120.22	111.75
1	C	45	ASP	CA-CB-CG	-6.61	105.99	112.60
1	A	6	LYS	O-C-N	-6.60	115.12	123.24
1	A	45	ASP	CA-CB-CG	-6.55	106.05	112.60
1	C	6	LYS	O-C-N	-6.55	115.18	123.24
1	C	114	LEU	CA-C-N	-6.49	114.64	123.14
1	C	114	LEU	C-N-CA	-6.49	114.64	123.14
1	A	114	LEU	CA-C-N	-6.44	114.71	123.14
1	A	114	LEU	C-N-CA	-6.44	114.71	123.14
1	A	136	GLN	OE1-CD-NE2	-6.40	116.20	122.60
1	C	136	GLN	OE1-CD-NE2	-6.36	116.24	122.60
1	A	67	ASP	N-CA-C	-6.30	104.41	111.28
1	C	67	ASP	N-CA-C	-6.30	104.42	111.28
2	E	82	ALA	CA-C-N	6.26	125.88	119.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	82	ALA	C-N-CA	6.26	125.88	119.56
1	C	142	GLU	CB-CA-C	-6.22	100.47	110.79
2	F	82	ALA	CA-C-N	6.21	125.83	119.56
2	F	82	ALA	C-N-CA	6.21	125.83	119.56
1	A	6	LYS	CA-C-N	6.17	131.69	123.05
1	A	6	LYS	C-N-CA	6.17	131.69	123.05
1	A	142	GLU	CB-CA-C	-6.17	100.56	110.79
2	E	84	GLY	CA-C-N	6.15	126.12	119.78
2	E	84	GLY	C-N-CA	6.15	126.12	119.78
1	C	6	LYS	CA-C-N	6.14	131.65	123.05
1	C	6	LYS	C-N-CA	6.14	131.65	123.05
2	F	84	GLY	CA-C-N	6.13	126.10	119.78
2	F	84	GLY	C-N-CA	6.13	126.10	119.78
1	A	171	PHE	CA-CB-CG	-6.13	107.67	113.80
1	C	50	GLY	N-CA-C	-6.10	102.15	111.24
1	A	50	GLY	N-CA-C	-6.09	102.17	111.24
1	C	111	PRO	CA-C-N	6.07	130.72	123.19
1	C	111	PRO	C-N-CA	6.07	130.72	123.19
1	C	171	PHE	CA-CB-CG	-6.07	107.73	113.80
1	C	129	ARG	CD-NE-CZ	6.04	132.86	124.40
1	A	63	GLN	CA-C-O	6.03	128.27	120.55
1	C	63	GLN	CA-C-O	6.03	128.27	120.55
1	A	129	ARG	CD-NE-CZ	6.01	132.81	124.40
1	C	76	ASP	CA-C-N	-6.00	111.43	121.39
1	C	76	ASP	C-N-CA	-6.00	111.43	121.39
2	F	74	GLY	N-CA-C	6.00	119.85	110.91
1	A	76	ASP	CA-C-N	-6.00	111.43	121.39
1	A	76	ASP	C-N-CA	-6.00	111.43	121.39
2	E	74	GLY	N-CA-C	5.99	119.84	110.91
1	A	118	LYS	CG-CD-CE	5.99	125.07	111.30
1	C	118	LYS	CG-CD-CE	5.97	125.04	111.30
1	A	111	PRO	CA-C-N	5.97	130.59	123.19
1	A	111	PRO	C-N-CA	5.97	130.59	123.19
1	C	167	VAL	N-CA-C	5.93	116.11	110.53
1	C	79	VAL	CA-C-O	-5.91	115.40	120.96
1	A	167	VAL	N-CA-C	5.90	116.07	110.53
1	A	103	VAL	CA-CB-CG2	5.89	120.41	110.40
1	C	31	PRO	O-C-N	-5.89	114.69	122.64
1	A	5	ARG	NE-CZ-NH1	5.88	127.38	121.50
1	C	103	VAL	CA-CB-CG2	5.87	120.38	110.40
1	A	176	ARG	CD-NE-CZ	5.87	132.62	124.40
1	C	176	ARG	CD-NE-CZ	5.84	132.58	124.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	31	PRO	O-C-N	-5.83	114.78	122.64
1	A	128	ARG	CB-CG-CD	5.83	124.70	111.30
1	A	79	VAL	CA-C-O	-5.82	115.49	120.96
1	C	74	TYR	O-C-N	-5.82	114.63	121.32
2	F	183	ASP	N-CA-C	5.80	115.68	108.19
1	C	5	ARG	NE-CZ-NH1	5.80	127.30	121.50
1	C	75	PRO	CA-C-O	-5.80	115.00	121.32
1	C	128	ARG	CB-CG-CD	5.79	124.62	111.30
2	E	183	ASP	N-CA-C	5.77	115.64	108.19
1	C	162	LYS	N-CA-CB	5.77	118.70	110.16
1	C	119	LYS	CA-C-N	5.76	130.34	120.72
1	C	119	LYS	C-N-CA	5.76	130.34	120.72
