



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:56 AM UTC

PDB ID : 5CA9 / pdb_00005ca9
Title : Structures of the candida albicans sey1p GTPase in complex with GDPAlF4-
Authors : Yan, L.
Deposited on : 2015-06-29
Resolution : 2.80 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

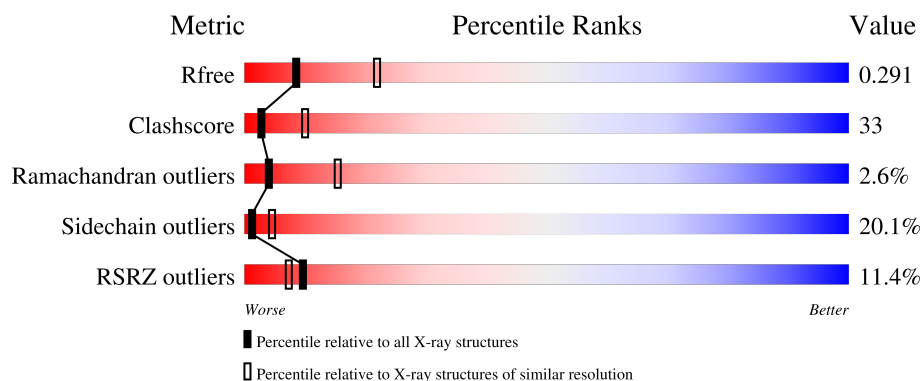
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	692	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5452 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 Protein SEY1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	656	Total	C	N	O	S	0	0	0
			5303	3390	877	1025	11			

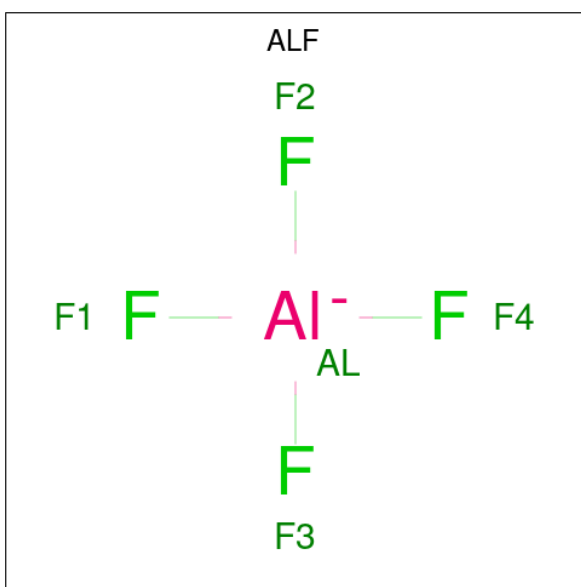
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	89	LEU	SER	see sequence details	UNP Q9C0L9
A	221	LEU	SER	see sequence details	UNP Q9C0L9
A	270	GLY	ASP	see sequence details	UNP Q9C0L9
A	337	THR	ALA	see sequence details	UNP Q9C0L9
A	479	VAL	ILE	see sequence details	UNP Q9C0L9
A	665	LEU	SER	see sequence details	UNP Q9C0L9

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

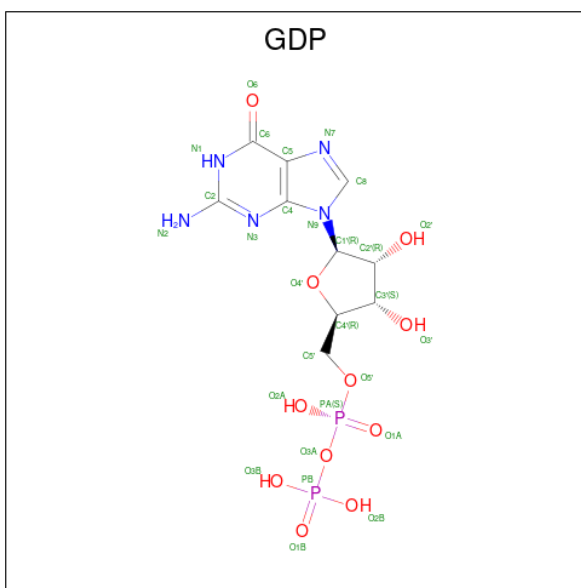
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is TETRAFLUOROALUMINATE ION (CCD ID: ALF) (formula: AlF_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Al	F	0	0
			5	1	4		

- Molecule 4 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: 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	
			28	10	5	11	2	

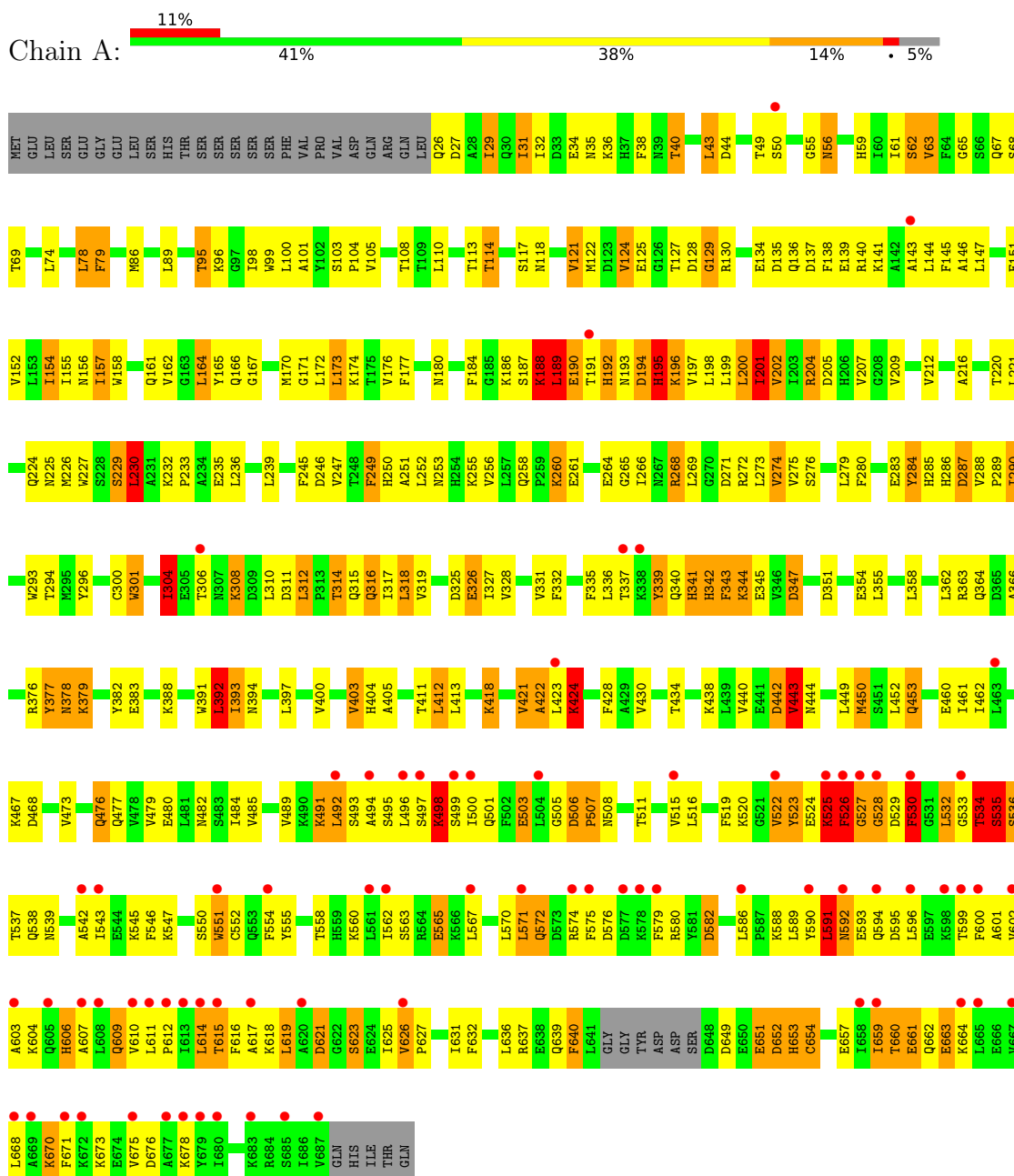
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	115	Total 115	O 115	0	0

