



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:03 PM UTC

PDB ID : 4PYG / pdb_00004pyg
Title : Transglutaminase2 complexed with GTP
Authors : Park, H.H.; Jang, T.H.
Deposited on : 2014-03-27
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

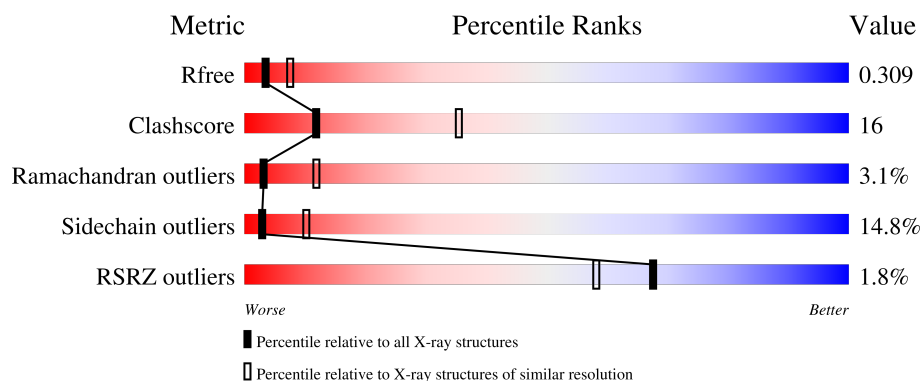
1 Overall quality at a glance

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	695	2% 64% 27% 7% .
1	B	695	2% 58% 32% 8% ..
1	E	695	2% 60% 31% 7% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16462 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-glutamine gamma-glutamyltransferase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	685	Total	C	N	O	S	0	0	0
			5419	3424	933	1032	30			
1	B	685	Total	C	N	O	S	0	0	0
			5419	3424	933	1032	30			
1	E	685	Total	C	N	O	S	0	0	0
			5419	3424	933	1032	30			

There are 24 discrepancies between the modelled and reference sequences:

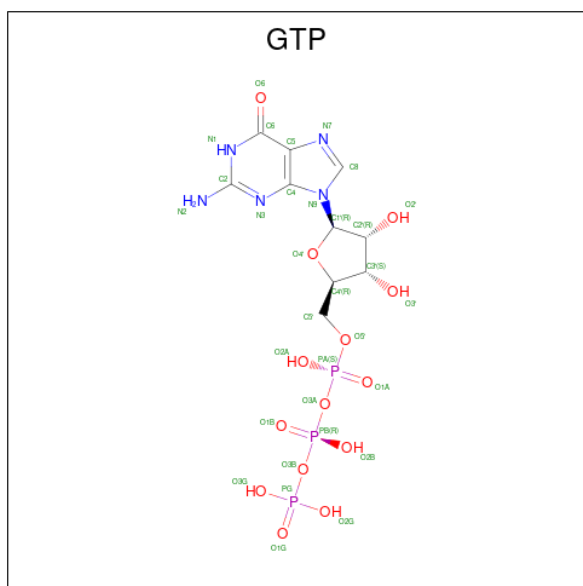
Chain	Residue	Modelled	Actual	Comment	Reference
A	688	LEU	-	expression tag	UNP P21980
A	689	GLU	-	expression tag	UNP P21980
A	690	HIS	-	expression tag	UNP P21980
A	691	HIS	-	expression tag	UNP P21980
A	692	HIS	-	expression tag	UNP P21980
A	693	HIS	-	expression tag	UNP P21980
A	694	HIS	-	expression tag	UNP P21980
A	695	HIS	-	expression tag	UNP P21980
B	688	LEU	-	expression tag	UNP P21980
B	689	GLU	-	expression tag	UNP P21980
B	690	HIS	-	expression tag	UNP P21980
B	691	HIS	-	expression tag	UNP P21980
B	692	HIS	-	expression tag	UNP P21980
B	693	HIS	-	expression tag	UNP P21980
B	694	HIS	-	expression tag	UNP P21980
B	695	HIS	-	expression tag	UNP P21980
E	688	LEU	-	expression tag	UNP P21980
E	689	GLU	-	expression tag	UNP P21980
E	690	HIS	-	expression tag	UNP P21980
E	691	HIS	-	expression tag	UNP P21980
E	692	HIS	-	expression tag	UNP P21980
E	693	HIS	-	expression tag	UNP P21980
E	694	HIS	-	expression tag	UNP P21980