1	A	75	PRO	CA-C-O	-5.75	115.06	121.32
1	A	162	LYS	N-CA-CB	5.74	118.66	110.16
1	A	119	LYS	CA-C-N	5.74	130.31	120.72
1	A	119	LYS	C-N-CA	5.74	130.31	120.72
1	C	124	ASP	CA-C-O	5.74	127.59	121.16
1	A	124	ASP	CA-C-O	5.74	127.58	121.16
1	A	74	TYR	O-C-N	-5.70	114.76	121.32
1	A	180	GLN	CG-CD-NE2	-5.70	107.85	116.40
1	A	49	ASP	N-CA-C	5.70	118.45	109.96
1	C	68	ARG	NH1-CZ-NH2	-5.68	111.91	119.30
1	C	49	ASP	N-CA-C	5.66	118.40	109.96
1	C	180	GLN	CG-CD-NE2	-5.66	107.91	116.40
1	C	39	PHE	CA-C-O	-5.64	114.55	120.58
1	A	39	PHE	CA-C-O	-5.62	114.56	120.58
1	A	68	ARG	NH1-CZ-NH2	-5.62	111.99	119.30
1	C	113	ILE	CA-C-O	-5.60	114.49	120.59
1	C	52	GLN	CA-C-O	-5.58	114.18	120.32
1	A	52	GLN	CA-C-O	-5.55	114.21	120.32
1	C	87	ASP	O-C-N	-5.53	115.26	122.39
1	A	113	ILE	CA-C-O	-5.52	114.57	120.59
1	C	115	VAL	CA-C-N	-5.51	117.38	122.29
1	C	115	VAL	C-N-CA	-5.51	117.38	122.29
1	A	163	THR	N-CA-C	-5.50	106.62	113.38
1	C	68	ARG	NE-CZ-NH1	5.50	127.00	121.50
1	C	163	THR	N-CA-C	-5.48	106.64	113.38
1	A	115	VAL	CA-C-N	-5.47	117.42	122.29
1	A	115	VAL	C-N-CA	-5.47	117.42	122.29
1	A	87	ASP	O-C-N	-5.45	115.36	122.39
1	C	176	ARG	NE-CZ-NH1	5.44	126.94	121.50
1	A	180	GLN	OE1-CD-NE2	5.42	128.02	122.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	137	VAL	N-CA-C	5.41	116.38	108.53
1	A	176	ARG	NE-CZ-NH1	5.38	126.88	121.50
2	E	137	VAL	N-CA-C	5.37	116.32	108.53
1	C	146	ASP	CA-CB-CG	-5.37	107.23	112.60
1	A	25	ASN	N-CA-CB	5.35	118.46	110.22
1	C	77	THR	CB-CA-C	5.33	119.28	109.46
1	C	180	GLN	OE1-CD-NE2	5.33	127.93	122.60
1	A	68	ARG	NE-CZ-NH1	5.33	126.83	121.50
1	A	77	THR	CB-CA-C	5.33	119.26	109.46
1	A	146	ASP	CA-CB-CG	-5.32	107.28	112.60
1	A	180	GLN	CB-CA-C	-5.30	100.02	110.10
1	C	25	ASN	N-CA-CB	5.30	118.39	110.22
1	C	180	GLN	CB-CA-C	-5.30	100.03	110.10
1	C	128	ARG	CA-CB-CG	-5.28	103.54	114.10
1	A	154	PHE	N-CA-CB	-5.28	101.63	110.39
1	C	154	PHE	N-CA-CB	-5.28	101.63	110.39
1	A	128	ARG	CA-CB-CG	-5.25	103.61	114.10
1	A	114	LEU	CA-C-O	-5.19	114.61	120.43
1	A	68	ARG	N-CA-C	-5.17	105.71	112.23
1	C	68	ARG	N-CA-C	-5.16	105.73	112.23
1	C	114	LEU	CA-C-O	-5.16	114.65	120.43
1	C	115	VAL	CA-C-O	-5.16	114.98	120.39
1	A	115	VAL	CA-C-O	-5.15	114.98	120.39
2	F	119	ASN	N-CA-C	5.15	119.45	112.04
2	E	119	ASN	N-CA-C	5.14	119.45	112.04
1	C	102	GLU	N-CA-CB	5.05	117.34	110.01
1	C	162	LYS	CA-C-O	-5.05	115.07	120.42
1	C	66	TYR	CA-C-O	5.04	127.71	120.51
1	C	125	GLU	O-C-N	-5.04	116.65	122.09
1	A	159	CYS	CA-C-O	5.04	126.70	121.36
1	C	159	CYS	CA-C-O	5.03	126.69	121.36
1	A	162	LYS	CA-C-O	-5.03	115.09	120.42
1	C	103	VAL	N-CA-CB	5.03	119.87	110.77
2	F	120	ARG	N-CA-C	5.03	119.62	112.93
1	A	102	GLU	N-CA-CB	5.02	117.29	110.01
1	C	137	GLU	N-CA-CB	-5.02	104.97	111.35
1	A	66	TYR	CA-C-O	5.01	127.68	120.51
1	A	103	VAL	N-CA-CB	5.01	119.84	110.77