3 Residue-property plots

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: Protein SEY1



4 Data and refinement statistics

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	76.27Å 120.53Å 190.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.76 – 2.80 48.76 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.9 (48.76-2.80) 98.9 (48.76-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.61 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.253 , 0.279 0.267 , 0.291	Depositor DCC
R_{free} test set	1121 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	64.6	Xtriage
Anisotropy	0.379	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 95.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	5452	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.29% 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: GDP, MG, ALF

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	1.09	11/5404 (0.2%)	1.38	81/7301 (1.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	56	ASN	N-CA	-8.54	1.35	1.46
1	A	200	LEU	CA-C	-7.58	1.43	1.52
1	A	288	VAL	C-O	-6.97	1.18	1.24
1	A	56	ASN	CA-C	6.46	1.61	1.52
1	A	195	HIS	CA-C	-5.67	1.45	1.52
1	A	284	TYR	N-CA	-5.28	1.39	1.46
1	A	260	LYS	N-CA	-5.21	1.40	1.46
1	A	63	VAL	C-O	-5.17	1.18	1.24
1	A	162	VAL	C-O	5.07	1.29	1.24
1	A	280	PHE	N-CA	5.02	1.52	1.46
1	A	65	GLY	N-CA	5.01	1.50	1.45

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	661	GLU	CB-CA-C	15.10	134.21	110.96
1	A	336	LEU	N-CA-C	13.92	127.81	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	532	LEU	N-CA-C	-13.63	89.58	110.17
1	A	522	VAL	CB-CA-C	-11.38	92.63	111.29
1	A	452	LEU	N-CA-C	11.31	124.14	110.91
1	A	424	LYS	N-CA-CB	-11.01	91.88	110.49
1	A	343	PHE	N-CA-CB	-10.79	95.42	110.95
1	A	530	PHE	N-CA-C	10.78	126.76	113.50
1	A	56	ASN	N-CA-C	-10.72	97.82	112.94
1	A	196	LYS	N-CA-C	-10.66	93.36	110.20
1	A	421	VAL	CB-CA-C	-9.61	95.53	111.29
1	A	276	SER	N-CA-C	-9.21	100.83	112.90
1	A	65	GLY	N-CA-C	9.05	122.72	110.69
1	A	204	ARG	N-CA-C	8.96	124.56	110.32
1	A	308	LYS	N-CA-C	8.86	120.55	111.07
1	A	501	GLN	N-CA-C	-8.78	101.67	111.07
1	A	528	GLY	N-CA-C	-8.48	102.06	112.33
1	A	498	LYS	CB-CA-C	-8.36	95.77	109.56
1	A	194	ASP	N-CA-C	-8.34	99.85	110.19
1	A	204	ARG	CB-CA-C	-8.26	95.38	109.51
1	A	79	PHE	N-CA-C	-8.26	97.56	110.36
1	A	79	PHE	CA-C-N	-8.03	111.30	122.87
1	A	79	PHE	C-N-CA	-8.03	111.30	122.87
1	A	301	TRP	N-CA-C	7.95	119.94	111.28
1	A	494	ALA	N-CA-C	7.77	119.53	111.14
1	A	287	ASP	N-CA-C	7.68	122.28	111.52
1	A	523	TYR	N-CA-C	-7.61	104.41	112.93
1	A	258	GLN	CA-C-N	7.43	127.79	119.32
1	A	258	GLN	C-N-CA	7.43	127.79	119.32
1	A	526	PHE	N-CA-C	-7.41	95.01	110.80
1	A	304	ILE	CB-CA-C	-7.16	102.54	111.92
1	A	337	THR	N-CA-C	-7.04	104.43	113.16
1	A	592	ASN	N-CA-C	-7.02	99.82	110.14
1	A	308	LYS	CB-CA-C	-6.81	100.19	110.88
1	A	129	GLY	N-CA-C	-6.73	103.54	112.82
1	A	393	ILE	CB-CA-C	-6.70	101.25	112.16
1	A	400	VAL	CB-CA-C	-6.60	103.38	112.02
1	A	614	LEU	N-CA-C	6.58	120.04	109.83
1	A	494	ALA	CB-CA-C	-6.51	100.61	110.90
1	A	525	LYS	N-CA-C	-6.51	96.93	110.80
1	A	62	SER	N-CA-C	6.47	119.24	109.41
1	A	532	LEU	CB-CA-C	-6.31	98.98	111.60
1	A	342	HIS	N-CA-C	-6.29	105.92	113.97
1	A	422	ALA	N-CA-C	-6.27	105.50	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	378	ASN	N-CA-C	-6.26	101.03	110.24
1	A	276	SER	CB-CA-C	6.17	122.08	109.67
1	A	194	ASP	CB-CA-C	-6.11	97.67	111.30
1	A	400	VAL	N-CA-C	6.10	116.26	110.53
1	A	378	ASN	CB-CA-C	6.09	118.98	109.84
1	A	392	LEU	N-CA-C	-6.09	104.72	111.36
1	A	530	PHE	N-CA-CB	-6.09	101.58	110.53
1	A	40	THR	N-CA-C	5.86	118.90	111.69
1	A	659	ILE	O-C-N	5.83	129.25	123.18
1	A	256	VAL	N-CA-C	5.82	116.55	110.62
1	A	452	LEU	CB-CA-C	-5.82	102.09	112.27
1	A	266	ILE	CB-CA-C	-5.79	104.56	111.97
1	A	191	THR	N-CA-C	5.65	119.45	110.70
1	A	336	LEU	CB-CA-C	-5.52	101.97	110.81
1	A	166	GLN	CA-C-N	5.52	127.23	120.22
1	A	166	GLN	C-N-CA	5.52	127.23	120.22
1	A	565	GLU	N-CA-C	5.44	117.07	111.03
1	A	651	GLU	CB-CA-C	5.41	121.19	110.42
1	A	535	SER	N-CA-C	-5.41	99.29	110.80
1	A	201	ILE	CB-CA-C	5.38	118.66	111.19
1	A	637	ARG	N-CA-C	5.36	122.21	110.80
1	A	249	PHE	N-CA-C	5.28	117.85	109.50
1	A	453	GLN	N-CA-C	-5.28	104.61	111.74
1	A	453	GLN	N-CA-CB	5.26	120.08	112.13
1	A	301	TRP	CB-CA-C	-5.24	102.08	110.79
1	A	527	GLY	N-CA-C	-5.21	98.20	113.30
1	A	157	ILE	N-CA-C	5.17	117.05	108.99
1	A	230	LEU	N-CA-C	5.17	118.49	110.17
1	A	495	SER	N-CA-C	-5.14	105.86	111.82
1	A	618	LYS	N-CA-C	5.12	115.05	108.34
1	A	312	LEU	C-N-CD	-5.11	104.07	125.00
1	A	591	LEU	N-CA-C	5.09	118.92	111.34
1	A	443	VAL	N-CA-C	-5.09	105.64	110.42
1	A	503	GLU	N-CA-C	-5.04	105.68	111.07
1	A	341	HIS	N-CA-CB	-5.03	103.94	110.88
1	A	616	PHE	N-CA-CB	-5.02	102.69	110.98
1	A	284	TYR	N-CA-C	-5.01	105.91	112.23

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	195	HIS	Peptide

5.2 Too-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 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	5303	0	5245	348	1
2	A	1	0	0	0	0
3	A	5	0	0	1	0
4	A	28	0	12	3	0
5	A	115	0	0	10	0
All	All	5452	0	5257	348	1

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 33.