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Chain	Residue	Modelled	Actual	Comment	Reference
E	695	HIS	-	expression tag	UNP P21980

- Molecule 2 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
2	B	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
2	E	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

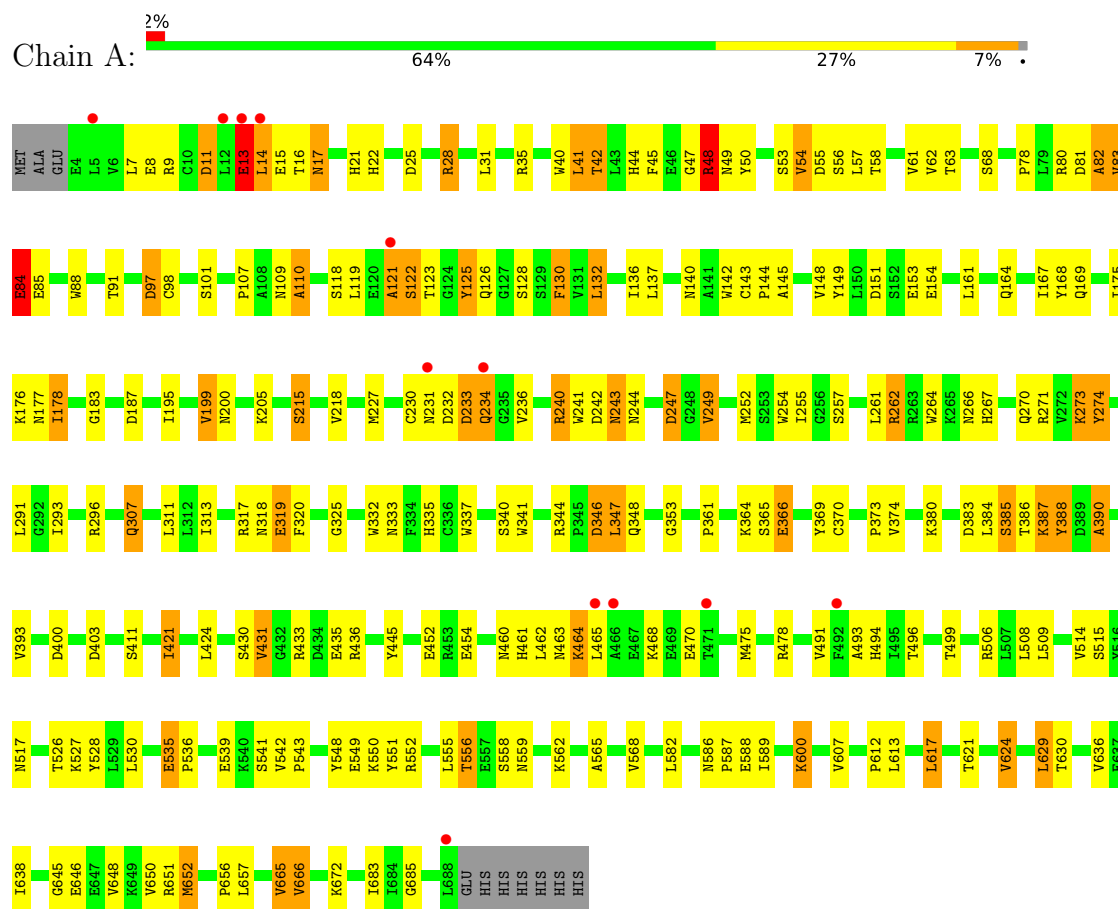
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	34	Total	O	0	0
			34	34		
3	B	42	Total	O	0	0
			42	42		
3	E	33	Total	O	0	0
			33	33		