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	59	7
1	C	1415	0	1394	61	16
2	E	1143	0	1100	35	20
2	F	1143	0	1100	38	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	146	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 (146) 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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:GLN:HE22	1:C:180:GLN:HE22	1.03	1.02
1:A:105:HIS:CD2	2:E:145:MET:HE2	1.96	1.01
1:A:71:PRO:CB	2:E:148:SER:CB	2.44	0.94
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:C:105:HIS:CD2	2:F:145:MET:HE2	2.07	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:A:105:HIS:NE2	2:E:145:MET:HE3	1.90	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: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: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:105:HIS:NE2	2:F:145:MET:HE3	2.01	0.74
1:C:128:ARG:HG2	1:C:128:ARG:HH11	1.54	0.73
1:A:71:PRO:HB3	2:E:148:SER:HB2	1.68	0.72
1:C:71:PRO:C	2:F:148:SER:HB2	2.15	0.72
1:A:128:ARG:HH11	1:A:128:ARG:HG2	1.54	0.71
1:C:105:HIS:CD2	2:F:145:MET:HE1	2.26	0.70
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: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:C:95:ILE:HB	1:C:96:PRO:HD3	1.82	0.62
1:C:128:ARG:HG2	1:C:128:ARG:NH1	2.13	0.62
2:E:69:ASN:ND2	2:E:121:GLU:H	1.98	0.61
1:C:68:ARG:HH11	2:F:34:SER:CA	2.11	0.61
2:F:69:ASN:ND2	2:F:121:GLU:H	1.98	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:62:GLY:C	1:C:64:GLU:N	2.57	0.60
1:A:62:GLY:C	1:A:64:GLU:N	2.57	0.59
1:A:128:ARG:HG2	1:A:128:ARG:NH1	2.13	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
1:A:119:LYS:NZ	1:A:165:ASP:OD2	2.26	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:65:ASP:C	1:A:67:ASP:H	2.13	0.57
1:A:180:GLN:O	1:A:181:ALA:CA	2.54	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:65:ASP:C	1:C:67:ASP:H	2.13	0.55
1:C:63:GLN:O	1:C:64:GLU:HB2	2.07	0.55
1:C:119:LYS:NZ	1:C:165:ASP:OD2	2.26	0.55
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
1:A:63:GLN:O	1:A:64:GLU:HB2	2.07	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
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
1:C:105:HIS:O	2:F:145:MET:HE2	2.12	0.50
2:E:146:VAL:HG12	2:E:149:TYR:CE1	2.46	0.50
2:F:126:MET:HB2	2:F:147:GLY:O	2.11	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:N	2.71	0.49
1:A:40:GLU:OE1	2:E:49:ARG:CA	2.61	0.49
2:E:134:ARG:HG2	2:E:134:ARG:HH11	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
1:A:65:ASP:C	1:A:67:ASP:N	2.71	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:93:GLU:O	1:A:96:PRO:HD2	2.15	0.47
1:C:169:GLU:OE1	1:C:169:GLU:N	2.45	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
1:A:169:GLU:OE1	1:A:169:GLU:N	2.45	0.46
2:E:117:ARG:HG2	2:E:119:ASN:ND2	2.31	0.46
1:C:8:LEU:C	1:C:8:LEU:HD23	2.41	0.46
1:A:8:LEU:C	1:A:8:LEU:HD23	2.41	0.45
1:A:99:TRP:O	1:A:103:VAL:HG13	2.16	0.45
1:C:22:LEU:CD1	1:C:59:ASP:HB2	2.46	0.45
1:C:190:CYS:CA	2:F:142:THR:HG23	2.47	0.45
1:C:105:HIS:CE1	2:F:145:MET:HE3	2.52	0.45
2:F:117:ARG:HG2	2:F:119:ASN:ND2	2.31	0.45
2:F:134:ARG:HG2	2:F:134:ARG:NH1	2.32	0.45
2:E:134:ARG:HG2	2:E:134:ARG:NH1	2.32	0.44
1:C:99:TRP:O	1:C:103:VAL:HG13	2.16	0.44
1:A:105:HIS:CD2	2:E:145:MET:HE1	2.46	0.44
1:A:66:TYR:OH	2:E:50:LYS:CA	2.66	0.44
1:C:74:TYR:O	1:C:75:PRO:C	2.59	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:69:LEU:HA	1:A:72:LEU:HD23	2.01	0.42
1:A:95:ILE:HB	1:A:96:PRO:CD	2.49	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
1:A:169:GLU:HG2	1:C:149:ASN:HD22	1.84	0.42
2:F:65:PRO:CA	2:F:120:ARG:NH2	2.82	0.42
1:C:9:VAL:HG21	1:C:77:THR:HG21	2.02	0.42
1:C:64:GLU:O	1:C:65:ASP:C	2.62	0.42
2:F:132:THR:HG23	2:F:177:ILE:HG13	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:GLU:O	1:A:65:ASP:C	2.62	0.42
1:A:51:LYS:CG	1:A:52:GLN:H	2.33	0.42
1:A:71:PRO:C	2:E:148:SER:HB2	2.45	0.42
1:C:51:LYS:HG3	1:C:52:GLN:H	1.85	0.42
1:C:69:LEU:HA	1:C:72:LEU:HD23	2.01	0.42
1:A:9:VAL:HG21	1:A:77:THR:HG21	2.02	0.42
1:A:105:HIS:CE1	2:E:145:MET:HE3	2.54	0.41
1:A:71:PRO:HB3	2:E:148:SER:HG	1.74	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:A:74:TYR:O	1:A:75:PRO:C	2.59	0.41
1:C:72:LEU:HD21	2:F:122:ILE:CG2	2.46	0.41
1:C:14:GLY:O	1:C:15:ALA:HB3	2.21	0.41
1:C:51:LYS:CG	1:C:52:GLN:H	2.33	0.41
2:E:67:VAL:CA	2:E:68:PRO:N	2.84	0.41
1:C:95:ILE:HB	1:C:96:PRO:CD	2.49	0.41
1:A:40:GLU:O	1:A:41:ASN:C	2.65	0.40