All (348) 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)
1:A:193:ASN:HD21	1:A:287:ASP:CB	1.14	1.59
1:A:590:TYR:C	1:A:591:LEU:HD23	1.43	1.43
1:A:193:ASN:ND2	1:A:287:ASP:HB2	1.08	1.40
1:A:193:ASN:ND2	1:A:287:ASP:CB	1.73	1.33
1:A:311:ASP:O	1:A:312:LEU:HD23	1.41	1.20
1:A:192:HIS:HB2	1:A:194:ASP:N	1.55	1.17
1:A:590:TYR:C	1:A:591:LEU:CD2	2.19	1.14
1:A:192:HIS:HB2	1:A:193:ASN:C	1.73	1.13
1:A:526:PHE:HD2	1:A:546:PHE:CE1	1.68	1.11
1:A:522:VAL:CG1	1:A:522:VAL:O	1.91	1.11
1:A:533:GLY:C	1:A:534:THR:HG23	1.74	1.08
1:A:193:ASN:O	1:A:286:HIS:HD2	1.36	1.08
1:A:522:VAL:O	1:A:522:VAL:HG12	1.28	1.08
1:A:188:LYS:O	1:A:190:GLU:CG	2.00	1.07
1:A:424:LYS:H	1:A:424:LYS:HD2	0.91	1.07
1:A:591:LEU:HD23	1:A:591:LEU:N	1.61	1.06
1:A:424:LYS:H	1:A:424:LYS:CD	1.51	1.06
1:A:424:LYS:HD2	1:A:424:LYS:N	1.71	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:533:GLY:O	1:A:534:THR:HG23	1.58	1.04
1:A:188:LYS:HD3	1:A:189:LEU:N	1.73	1.03
1:A:524:GLU:C	1:A:526:PHE:H	1.50	1.02
1:A:525:LYS:O	1:A:528:GLY:N	1.92	1.01
1:A:652:ASP:O	1:A:653:HIS:C	2.04	1.01
1:A:418:LYS:O	1:A:421:VAL:HG12	1.61	1.00
1:A:188:LYS:O	1:A:190:GLU:HG3	1.14	0.99
1:A:154:ILE:HD13	1:A:202:VAL:HG13	1.44	0.98
1:A:63:VAL:O	1:A:124:VAL:CG1	2.12	0.98
1:A:193:ASN:ND2	1:A:287:ASP:HB3	1.78	0.97
1:A:524:GLU:O	1:A:526:PHE:N	1.98	0.96
1:A:545:LYS:HG2	1:A:640:PHE:HD2	1.31	0.96
1:A:190:GLU:O	1:A:192:HIS:CD2	2.19	0.95
1:A:535:SER:HB3	1:A:538:GLN:HB2	1.45	0.95
1:A:450:MET:O	1:A:450:MET:HG3	1.62	0.94
1:A:188:LYS:CD	1:A:189:LEU:N	2.30	0.94
1:A:530:PHE:N	1:A:530:PHE:CD2	2.35	0.94
1:A:590:TYR:O	1:A:591:LEU:CD2	2.15	0.93
1:A:187:SER:O	1:A:188:LYS:HB2	1.68	0.93
1:A:524:GLU:C	1:A:526:PHE:N	2.19	0.91
1:A:526:PHE:CD2	1:A:546:PHE:CD1	2.49	0.91
1:A:154:ILE:HD13	1:A:202:VAL:CG1	2.00	0.91
1:A:188:LYS:HD3	1:A:188:LYS:C	1.94	0.90
1:A:192:HIS:CD2	1:A:192:HIS:H	1.88	0.90
1:A:526:PHE:CD2	1:A:546:PHE:CZ	2.56	0.90
1:A:526:PHE:CD2	1:A:546:PHE:CE1	2.59	0.89
1:A:572:GLN:HA	1:A:575:PHE:HB3	1.56	0.88
1:A:526:PHE:HD2	1:A:546:PHE:CZ	1.81	0.87
1:A:533:GLY:C	1:A:534:THR:CG2	2.47	0.86
1:A:535:SER:O	1:A:538:GLN:N	2.08	0.86
1:A:525:LYS:O	1:A:527:GLY:CA	2.24	0.85
1:A:525:LYS:O	1:A:527:GLY:C	2.20	0.84
1:A:530:PHE:H	1:A:530:PHE:HD2	1.24	0.84
1:A:193:ASN:O	1:A:286:HIS:CD2	2.27	0.84
1:A:590:TYR:O	1:A:591:LEU:HD22	1.76	0.84
1:A:520:LYS:HA	1:A:523:TYR:HB3	1.58	0.83
1:A:188:LYS:N	1:A:190:GLU:OE1	2.12	0.83
1:A:193:ASN:HD22	1:A:287:ASP:CB	1.90	0.83
1:A:526:PHE:HD2	1:A:546:PHE:CD1	1.87	0.82
1:A:529:ASP:OD1	1:A:529:ASP:C	2.20	0.82
1:A:192:HIS:CB	1:A:193:ASN:C	2.51	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:499:SER:O	1:A:503:GLU:HG2	1.81	0.81
1:A:314:THR:OG1	1:A:316:GLN:N	2.12	0.81
1:A:533:GLY:O	1:A:534:THR:CG2	2.30	0.80
1:A:155:ILE:O	1:A:201:ILE:HD12	1.81	0.79
1:A:300:CYS:O	1:A:304:ILE:HG12	1.82	0.79
1:A:582:ASP:HA	1:A:588:LYS:HG3	1.65	0.79
1:A:274:VAL:HG12	1:A:275:VAL:HG23	1.65	0.78
1:A:189:LEU:O	1:A:189:LEU:CD2	2.30	0.78
1:A:534:THR:O	1:A:535:SER:HB2	1.81	0.78
1:A:193:ASN:HD21	1:A:287:ASP:CG	1.91	0.78
1:A:619:LEU:HD23	1:A:625:ILE:HG12	1.65	0.77
1:A:63:VAL:HG23	1:A:154:ILE:HG13	1.66	0.77
1:A:235:GLU:HG2	1:A:236:LEU:HG	1.66	0.77
1:A:193:ASN:HD22	1:A:287:ASP:HB3	1.47	0.76
1:A:516:LEU:HA	1:A:519:PHE:HB3	1.65	0.76
1:A:78:LEU:HD22	1:A:269:LEU:HD23	1.68	0.76
1:A:95:THR:N	3:A:702:ALF:F4	2.07	0.76
1:A:144:LEU:HD23	1:A:304:ILE:HD12	1.66	0.76
1:A:421:VAL:CG1	1:A:422:ALA:N	2.48	0.75
1:A:68:SER:HB3	1:A:86:MET:HE1	1.68	0.75
1:A:193:ASN:CG	1:A:287:ASP:HB2	2.10	0.74
1:A:449:LEU:HB2	5:A:803:HOH:O	1.85	0.74
1:A:194:ASP:OD2	1:A:195:HIS:C	2.29	0.74
1:A:154:ILE:CD1	1:A:202:VAL:HG13	2.17	0.73
1:A:63:VAL:O	1:A:124:VAL:HG13	1.86	0.73
1:A:189:LEU:O	1:A:189:LEU:HD22	1.89	0.72
1:A:476:GLN:HA	1:A:476:GLN:HE21	1.54	0.72