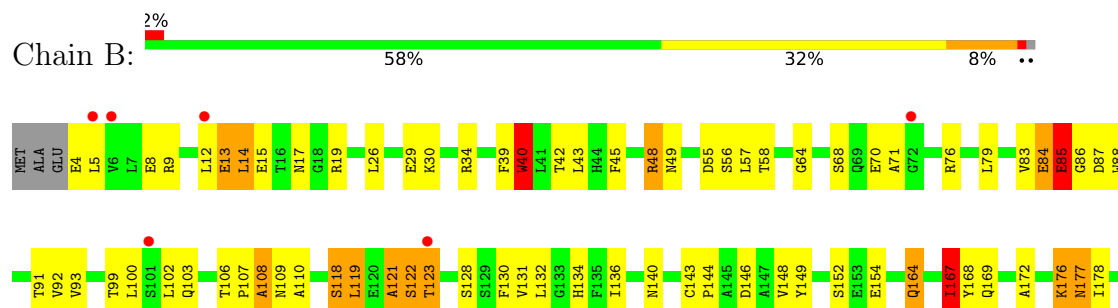
3 Residue-property plots

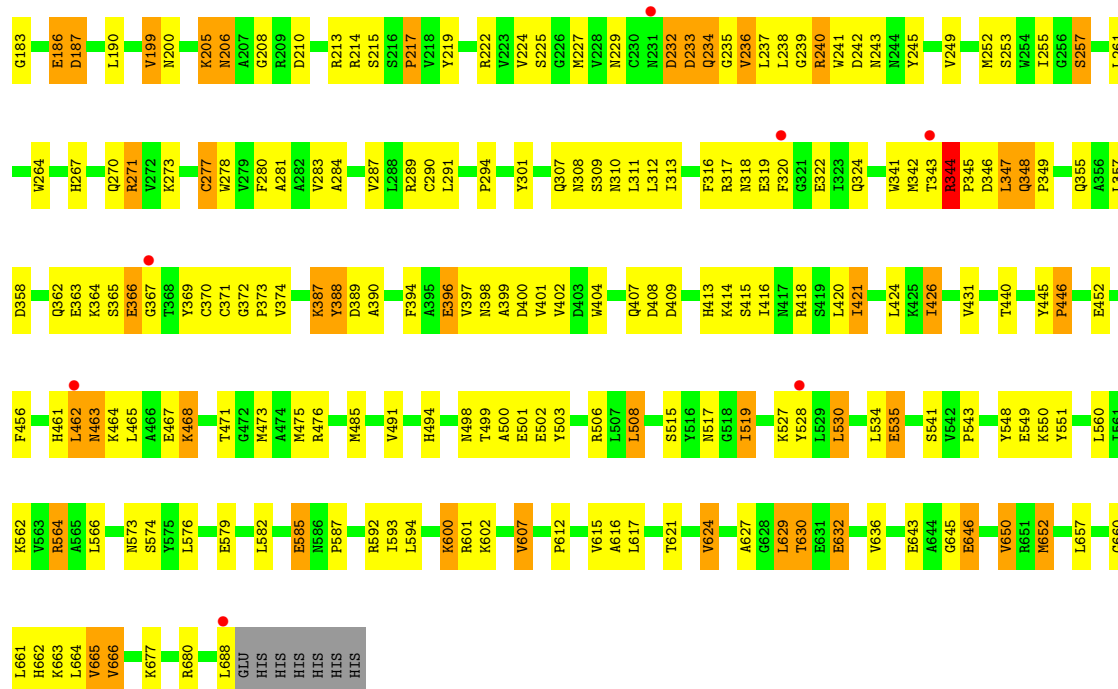
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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-glutamine gamma-glutamyltransferase 2