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
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	7	34
1	C	175/190 (92%)	164 (94%)	8 (5%)	3 (2%)	7	34
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%)	12	47

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%)	139 (89%)	17 (11%)	6	21
1	C	156/164 (95%)	139 (89%)	17 (11%)	6	21
2	E	122/180 (68%)	110 (90%)	12 (10%)	7	24
2	F	122/180 (68%)	110 (90%)	12 (10%)	7	24
All	All	556/688 (81%)	498 (90%)	58 (10%)	7	22

All (58) 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	110	VAL
1	A	123	ASN
1	A	128	ARG
1	A	162	LYS
1	A	164	LYS
1	A	168	ARG
1	A	179	LEU
1	A	180	GLN
2	E	76	THR
2	E	77	LEU
2	E	80	SER
2	E	81	SER
2	E	86	LEU
2	E	94	LEU
2	E	104	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	145	MET
2	E	152	ARG
2	E	161	PRO
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	110	VAL
1	C	123	ASN
1	C	128	ARG
1	C	162	LYS
1	C	164	LYS
1	C	168	ARG
1	C	179	LEU
1	C	180	GLN
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	104	LEU
2	F	145	MET
2	F	152	ARG
2	F	161	PRO
2	F	170	LEU
2	F	190	LEU

Sometimes 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

Continued on next page...

Continued from previous page...

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	29,30,30	1.24	2 (6%)	45,47,47	1.38	6 (13%)
4	GDP	C	202	3	29,30,30	1.25	2 (6%)	45,47,47	1.38	6 (13%)

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	202	GDP	PA-O3A	3.35	1.63	1.59
4	A	201	GDP	PA-O3A	3.25	1.63	1.59
4	C	202	GDP	C5-C4	-3.00	1.30	1.38
4	A	201	GDP	C5-C4	-2.97	1.30	1.38

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	201	GDP	O3B-PB-O2B	3.78	121.96	107.80
4	C	202	GDP	O3B-PB-O2B	3.76	121.92	107.80
4	A	201	GDP	O2'-C2'-C1'	-3.27	98.85	110.10
4	C	202	GDP	O2'-C2'-C1'	-3.26	98.89	110.10
4	A	201	GDP	O3A-PB-O1B	-2.84	96.09	111.04
4	C	202	GDP	O3A-PB-O1B	-2.84	96.12	111.04
4	A	201	GDP	O4'-C1'-C2'	-2.07	102.19	106.62
4	C	202	GDP	O2A-PA-O1A	2.07	122.06	112.44
4	C	202	GDP	O4'-C1'-C2'	-2.06	102.21	106.62
4	A	201	GDP	O2A-PA-O1A	2.05	121.99	112.44
4	C	202	GDP	C6-C5-N7	-2.02	126.62	130.29
4	A	201	GDP	C6-C5-N7	-2.01	126.64	130.29

There are no chirality outliers.

All (2) torsion outliers are listed below:

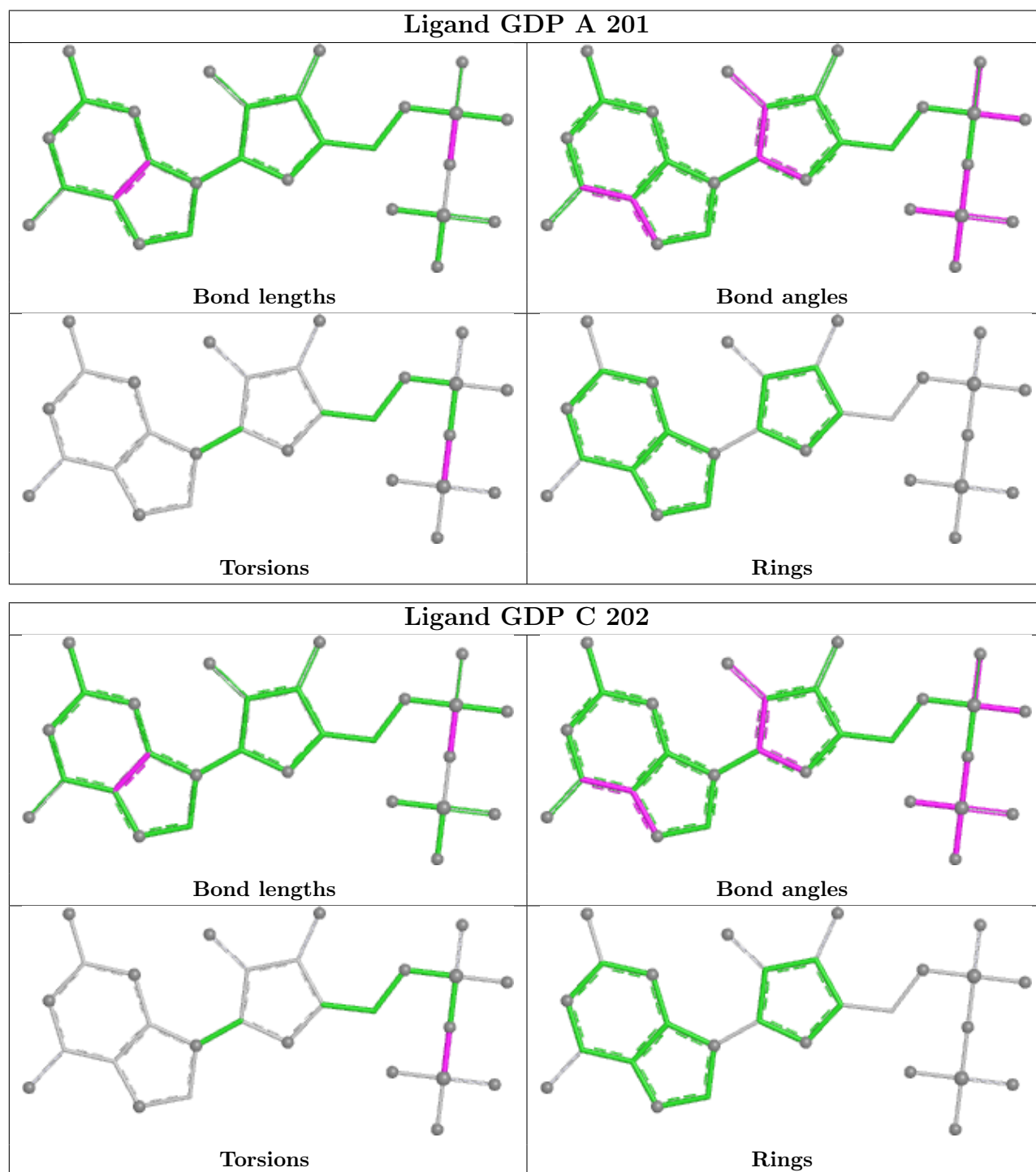
Mol	Chain	Res	Type	Atoms
4	A	201	GDP	PA-O3A-PB-O1B
4	C	202	GDP	PA-O3A-PB-O1B