1:A:154:ILE:HD11	1:A:156:ASN:HB2	1.71	0.71
1:A:38:PHE:HB2	1:A:301:TRP:CD1	2.26	0.71
1:A:154:ILE:HA	1:A:200:LEU:O	1.90	0.71
1:A:135:ASP:OD1	1:A:135:ASP:O	2.07	0.71
1:A:233:PRO:HG2	1:A:236:LEU:HD12	1.73	0.71
1:A:55:GLY:O	1:A:289:PRO:HA	1.90	0.71
1:A:188:LYS:C	1:A:190:GLU:HG3	2.11	0.71
1:A:507:PRO:HB3	1:A:610:VAL:HG23	1.71	0.70
1:A:563:SER:O	1:A:567:LEU:HB2	1.91	0.70
1:A:190:GLU:O	1:A:192:HIS:HD2	1.74	0.70
1:A:315:GLN:O	1:A:319:VAL:HG23	1.91	0.69
1:A:311:ASP:C	1:A:312:LEU:HD23	2.17	0.69
1:A:422:ALA:O	1:A:423:LEU:HD12	1.92	0.69
1:A:523:TYR:O	1:A:523:TYR:CD1	2.46	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:PHE:HB3	1:A:103:SER:HB2	1.75	0.68
1:A:589:LEU:HD23	1:A:591:LEU:HD21	1.75	0.68
1:A:525:LYS:O	1:A:527:GLY:N	2.27	0.68
1:A:63:VAL:HG23	1:A:154:ILE:CG1	2.24	0.68
1:A:534:THR:O	1:A:535:SER:CB	2.41	0.67
1:A:631:ILE:HG22	1:A:632:PHE:H	1.57	0.67
1:A:38:PHE:HB2	1:A:301:TRP:HD1	1.59	0.67
1:A:108:THR:HB	1:A:271:ASP:OD1	1.95	0.67
1:A:525:LYS:O	1:A:526:PHE:C	2.37	0.67
1:A:499:SER:O	1:A:503:GLU:CG	2.42	0.67
1:A:157:ILE:HG12	1:A:201:ILE:HD11	1.75	0.66
1:A:535:SER:O	1:A:536:SER:C	2.36	0.66
1:A:188:LYS:CD	1:A:189:LEU:H	2.08	0.66
1:A:421:VAL:HG13	1:A:422:ALA:N	2.08	0.66
1:A:193:ASN:HD21	1:A:287:ASP:HB2	0.49	0.65
1:A:626:VAL:HG12	1:A:627:PRO:HD2	1.78	0.65
1:A:662:GLN:N	1:A:662:GLN:OE1	2.29	0.65
1:A:388:LYS:O	1:A:392:LEU:HD12	1.95	0.65
1:A:189:LEU:O	1:A:189:LEU:HD23	1.95	0.65
1:A:192:HIS:CB	1:A:194:ASP:N	2.49	0.65
1:A:192:HIS:C	1:A:194:ASP:H	2.02	0.65
1:A:193:ASN:O	1:A:286:HIS:HA	1.97	0.65
1:A:545:LYS:HG2	1:A:640:PHE:CD2	2.23	0.65
1:A:192:HIS:HB2	1:A:194:ASP:CA	2.26	0.65
1:A:194:ASP:OD2	1:A:196:LYS:N	2.30	0.65
1:A:311:ASP:O	1:A:312:LEU:CD2	2.33	0.64
1:A:377:TYR:N	1:A:377:TYR:CD1	2.62	0.64
1:A:68:SER:CB	1:A:86:MET:HE1	2.28	0.64
1:A:68:SER:HB3	1:A:86:MET:CE	2.28	0.64
1:A:376:ARG:HB2	1:A:377:TYR:CD1	2.33	0.63
1:A:535:SER:HB3	1:A:538:GLN:CB	2.26	0.63
1:A:156:ASN:HD21	1:A:204:ARG:HH11	1.45	0.63
1:A:193:ASN:OD1	1:A:285:HIS:O	2.16	0.63
1:A:227:TRP:O	1:A:230:LEU:HD12	1.99	0.63
1:A:551:TRP:CE3	1:A:627:PRO:HA	2.34	0.63
1:A:56:ASN:ND2	1:A:287:ASP:OD1	2.28	0.62
1:A:551:TRP:CZ3	1:A:627:PRO:HA	2.33	0.62
1:A:377:TYR:HD1	1:A:377:TYR:H	1.47	0.62
1:A:165:TYR:O	1:A:170:MET:HB2	2.00	0.62
1:A:449:LEU:N	5:A:803:HOH:O	2.32	0.62
1:A:529:ASP:OD1	1:A:529:ASP:O	2.16	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:LEU:HD23	1:A:304:ILE:HG23	1.82	0.62
1:A:534:THR:OG1	1:A:535:SER:N	2.29	0.62
1:A:428:PHE:HB3	1:A:532:LEU:HA	1.82	0.62
1:A:660:THR:OG1	1:A:661:GLU:N	2.30	0.61
1:A:533:GLY:O	1:A:534:THR:CB	2.46	0.61
1:A:562:ILE:HG23	1:A:567:LEU:HD13	1.80	0.61
1:A:438:LYS:O	1:A:442:ASP:HB2	2.01	0.61
1:A:554:PHE:O	1:A:558:THR:HG23	2.01	0.61
1:A:507:PRO:HB3	1:A:610:VAL:CG2	2.31	0.60
1:A:619:LEU:HD23	1:A:625:ILE:CG1	2.30	0.60
1:A:588:LYS:HE2	1:A:599:THR:HG21	1.84	0.60
1:A:144:LEU:CD2	1:A:304:ILE:HD12	2.30	0.60
1:A:192:HIS:C	1:A:194:ASP:N	2.60	0.60
1:A:27:ASP:HB2	5:A:859:HOH:O	2.02	0.59
1:A:671:PHE:O	1:A:675:VAL:HB	2.02	0.59
1:A:157:ILE:CD1	1:A:201:ILE:HD11	2.32	0.59
1:A:547:LYS:O	1:A:551:TRP:HD1	1.85	0.59
1:A:428:PHE:HE2	1:A:477:GLN:HG2	1.68	0.59
1:A:476:GLN:HA	1:A:476:GLN:NE2	2.17	0.59
1:A:450:MET:O	1:A:450:MET:CG	2.39	0.59
1:A:473:VAL:O	1:A:477:GLN:HG3	2.03	0.58
1:A:571:LEU:HB2	1:A:572:GLN:OE1	2.02	0.58
1:A:147:LEU:HD11	1:A:245:PHE:CE1	2.38	0.58
1:A:619:LEU:HD21	1:A:623:SER:O	2.02	0.58
1:A:314:THR:HG23	1:A:317:ILE:HG12	1.84	0.58
1:A:673:LYS:HB2	5:A:813:HOH:O	2.03	0.58
1:A:250:HIS:CD2	1:A:269:LEU:HB2	2.39	0.58
1:A:339:TYR:C	1:A:341:HIS:H	2.10	0.58
1:A:619:LEU:HD12	1:A:621:ASP:HB2	1.86	0.58
1:A:574:ARG:HH22	1:A:609:GLN:HG3	1.69	0.58
1:A:673:LYS:CB	5:A:813:HOH:O	2.52	0.57
1:A:403:VAL:HG12	1:A:404:HIS:N	2.19	0.57