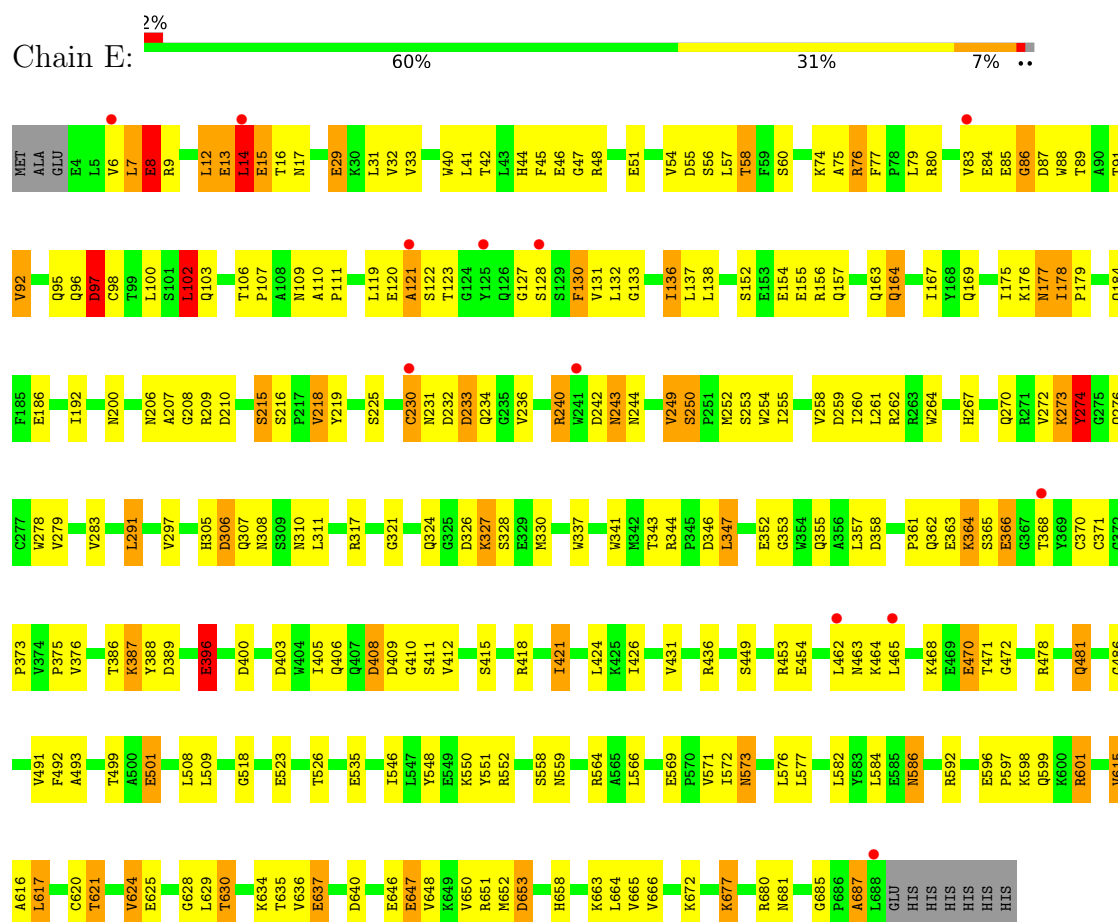


- Molecule 1: Protein-glutamine gamma-glutamyltransferase 2





• Molecule 1: Protein-glutamine gamma-glutamyltransferase 2



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	133.55Å 216.22Å 165.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.92 – 2.80 39.92 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.5 (39.92-2.80) 99.4 (39.92-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.88 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.236 , 0.319 0.230 , 0.309	Depositor DCC
R_{free} test set	2961 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	71.1	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 30.4	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	0.93	EDS
Total number of atoms	16462	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% 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: GTP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.83	0/5537	1.09	16/7515 (0.2%)
1	B	0.79	0/5537	1.07	14/7515 (0.2%)
1	E	0.80	0/5537	1.09	28/7515 (0.4%)
All	All	0.81	0/16611	1.08	58/22545 (0.3%)

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	2
1	B	0	1
1	E	0	2
All	All	0	5

There are no bond length outliers.