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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%)	1.86	75 (40%) 0 3	35, 35, 35, 35	0
1	C	187/190 (98%)	1.88	67 (35%) 1 4	35, 35, 35, 35	0
2	E	180/204 (88%)	2.89	98 (54%) 0 2	35, 35, 35, 35	0
2	F	180/204 (88%)	3.00	101 (56%) 0 2	35, 35, 35, 35	0
All	All	734/788 (93%)	2.39	341 (46%) 0 2	35, 35, 35, 35	0

All (341) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	57	GLY	17.5
1	C	189	GLY	14.4
2	E	57	GLY	14.1
2	E	26	ASN	10.6
2	F	27	TYR	10.5
2	E	30	PRO	10.4
2	F	26	ASN	10.3
2	F	58	ARG	10.3
2	F	24	SER	10.3
2	F	46	GLU	10.0
2	E	27	TYR	10.0
2	E	29	PRO	9.8
2	E	25	VAL	9.7
2	F	66	ASN	9.7
2	F	29	PRO	9.6
1	C	190	CYS	9.6
2	E	114	ILE	9.6
2	F	59	VAL	9.5
2	F	34	SER	9.3
2	E	24	SER	9.2
2	F	25	VAL	9.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	188	SER	8.7
1	A	190	CYS	8.4
2	F	28	LYS	8.4
2	F	54	ALA	8.3
2	E	122	ILE	8.2
2	F	124	SER	8.0
2	E	54	ALA	8.0
2	E	60	ALA	7.8
2	F	39	GLN	7.7
1	A	69	LEU	7.5
2	F	30	PRO	7.4
2	E	53	GLU	7.4
2	E	63	ALA	7.4
2	E	59	VAL	7.3
2	E	145	MET	7.3
2	E	32	GLN	7.0
2	E	61	VAL	6.9
1	C	29	GLN	6.8
2	F	37	GLU	6.8
2	E	56	LEU	6.8
2	E	62	SER	6.7
2	F	181	PHE	6.7
2	E	64	ASP	6.6
2	F	32	GLN	6.5
1	A	68	ARG	6.5
2	E	34	SER	6.5
2	F	50	LYS	6.4
2	E	127	LYS	6.3
2	F	33	LYS	6.3
2	E	28	LYS	6.2
1	A	38	VAL	6.1
2	F	44	ASP	6.0
2	F	193	GLU	5.9
1	C	66	TYR	5.9
2	F	53	GLU	5.9
1	A	188	SER	5.8
2	E	55	LEU	5.8
1	C	155	GLY	5.8
2	E	148	SER	5.8
1	C	182	ARG	5.6
2	E	49	ARG	5.6
2	F	56	LEU	5.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	E	158	PHE	5.5
2	F	36	GLN	5.5
1	A	83	CYS	5.5
1	A	158	GLU	5.5
2	E	46	GLU	5.5
2	E	175	TYR	5.5
2	F	49	ARG	5.4
2	E	58	ARG	5.4
2	F	121	GLU	5.4
2	F	170	LEU	5.3
2	F	47	SER	5.2
2	F	62	SER	5.2
2	E	52	LYS	5.1
2	F	90	LEU	5.0
1	A	117	ASN	5.0
2	E	51	TYR	5.0
1	A	187	LYS	4.9
1	A	189	GLY	4.9
1	C	149	ASN	4.9
1	A	159	CYS	4.9
1	C	57	LEU	4.9
2	E	50	LYS	4.9
1	A	182	ARG	4.9
1	C	117	ASN	4.8
2	E	38	ILE	4.7
2	F	117	ARG	4.7
2	F	64	ASP	4.7
2	E	124	SER	4.7
2	F	187	THR	4.7
2	E	149	TYR	4.6
2	E	41	LEU	4.6
2	E	146	VAL	4.6
2	F	145	MET	4.6
2	F	78	VAL	4.5
1	C	183	ARG	4.5
2	F	60	ALA	4.5
2	E	203	LYS	4.5
2	F	179	SER	4.5
2	E	33	LYS	4.5
1	C	87	ASP	4.5
2	E	35	ILE	4.4
1	C	184	GLY	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	181	ALA	4.4
2	E	199	LYS	4.4
2	F	184	ASP	4.3
1	C	159	CYS	4.3
1	C	58	TRP	4.3
2	F	35	ILE	4.2
1	C	9	VAL	4.2
2	F	48	LEU	4.2
1	C	158	GLU	4.2
2	F	61	VAL	4.2
2	F	72	VAL	4.1
1	A	10	ILE	4.1
2	F	38	ILE	4.1
1	A	151	ILE	4.0
2	E	47	SER	4.0
1	C	128	ARG	4.0
1	A	130	GLU	4.0
1	A	60	THR	4.0
2	F	31	ALA	4.0
2	F	70	VAL	3.9
2	F	55	LEU	3.9
2	F	94	LEU	3.9
1	C	62	GLY	3.9
1	A	127	THR	3.8
2	E	198	ILE	3.8
2	F	71	VAL	3.8
2	E	37	GLU	3.8
2	E	202	TRP	3.8
1	C	133	LYS	3.8
2	E	70	VAL	3.7
1	A	40	GLU	3.7
1	A	181	ALA	3.7
1	A	94	ASN	3.6
2	F	80	SER	3.6
2	E	91	THR	3.6
2	F	189	HIS	3.6
2	F	165	ALA	3.6
2	E	108	VAL	3.6
2	F	63	ALA	3.6
2	F	171	ALA	3.6
2	E	100	GLN	3.6
1	A	175	THR	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	68	ARG	3.5
2	E	112	ILE	3.5
1	C	151	ILE	3.5
2	F	130	GLN	3.5
2	E	44	ASP	3.5
1	C	83	CYS	3.5
1	C	77	THR	3.5
1	C	113	ILE	3.5
2	F	112	ILE	3.5
2	F	192	TRP	3.4
2	E	130	GLN	3.4