1:A:68:SER:CB	1:A:86:MET:CE	2.83	0.57
1:A:326:GLU:HG2	1:A:327:ILE:N	2.19	0.57
1:A:652:ASP:O	1:A:654:CYS:N	2.38	0.57
1:A:253:ASN:OD1	1:A:261:GLU:HB3	2.05	0.57
1:A:67:GLN:OE1	1:A:129:GLY:HA3	2.04	0.56
1:A:424:LYS:CD	1:A:424:LYS:N	2.32	0.56
1:A:157:ILE:CG1	1:A:201:ILE:HD11	2.35	0.56
1:A:391:TRP:HA	1:A:394:ASN:HB2	1.87	0.56
1:A:377:TYR:N	1:A:377:TYR:HD1	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:LYS:HD2	1:A:189:LEU:N	2.19	0.55
1:A:498:LYS:HG2	1:A:499:SER:N	2.10	0.55
1:A:603:ALA:O	1:A:607:ALA:N	2.40	0.55
1:A:127:THR:O	1:A:128:ASP:HB3	2.05	0.54
1:A:154:ILE:HD12	1:A:154:ILE:C	2.33	0.54
1:A:216:ALA:O	1:A:220:THR:HG23	2.07	0.54
1:A:127:THR:O	1:A:128:ASP:CB	2.55	0.54
1:A:177:PHE:O	1:A:180:ASN:HB3	2.08	0.54
1:A:592:ASN:HB3	1:A:594:GLN:HB2	1.90	0.54
1:A:676:ASP:C	1:A:678:LYS:H	2.14	0.54
1:A:155:ILE:HG22	1:A:201:ILE:HD13	1.90	0.54
1:A:161:GLN:HA	1:A:164:LEU:HD22	1.89	0.54
1:A:314:THR:OG1	1:A:315:GLN:N	2.36	0.54
1:A:29:ILE:HD12	1:A:29:ILE:H	1.72	0.54
1:A:265:GLY:HA2	1:A:268:ARG:NH1	2.24	0.53
1:A:526:PHE:C	1:A:526:PHE:HD1	2.17	0.53
1:A:536:SER:HA	1:A:539:ASN:HB2	1.91	0.53
1:A:593:GLU:HA	1:A:596:LEU:HB3	1.90	0.53
1:A:492:LEU:O	1:A:496:LEU:HB2	2.09	0.53
1:A:140:ARG:HA	1:A:172:LEU:HD11	1.90	0.53
1:A:68:SER:OG	1:A:86:MET:CE	2.57	0.52
1:A:602:VAL:O	1:A:606:HIS:HB2	2.09	0.52
1:A:508:ASN:H	1:A:511:THR:HG23	1.73	0.52
1:A:524:GLU:O	1:A:525:LYS:C	2.51	0.52
1:A:205:ASP:OD2	4:A:703:GDP:N2	2.35	0.52
1:A:212:VAL:CG2	1:A:251:ALA:HB2	2.39	0.52
1:A:192:HIS:CD2	1:A:192:HIS:N	2.67	0.52
1:A:507:PRO:CB	1:A:610:VAL:HG23	2.40	0.52
1:A:528:GLY:C	1:A:529:ASP:O	2.49	0.52
1:A:296:TYR:O	1:A:300:CYS:SG	2.68	0.51
1:A:619:LEU:CD1	1:A:621:ASP:HB2	2.39	0.51
1:A:343:PHE:O	1:A:344:LYS:C	2.51	0.51
1:A:543:ILE:HG22	1:A:547:LYS:HG3	1.93	0.51
1:A:505:GLY:O	1:A:506:ASP:HB2	2.10	0.51
1:A:139:GLU:OE2	1:A:172:LEU:HD22	2.11	0.50
1:A:449:LEU:CA	5:A:803:HOH:O	2.59	0.50
1:A:535:SER:O	1:A:537:THR:N	2.44	0.50
1:A:611:LEU:HB2	1:A:612:PRO:HD3	1.92	0.50
1:A:250:HIS:NE2	1:A:269:LEU:HB2	2.27	0.50
1:A:533:GLY:O	1:A:534:THR:OG1	2.29	0.50
1:A:225:ASN:O	1:A:226:MET:C	2.53	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:ASP:HB3	1:A:354:GLU:HB2	1.93	0.50
1:A:377:TYR:O	1:A:378:ASN:C	2.52	0.50
1:A:589:LEU:HD23	1:A:591:LEU:CD2	2.41	0.50
1:A:113:THR:HG22	1:A:114:THR:O	2.12	0.49
1:A:351:ASP:HB3	1:A:354:GLU:CD	2.37	0.49
1:A:522:VAL:C	1:A:524:GLU:H	2.18	0.49
1:A:670:LYS:NZ	5:A:802:HOH:O	2.32	0.49
1:A:161:GLN:NE2	1:A:167:GLY:O	2.27	0.49
1:A:339:TYR:C	1:A:341:HIS:N	2.71	0.49
1:A:489:VAL:HG12	1:A:489:VAL:O	2.11	0.49
1:A:526:PHE:C	1:A:526:PHE:CD1	2.91	0.49
1:A:193:ASN:ND2	1:A:287:ASP:CG	2.62	0.49
1:A:519:PHE:O	1:A:523:TYR:HB2	2.13	0.49
1:A:342:HIS:HD2	1:A:358:LEU:HD11	1.77	0.49
1:A:575:PHE:HE1	1:A:675:VAL:HG13	1.78	0.49
1:A:619:LEU:C	1:A:621:ASP:H	2.21	0.49
1:A:59:HIS:HD2	1:A:151:GLU:OE2	1.96	0.48
1:A:376:ARG:HB2	1:A:377:TYR:CE1	2.48	0.48
1:A:212:VAL:HG22	1:A:251:ALA:HB2	1.95	0.48
1:A:525:LYS:O	1:A:527:GLY:HA2	2.07	0.48
1:A:50:SER:OG	1:A:118:ASN:ND2	2.47	0.48
1:A:29:ILE:HD12	1:A:29:ILE:N	2.29	0.48
1:A:575:PHE:CE1	1:A:675:VAL:HG13	2.49	0.48
1:A:317:ILE:O	1:A:318:LEU:C	2.56	0.48
1:A:659:ILE:HG13	1:A:663:GLU:HB2	1.96	0.48
1:A:63:VAL:O	1:A:124:VAL:HG11	2.08	0.47
1:A:136:GLN:O	1:A:140:ARG:HG3	2.13	0.47
1:A:141:LYS:HG2	1:A:304:ILE:HG22	1.97	0.47
1:A:601:ALA:HA	1:A:604:LYS:HG3	1.95	0.47
1:A:404:HIS:O	1:A:405:ALA:C	2.55	0.47
1:A:99:TRP:O	1:A:122:MET:HA	2.15	0.47
1:A:283:GLU:H	1:A:283:GLU:CD	2.21	0.47
1:A:332:PHE:O	1:A:335:PHE:N	2.45	0.47
1:A:100:LEU:HD12	1:A:122:MET:HG3	1.97	0.47
1:A:157:ILE:HD11	1:A:201:ILE:HD11	1.97	0.47
1:A:522:VAL:O	1:A:522:VAL:HG13	2.05	0.47
1:A:101:ALA:O	1:A:121:VAL:HG13	2.15	0.46
1:A:205:ASP:CG	4:A:703:GDP:HN1	2.20	0.46