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	29	GLU	N-CA-C	-8.18	103.90	114.04
1	A	13	GLU	N-CA-C	-7.63	104.47	114.31
1	E	178	ILE	CA-C-N	7.61	129.35	119.84
1	E	178	ILE	C-N-CA	7.61	129.35	119.84
1	A	130	PHE	N-CA-C	7.32	118.19	107.88
1	B	646	GLU	N-CA-C	7.32	119.26	110.19
1	A	390	ALA	CA-C-N	-7.28	112.14	119.56
1	A	390	ALA	C-N-CA	-7.28	112.14	119.56
1	B	666	VAL	N-CA-C	7.02	118.23	108.12
1	E	324	GLN	N-CA-C	6.96	120.26	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	348	GLN	CA-C-N	-6.77	113.71	120.21
1	A	348	GLN	C-N-CA	-6.77	113.71	120.21
1	E	685	GLY	CA-C-N	6.74	128.27	119.84
1	E	685	GLY	C-N-CA	6.74	128.27	119.84
1	B	390	ALA	CA-C-N	-6.66	112.84	119.56
1	B	390	ALA	C-N-CA	-6.66	112.84	119.56
1	E	687	ALA	N-CA-C	6.64	121.72	111.56
1	A	685	GLY	CA-C-N	6.51	126.27	119.76
1	A	685	GLY	C-N-CA	6.51	126.27	119.76
1	B	224	VAL	N-CA-C	6.35	117.09	110.62
1	E	250	SER	CA-C-N	6.24	125.73	119.24
1	E	250	SER	C-N-CA	6.24	125.73	119.24
1	B	348	GLN	CA-C-N	6.22	127.61	119.84
1	B	348	GLN	C-N-CA	6.22	127.61	119.84
1	B	167	ILE	CB-CA-C	-6.16	102.02	110.77
1	E	14	LEU	N-CA-C	6.11	123.81	110.80
1	B	344	ARG	CA-C-N	6.01	127.36	119.84
1	B	344	ARG	C-N-CA	6.01	127.36	119.84
1	E	86	GLY	N-CA-C	-5.92	107.25	113.58
1	A	48	ARG	N-CA-C	5.86	118.32	110.35
1	A	215	SER	N-CA-C	-5.86	106.30	113.50
1	E	77	PHE	CA-C-N	5.86	127.16	119.84
1	E	77	PHE	C-N-CA	5.86	127.16	119.84
1	E	8	GLU	N-CA-C	5.74	118.75	109.40
1	A	110	ALA	CA-C-N	-5.66	114.43	120.03
1	A	110	ALA	C-N-CA	-5.66	114.43	120.03
1	E	15	GLU	CA-C-N	5.66	129.30	120.82
1	E	15	GLU	C-N-CA	5.66	129.30	120.82
1	B	177	ASN	N-CA-C	5.65	117.51	108.41
1	E	102	LEU	N-CA-C	5.62	118.76	109.94
1	E	156	ARG	N-CA-C	-5.59	104.57	111.40
1	E	178	ILE	CB-CA-C	5.54	117.22	110.85
1	E	449	SER	N-CA-C	5.44	117.31	110.24
1	E	586	ASN	CA-C-N	-5.30	114.49	119.85
1	E	586	ASN	C-N-CA	-5.30	114.49	119.85
1	B	93	VAL	N-CA-C	-5.29	107.68	112.12
1	E	274	TYR	N-CA-C	5.19	121.86	110.80
1	E	646	GLU	N-CA-C	5.19	117.03	110.33
1	A	646	GLU	N-CA-C	5.18	117.87	109.79
1	A	161	LEU	N-CA-C	5.17	119.64	113.23
1	E	215	SER	N-CA-C	-5.15	106.85	113.23
1	E	370	CYS	N-CA-C	5.10	116.51	110.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	277	CYS	N-CA-C	5.09	116.83	111.28
1	B	39	PHE	N-CA-C	5.09	116.69	108.34
1	E	130	PHE	N-CA-C	5.05	116.66	109.14
1	E	368	THR	N-CA-C	5.04	116.84	108.02
1	A	588	GLU	CA-C-N	-5.01	116.74	122.95
1	A	588	GLU	C-N-CA	-5.01	116.74	122.95