1	A	139	VAL	3.4
2	E	81	SER	3.4
1	C	86	ILE	3.4
1	C	84	PHE	3.4
2	E	31	ALA	3.4
2	E	80	SER	3.4
1	C	172	GLU	3.4
1	A	66	TYR	3.3
1	A	114	LEU	3.3
2	E	96	SER	3.3
1	A	123	ASN	3.3
1	C	114	LEU	3.3
2	F	104	LEU	3.3
1	A	174	ALA	3.3
1	A	65	ASP	3.3
1	A	178	ALA	3.3
1	C	24	VAL	3.3
1	C	187	LYS	3.3
2	E	153	ALA	3.2
2	E	42	ASP	3.2
1	A	41	ASN	3.2
1	C	69	LEU	3.2
2	F	79	CYS	3.2
2	E	99	LYS	3.2
1	A	4	ILE	3.2
2	E	171	ALA	3.2
2	E	118	VAL	3.1
2	F	52	LYS	3.1
1	A	88	SER	3.1
2	F	190	LEU	3.1
1	A	184	GLY	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	72	LEU	3.1
1	A	100	THR	3.1
2	F	123	VAL	3.1
1	A	121	LEU	3.1
2	E	126	MET	3.1
2	F	125	GLY	3.0
1	A	87	ASP	3.0
2	E	65	PRO	3.0
2	F	41	LEU	3.0
1	A	145	ARG	3.0
1	C	60	THR	3.0
2	E	45	ASP	3.0
2	F	180	ARG	3.0
1	A	17	GLY	3.0
1	C	178	ALA	3.0
2	F	91	THR	3.0
1	C	71	PRO	3.0
1	A	14	GLY	2.9
2	F	148	SER	2.9
2	E	86	LEU	2.9
2	E	87	GLU	2.9
1	C	118	LYS	2.9
2	F	97	PHE	2.9
2	E	79	CYS	2.9
1	A	20	CYS	2.9
2	E	182	THR	2.9
2	F	101	SER	2.9
1	C	145	ARG	2.8
1	A	28	ASP	2.8
1	A	129	ARG	2.8
2	F	110	TYR	2.8
1	A	104	LYS	2.8
1	C	6	LYS	2.8
1	C	56	ALA	2.8
1	A	24	VAL	2.7
1	C	10	ILE	2.7
1	A	18	LYS	2.7
1	A	119	LYS	2.7
1	A	9	VAL	2.7
1	A	110	VAL	2.7
1	C	81	LEU	2.7
2	E	48	LEU	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	F	114	ILE	2.7
1	A	91	SER	2.7
1	A	59	ASP	2.7
1	A	39	PHE	2.7
2	E	117	ARG	2.6
2	E	166	PRO	2.6
1	C	55	LEU	2.6
2	E	36	GLN	2.6
2	E	133	TYR	2.6
1	C	67	ASP	2.6
2	E	165	ALA	2.6
2	E	77	LEU	2.6
2	F	65	PRO	2.6
1	C	16	CYS	2.6
1	A	143	GLU	2.6
2	F	77	LEU	2.6
1	C	18	LYS	2.6
1	A	32	GLU	2.6
2	F	196	LEU	2.5
1	A	53	VAL	2.5
1	C	20	CYS	2.5
2	E	69	ASN	2.5
2	F	76	THR	2.5
1	A	44	ALA	2.5
2	E	71	VAL	2.5
2	F	102	PHE	2.5
1	C	167	VAL	2.5
1	A	73	SER	2.5
1	A	85	SER	2.5
2	F	108	VAL	2.5
2	F	107	GLY	2.5
2	F	153	ALA	2.5
2	E	178	LYS	2.5
1	A	84	PHE	2.5
1	A	124	ASP	2.5
2	F	194	TRP	2.5
1	C	34	TYR	2.4
1	C	74	TYR	2.4
2	E	72	VAL	2.4
2	E	181	PHE	2.4
2	E	78	VAL	2.4
2	F	67	VAL	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	F	182	THR	2.4
2	E	143	ASP	2.4
1	C	170	VAL	2.4
2	E	174	SER	2.4
2	F	75	LEU	2.4
2	F	88	LEU	2.4
2	F	81	SER	2.3
1	C	35	VAL	2.3
2	F	69	ASN	2.3
1	A	118	LYS	2.3
2	E	109	GLU	2.3
2	F	166	PRO	2.3
1	A	179	LEU	2.3
1	C	121	LEU	2.3
1	C	95	ILE	2.3
2	E	104	LEU	2.3
2	F	159	LEU	2.3
1	C	93	GLU	2.3
1	C	106	PHE	2.3
2	F	191	SER	2.3
1	C	61	ALA	2.3
1	A	8	LEU	2.2
2	E	189	HIS	2.2
2	F	195	ASN	2.2
1	A	162	LYS	2.2
1	A	33	VAL	2.2
2	E	116	PHE	2.2
2	E	147	GLY	2.2
2	F	129	ILE	2.2
2	E	170	LEU	2.2
2	F	177	ILE	2.2
1	C	104	LYS	2.2
2	F	43	LYS	2.2
1	A	46	ILE	2.2
1	A	126	HIS	2.2
2	E	98	LYS	2.2
2	F	203	LYS	2.2
1	A	11	VAL	2.2
1	C	8	LEU	2.2
1	C	88	SER	2.2
1	A	29	GLN	2.2
2	F	152	ARG	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	F	169	MET	2.2
1	C	17	GLY	2.1
1	A	164	LYS	2.1
2	E	66	ASN	2.1
2	F	51	TYR	2.1
1	C	102	GLU	2.1
1	C	98	LYS	2.1
1	C	171	PHE	2.1
1	C	64	GLU	2.1
1	C	115	VAL	2.1
1	A	128	ARG	2.1
2	E	128	TYR	2.1
2	F	98	LYS	2.1
2	E	144	TYR	2.1
1	C	25	ASN	2.1
2	E	43	LYS	2.0
2	E	110	TYR	2.0
1	A	61	ALA	2.0
2	E	111	ARG	2.0
1	A	51	LYS	2.0
1	A	63	GLN	2.0
2	E	67	VAL	2.0
1	A	81	LEU	2.0
2	F	128	TYR	2.0
1	A	109	ASN	2.0
2	F	178	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