1:A:619:LEU:CD2	1:A:625:ILE:HG12	2.40	0.46
1:A:61:ILE:HG23	1:A:61:ILE:O	2.15	0.46
1:A:428:PHE:CB	1:A:532:LEU:HA	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:LEU:HD11	1:A:245:PHE:HE1	1.80	0.46
1:A:422:ALA:C	1:A:423:LEU:HD12	2.39	0.46
1:A:550:SER:C	1:A:552:CYS:H	2.23	0.46
1:A:325:ASP:O	1:A:326:GLU:C	2.58	0.46
1:A:450:MET:N	5:A:803:HOH:O	2.48	0.46
1:A:379:LYS:O	1:A:383:GLU:N	2.45	0.46
1:A:136:GLN:O	1:A:137:ASP:C	2.59	0.46
1:A:293:TRP:O	1:A:294:THR:C	2.59	0.45
1:A:335:PHE:CZ	1:A:393:ILE:HG23	2.52	0.45
1:A:546:PHE:CD1	1:A:546:PHE:C	2.94	0.45
1:A:428:PHE:CE2	1:A:477:GLN:HG2	2.48	0.45
1:A:174:LYS:HD2	1:A:229:SER:OG	2.17	0.45
1:A:652:ASP:O	1:A:653:HIS:O	2.33	0.45
1:A:34:GLU:HG3	1:A:96:LYS:HB3	1.98	0.45
1:A:62:SER:HB3	1:A:122:MET:HB2	1.99	0.44
1:A:379:LYS:HB3	1:A:379:LYS:HE2	1.73	0.44
1:A:582:ASP:CA	1:A:588:LYS:HG3	2.41	0.44
1:A:631:ILE:O	1:A:632:PHE:HB2	2.17	0.44
1:A:100:LEU:HD12	1:A:122:MET:CG	2.47	0.44
1:A:199:LEU:HB2	1:A:247:VAL:HG12	1.99	0.44
1:A:43:LEU:HG	1:A:294:THR:HG21	2.00	0.44
1:A:485:VAL:HG22	1:A:542:ALA:O	2.17	0.44
1:A:49:THR:OG1	1:A:50:SER:N	2.50	0.44
1:A:306:THR:HG23	1:A:306:THR:O	2.17	0.44
1:A:421:VAL:HG12	1:A:422:ALA:N	2.29	0.44
1:A:331:VAL:HG12	1:A:366:ALA:HB1	1.99	0.44
1:A:393:ILE:O	1:A:393:ILE:CG2	2.64	0.44
1:A:412:LEU:O	1:A:413:LEU:C	2.60	0.44
1:A:555:TYR:HH	1:A:632:PHE:HZ	1.64	0.44
1:A:143:ALA:HB3	1:A:176:VAL:HG21	2.00	0.43
1:A:312:LEU:HD23	1:A:312:LEU:HA	1.66	0.43
1:A:418:LYS:HZ2	1:A:421:VAL:HG11	1.83	0.43
1:A:327:ILE:O	1:A:328:VAL:C	2.59	0.43
1:A:331:VAL:CG1	1:A:366:ALA:HB1	2.48	0.43
1:A:138:PHE:CD1	1:A:138:PHE:C	2.97	0.43
1:A:491:LYS:HA	1:A:491:LYS:HD3	1.56	0.43
1:A:393:ILE:O	1:A:393:ILE:HG22	2.16	0.43
1:A:611:LEU:HB3	1:A:615:THR:HG23	1.99	0.43
1:A:424:LYS:HA	1:A:480:GLU:OE1	2.19	0.43
1:A:443:VAL:O	1:A:444:ASN:C	2.63	0.42
1:A:347:ASP:OD1	1:A:347:ASP:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:ASN:O	1:A:382:TYR:HB3	2.19	0.42
1:A:654:CYS:HB3	1:A:657:GLU:HB2	2.00	0.42
1:A:673:LYS:HB3	5:A:813:HOH:O	2.18	0.42
1:A:61:ILE:CD1	1:A:152:VAL:HB	2.50	0.42
1:A:63:VAL:O	1:A:124:VAL:HG12	2.11	0.42
1:A:171:GLY:O	1:A:172:LEU:C	2.61	0.42
1:A:411:THR:HG22	1:A:412:LEU:N	2.34	0.42
1:A:572:GLN:CD	1:A:572:GLN:N	2.78	0.42
1:A:61:ILE:HG23	1:A:121:VAL:HA	2.00	0.42
1:A:187:SER:O	1:A:188:LYS:CB	2.46	0.42
1:A:579:PHE:CE1	1:A:600:PHE:HA	2.54	0.42
1:A:145:PHE:O	1:A:146:ALA:C	2.62	0.42
1:A:639:GLN:HB2	1:A:640:PHE:CE1	2.55	0.42
1:A:134:GLU:HG2	1:A:314:THR:HB	2.01	0.42
1:A:31:ILE:HD11	1:A:98:ILE:HG22	2.01	0.42
1:A:69:THR:HA	1:A:158:TRP:CZ2	2.55	0.42
1:A:335:PHE:CE1	1:A:393:ILE:HG23	2.55	0.42
1:A:364:GLN:O	1:A:364:GLN:NE2	2.53	0.42
1:A:61:ILE:HD12	1:A:152:VAL:HB	2.02	0.41
1:A:652:ASP:O	1:A:652:ASP:CG	2.63	0.41
1:A:152:VAL:HG22	1:A:198:LEU:HB3	2.02	0.41
1:A:260:LYS:O	1:A:264:GLU:HG3	2.20	0.41
1:A:467:LYS:HG3	1:A:468:ASP:N	2.35	0.41
1:A:424:LYS:HG2	1:A:424:LYS:O	2.20	0.41
1:A:188:LYS:HD2	1:A:189:LEU:H	1.80	0.41
1:A:193:ASN:C	1:A:194:ASP:O	2.59	0.41
1:A:226:MET:HE2	1:A:226:MET:HB3	1.89	0.41
1:A:515:VAL:HG12	1:A:516:LEU:HD12	2.01	0.41
1:A:173:LEU:O	1:A:174:LYS:C	2.64	0.41
1:A:201:ILE:HG12	1:A:249:PHE:CE1	2.56	0.41
1:A:523:TYR:O	1:A:523:TYR:CG	2.73	0.41
1:A:246:ASP:OD2	1:A:284:TYR:OH	2.32	0.41
1:A:507:PRO:CB	1:A:610:VAL:CG2	2.98	0.41
1:A:659:ILE:O	1:A:659:ILE:HG23	2.21	0.40
1:A:155:ILE:O	1:A:201:ILE:CD1	2.61	0.40
1:A:232:LYS:HA	1:A:233:PRO:HD2	1.94	0.40
1:A:255:LYS:HD3	4:A:703:GDP:C5	2.57	0.40
1:A:290:ILE:O	1:A:294:THR:HG23	2.21	0.40
1:A:212:VAL:HG21	1:A:251:ALA:HB2	2.04	0.40
1:A:339:TYR:O	1:A:343:PHE:HB2	2.22	0.40
1:A:393:ILE:O	1:A:397:LEU:HG	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:489:VAL:O	1:A:489:VAL:CG1	2.69	0.40
1:A:579:PHE:HD2	5:A:816:HOH:O	2.04	0.40