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	273	LYS	Peptide
1	A	645	GLY	Peptide
1	B	645	GLY	Peptide
1	E	13	GLU	Peptide
1	E	273	LYS	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	5419	0	5312	154	0
1	B	5419	0	5312	197	0
1	E	5419	0	5312	173	0
2	A	32	0	12	1	0
2	B	32	0	12	1	0
2	E	32	0	12	0	0
3	A	34	0	0	1	0
3	B	42	0	0	5	0
3	E	33	0	0	0	0
All	All	16462	0	15972	509	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

All (509) 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:346:ASP:OD1	1:A:387:LYS:HE3	1.50	1.10
1:A:463:ASN:O	1:A:464:LYS:HG2	1.57	1.04
1:E:55:ASP:HA	1:E:123:THR:OG1	1.64	0.95
1:E:225:SER:HB2	1:E:357:LEU:HD23	1.48	0.92
1:E:344:ARG:HH21	1:E:387:LYS:HZ3	1.10	0.92
1:A:14:LEU:HB2	1:A:17:ASN:HD21	1.36	0.90
1:A:344:ARG:HB3	1:A:347:LEU:HD11	1.54	0.88
1:E:421:ILE:HG13	1:E:424:LEU:HD21	1.56	0.87
1:A:311:LEU:HD23	1:A:461:HIS:CD2	2.10	0.87
1:B:164:GLN:HG3	1:B:663:LYS:HB2	1.57	0.85
1:A:307:GLN:HE21	1:A:307:GLN:HA	1.41	0.85
1:E:87:ASP:HB3	1:E:107:PRO:HB3	1.57	0.85
1:E:344:ARG:HH21	1:E:387:LYS:NZ	1.73	0.85
1:E:267:HIS:O	1:E:270:GLN:HG2	1.77	0.84
1:B:241:TRP:CD1	1:B:517:ASN:ND2	2.46	0.82
1:B:452:GLU:HG2	1:B:456:PHE:CE1	2.15	0.81
1:A:344:ARG:HH21	1:A:387:LYS:NZ	1.78	0.81
1:A:252:MET:HE3	1:A:558:SER:OG	1.82	0.79
1:A:311:LEU:HD23	1:A:461:HIS:HD2	1.47	0.79
1:B:320:PHE:CE1	1:B:528:TYR:CZ	2.70	0.79
1:E:186:GLU:OE1	1:E:258:VAL:HG21	1.84	0.78
1:B:615:VAL:HG12	1:B:616:ALA:H	1.49	0.77
1:B:210:ASP:OD2	1:B:219:TYR:OH	2.03	0.76
1:E:230:CYS:HB3	1:E:361:PRO:HB3	1.68	0.75
1:B:407:GLN:HE22	1:B:573:ASN:HD21	1.34	0.75
1:B:283:VAL:O	1:B:287:VAL:HG23	1.87	0.75
1:A:109:ASN:O	1:A:215:SER:HB2	1.85	0.74
1:B:508:LEU:HA	1:B:528:TYR:CD2	2.21	0.74
1:E:74:LYS:HE3	1:E:76:ARG:HD2	1.68	0.74
1:E:344:ARG:NH2	1:E:387:LYS:HZ3	1.85	0.74
1:A:344:ARG:NH2	1:A:387:LYS:HZ1	1.85	0.74