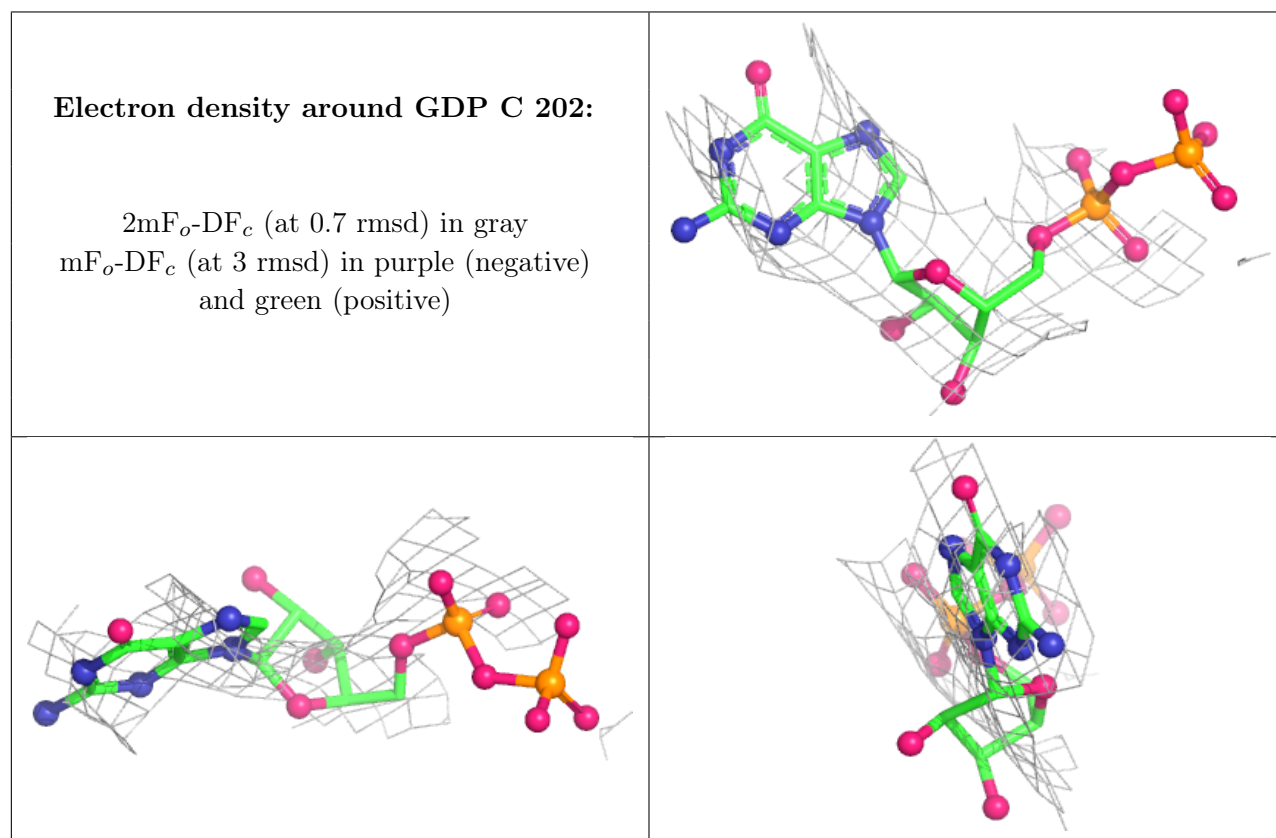
There are no oligosaccharides in this entry.