All (1) 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)
1:A:224:GLN:OE1	1:A:453:GLN:NE2[4_555]	2.00	0.20

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	652/692 (94%)	543 (83%)	92 (14%)	17 (3%)	4	15

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	188	LYS
1	A	189	LEU
1	A	506	ASP
1	A	534	THR
1	A	535	SER
1	A	536	SER
1	A	660	THR
1	A	663	GLU
1	A	617	ALA
1	A	652	ASP
1	A	653	HIS
1	A	525	LYS
1	A	551	TRP
1	A	582	ASP

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Mol	Chain	Res	Type
1	A	507	PRO
1	A	104	PRO
1	A	403	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	588/621 (95%)	470 (80%)	118 (20%)	1 4

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	29	ILE
1	A	31	ILE
1	A	32	ILE
1	A	35	ASN
1	A	36	LYS
1	A	40	THR
1	A	43	LEU
1	A	44	ASP
1	A	74	LEU
1	A	78	LEU
1	A	89	LEU
1	A	95	THR
1	A	105	VAL
1	A	110	LEU
1	A	114	THR
1	A	117	SER
1	A	121	VAL
1	A	124	VAL
1	A	125	GLU
1	A	130	ARG
1	A	154	ILE
1	A	164	LEU

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Mol	Chain	Res	Type
1	A	173	LEU
1	A	184	PHE
1	A	186	LYS
1	A	188	LYS
1	A	189	LEU
1	A	190	GLU
1	A	192	HIS
1	A	195	HIS
1	A	197	VAL
1	A	201	ILE
1	A	202	VAL
1	A	207	VAL
1	A	209	VAL
1	A	221	LEU
1	A	229	SER
1	A	230	LEU
1	A	239	LEU
1	A	252	LEU
1	A	268	ARG
1	A	272	ARG
1	A	273	LEU
1	A	274	VAL
1	A	279	LEU
1	A	290	ILE
1	A	304	ILE
1	A	308	LYS
1	A	310	LEU
1	A	314	THR
1	A	316	GLN
1	A	318	LEU
1	A	326	GLU
1	A	339	TYR
1	A	340	GLN
1	A	344	LYS
1	A	345	GLU
1	A	347	ASP
1	A	355	LEU
1	A	362	LEU
1	A	363	ARG
1	A	377	TYR
1	A	379	LYS
1	A	392	LEU

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Mol	Chain	Res	Type
1	A	412	LEU
1	A	418	LYS
1	A	424	LYS
1	A	430	VAL
1	A	434	THR
1	A	440	VAL
1	A	442	ASP
1	A	443	VAL
1	A	450	MET
1	A	460	GLU
1	A	461	ILE
1	A	462	ILE
1	A	476	GLN
1	A	479	VAL
1	A	482	ASN
1	A	484	ILE
1	A	491	LYS
1	A	492	LEU
1	A	493	SER
1	A	497	SER
1	A	498	LYS
1	A	500	ILE
1	A	525	LYS
1	A	526	PHE
1	A	530	PHE
1	A	534	THR
1	A	535	SER
1	A	560	LYS
1	A	565	GLU
1	A	570	LEU
1	A	571	LEU
1	A	572	GLN
1	A	576	ASP
1	A	580	ARG
1	A	586	LEU
1	A	591	LEU
1	A	595	ASP
1	A	606	HIS
1	A	609	GLN
1	A	614	LEU
1	A	615	THR
1	A	619	LEU

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Mol	Chain	Res	Type
1	A	621	ASP
1	A	623	SER
1	A	626	VAL
1	A	636	LEU
1	A	640	PHE
1	A	649	ASP
1	A	651	GLU
1	A	654	CYS
1	A	664	LYS
1	A	668	LEU
1	A	670	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	59	HIS
1	A	92	GLN
1	A	118	ASN
1	A	166	GLN
1	A	169	ASN
1	A	192	HIS
1	A	193	ASN
1	A	206	HIS
1	A	238	HIS
1	A	258	GLN
1	A	286	HIS
1	A	315	GLN
1	A	316	GLN
1	A	340	GLN
1	A	444	ASN
1	A	476	GLN
1	A	482	ASN
1	A	486	ASN
1	A	501	GLN
1	A	508	ASN
1	A	541	GLN
1	A	639	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 1 is 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	703	2	29,30,30	1.93	7 (24%)	45,47,47	2.06	11 (24%)
3	ALF	A	702	-	4,4,4	1.19	0	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GDP	A	703	2	-	1/16/32/32	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	703	GDP	PA-O3A	5.66	1.65	1.59
4	A	703	GDP	C5-N7	-4.33	1.30	1.39
4	A	703	GDP	C5-C4	3.50	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	703	GDP	C6-N1	-2.72	1.33	1.38
4	A	703	GDP	C2'-C1'	-2.20	1.46	1.53
4	A	703	GDP	C8-N7	2.15	1.38	1.32
4	A	703	GDP	C1'-N9	-2.13	1.41	1.47

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	703	GDP	C5-C4-N3	-5.46	119.69	128.39
4	A	703	GDP	N9-C4-N3	5.30	136.56	125.95
4	A	703	GDP	O2A-PA-O3A	4.82	120.31	107.27
4	A	703	GDP	O5'-PA-O1A	-4.20	92.29	108.94
4	A	703	GDP	O6-C6-C5	-3.99	116.00	126.53
4	A	703	GDP	C2-N3-C4	3.36	118.09	112.30
4	A	703	GDP	O6-C6-N1	3.16	126.06	120.11
4	A	703	GDP	C2-N1-C6	-2.28	120.97	125.11
4	A	703	GDP	O3B-PB-O2B	2.21	116.08	107.80
4	A	703	GDP	O3'-C3'-C2'	-2.09	105.11	111.82
4	A	703	GDP	O3A-PB-O1B	-2.04	100.30	111.04

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	703	GDP	C3'-C4'-C5'-O5'

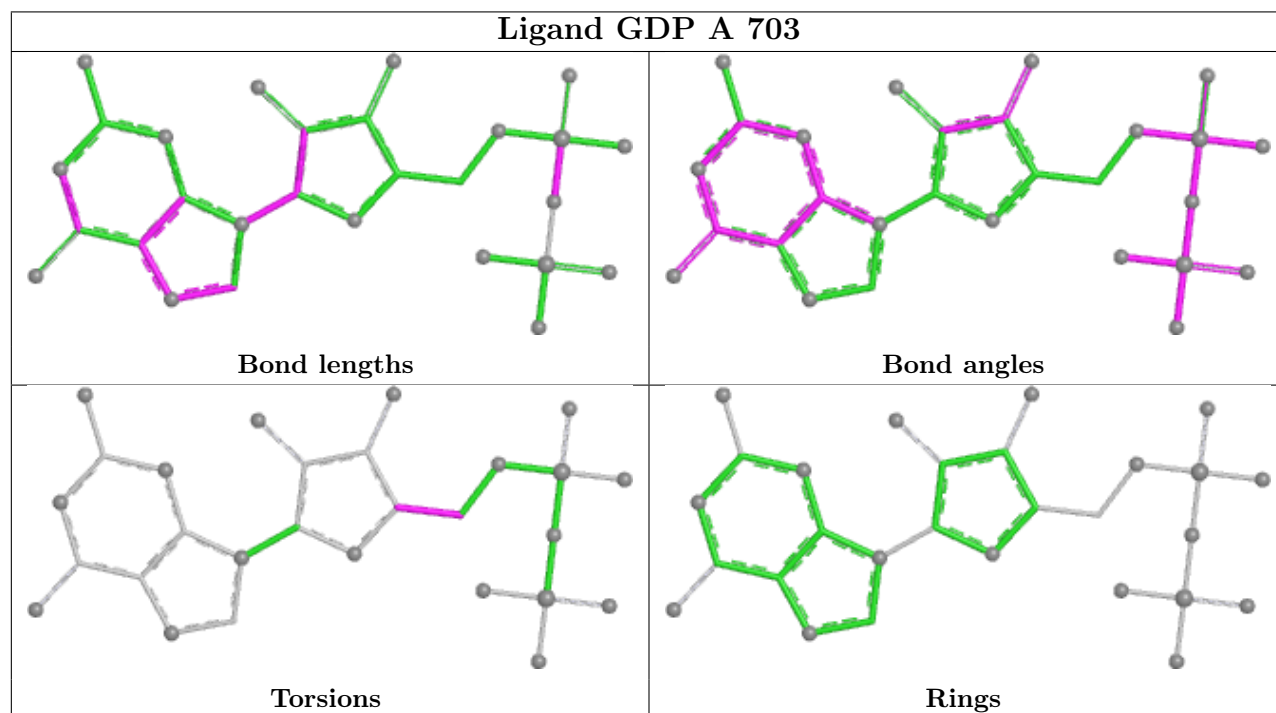
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	703	GDP	3	0
3	A	702	ALF	1	0

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	656/692 (94%)	0.49	75 (11%) 10 7	33, 77, 188, 281	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	605	GLN	5.0
1	A	551	TRP	4.9
1	A	603	ALA	4.9
1	A	614	LEU	4.8
1	A	608	LEU	4.7
1	A	680	ILE	4.4
1	A	668	LEU	4.0
1	A	527	GLY	4.0
1	A	665	LEU	4.0
1	A	667	VAL	3.7
1	A	571	LEU	3.6
1	A	500	ILE	3.6
1	A	542	ALA	3.5
1	A	423	LEU	3.5
1	A	528	GLY	3.4
1	A	659	ILE	3.3
1	A	611	LEU	3.3
1	A	515	VAL	3.3
1	A	675	VAL	3.3
1	A	615	THR	3.3
1	A	578	LYS	3.2
1	A	610	VAL	3.2
1	A	579	PHE	3.2
1	A	617	ALA	3.2
1	A	598	LYS	3.2
1	A	492	LEU	3.1
1	A	664	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	577	ASP	3.0
1	A	612	PRO	3.0
1	A	687	VAL	2.9
1	A	672	LYS	2.9
1	A	683	LYS	2.9
1	A	671	PHE	2.9
1	A	554	PHE	2.8
1	A	522	VAL	2.8
1	A	504	LEU	2.8
1	A	525	LYS	2.7
1	A	679	TYR	2.7
1	A	338	LYS	2.6
1	A	562	ILE	2.6
1	A	50	SER	2.6
1	A	669	ALA	2.6
1	A	543	ILE	2.6
1	A	530	PHE	2.6
1	A	677	ALA	2.6
1	A	567	LEU	2.6
1	A	526	PHE	2.6
1	A	596	LEU	2.6
1	A	613	ILE	2.6
1	A	599	THR	2.5
1	A	575	PHE	2.5
1	A	494	ALA	2.5
1	A	607	ALA	2.5
1	A	678	LYS	2.4
1	A	594	GLN	2.4
1	A	626	VAL	2.3
1	A	497	SER	2.3
1	A	561	LEU	2.3
1	A	602	VAL	2.3
1	A	496	LEU	2.2
1	A	620	ALA	2.2
1	A	191	THR	2.2
1	A	574	ARG	2.1
1	A	463	LEU	2.1
1	A	337	THR	2.1
1	A	499	SER	2.1
1	A	685	SER	2.1
1	A	592	ASN	2.1
1	A	533	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	143	ALA	2.1
1	A	658	ILE	2.1
1	A	600	PHE	2.0
1	A	306	THR	2.0
1	A	590	TYR	2.0
1	A	586	LEU	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](#)

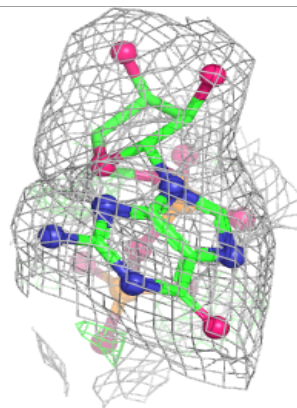
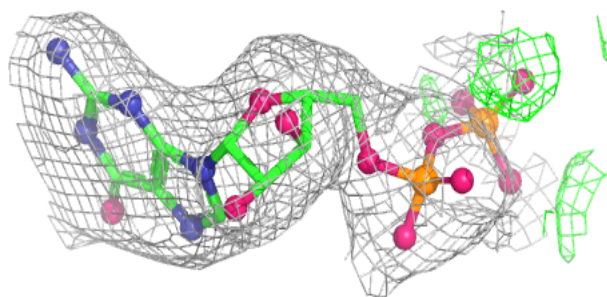
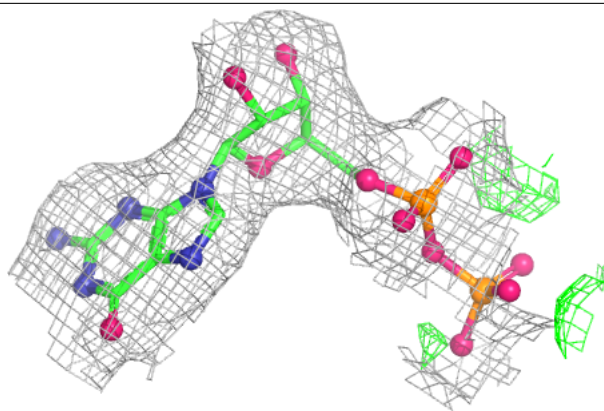
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
2	MG	A	701	1/1	0.97	0.07	30,30,30,30	0
3	ALF	A	702	5/5	0.97	0.08	31,32,40,41	0
4	GDP	A	703	28/28	0.97	0.06	22,29,38,42	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.

Electron density around GDP A 703:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.