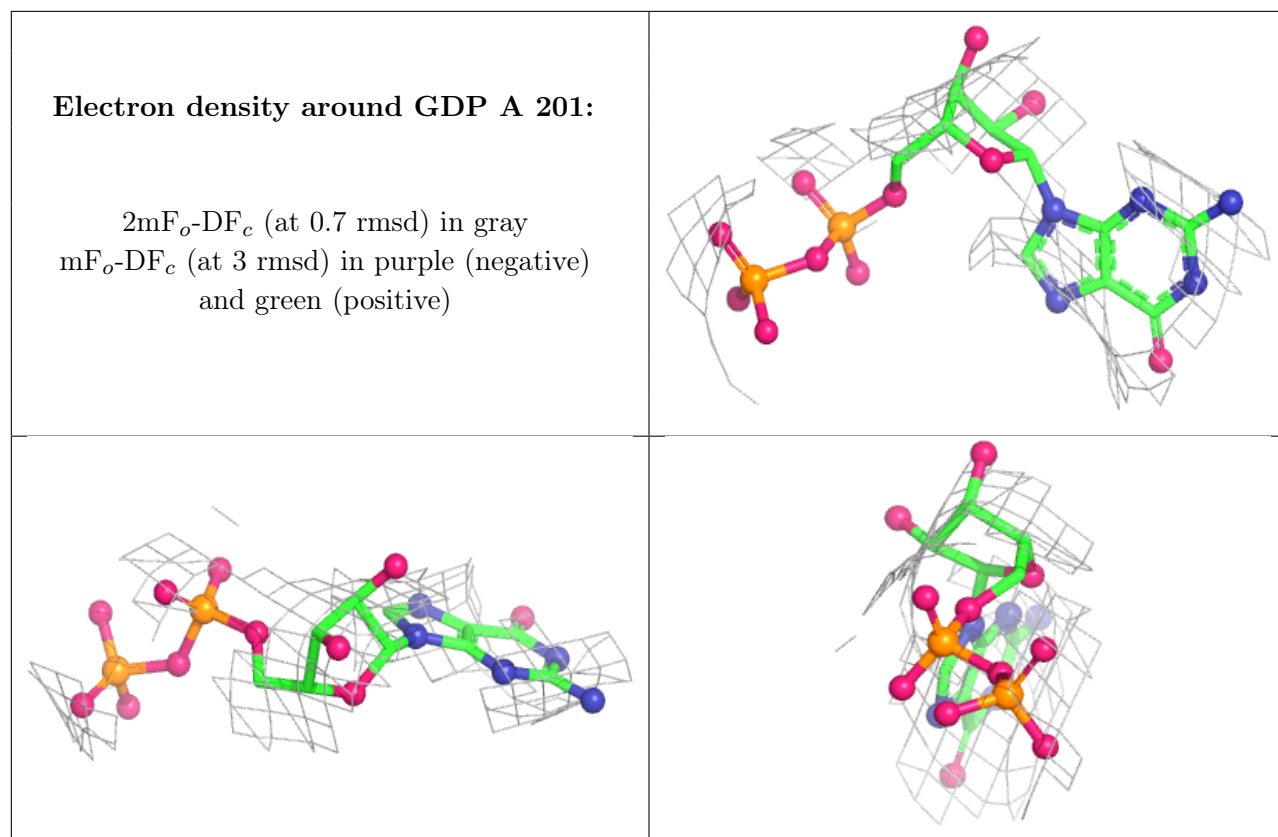
6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MG	C	302	1/1	-0.17	0.27	35,35,35,35	0
3	MG	A	301	1/1	0.45	0.38	35,35,35,35	0
4	GDP	C	202	28/28	0.77	0.24	35,35,35,35	0
4	GDP	A	201	28/28	0.91	0.17	35,35,35,35	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





6.5 Other polymers [i](#)

There are no such residues in this entry.