1:A:320:PHE:HZ	1:B:528:TYR:CE1	2.06	0.73
1:E:636:VAL:HG11	1:E:650:VAL:HG21	1.71	0.72
1:A:344:ARG:HH12	1:A:373:PRO:HB2	1.55	0.72
1:E:624:VAL:HG13	1:E:664:LEU:HD11	1.72	0.72
1:A:650:VAL:HG22	1:A:651:ARG:H	1.55	0.71
1:A:344:ARG:NH2	1:A:387:LYS:NZ	2.38	0.71
1:E:138:LEU:HD22	1:E:291:LEU:HA	1.72	0.71
1:E:240:ARG:HG3	1:E:274:TYR:CE1	2.25	0.71
1:B:13:GLU:CD	1:B:13:GLU:H	1.98	0.71
1:A:232:ASP:O	1:A:271:ARG:NH1	2.18	0.71
1:B:373:PRO:O	1:B:388:TYR:HB2	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:320:PHE:HE1	1:B:528:TYR:CZ	2.07	0.71
1:B:358:ASP:HB3	1:B:371:CYS:HB2	1.70	0.71
1:E:615:VAL:HG12	1:E:616:ALA:H	1.56	0.70
1:B:169:GLN:OE1	1:B:252:MET:HE1	1.91	0.70
1:B:119:LEU:HB3	1:B:132:LEU:HD11	1.72	0.70
1:B:348:GLN:HG2	3:B:832:HOH:O	1.92	0.70
1:B:607:VAL:HG23	1:B:650:VAL:HG12	1.74	0.70
1:A:320:PHE:CZ	1:B:528:TYR:CE1	2.81	0.69
1:E:347:LEU:HD21	1:E:387:LYS:HZ2	1.57	0.69
1:B:40:TRP:CD1	1:B:103:GLN:HE21	2.10	0.69
1:A:344:ARG:HB3	1:A:347:LEU:CD1	2.23	0.69
1:A:506:ARG:HD2	1:B:530:LEU:HD13	1.73	0.69
1:E:164:GLN:HG3	1:E:663:LYS:HB2	1.74	0.69
1:B:508:LEU:HA	1:B:528:TYR:HD2	1.57	0.68
1:B:320:PHE:CD1	1:B:528:TYR:CZ	2.81	0.68
1:B:636:VAL:HG11	1:B:650:VAL:HG21	1.74	0.68
1:E:210:ASP:OD2	1:E:219:TYR:OH	2.12	0.68
1:A:255:ILE:HB	1:A:665:VAL:HG22	1.74	0.68
1:E:255:ILE:HG13	1:E:625:GLU:OE1	1.94	0.68
1:A:17:ASN:H	1:A:17:ASN:ND2	1.90	0.67
1:E:615:VAL:HG12	1:E:616:ALA:N	2.09	0.67
1:E:17:ASN:HD21	1:E:40:TRP:HB2	1.60	0.67
1:A:509:LEU:HD12	1:A:527:LYS:HB3	1.77	0.67
1:B:491:VAL:HG11	1:B:582:LEU:HD11	1.77	0.66
1:E:559:ASN:ND2	1:E:586:ASN:OD1	2.29	0.66
1:B:241:TRP:CD1	1:B:517:ASN:HD21	2.12	0.66
1:B:680:ARG:NH2	1:E:154:GLU:OE1	2.28	0.65
1:E:122:SER:HA	1:E:127:GLY:HA2	1.78	0.65
1:B:154:GLU:OE1	1:E:680:ARG:NH2	2.30	0.64
1:E:57:LEU:HD22	1:E:119:LEU:HD11	1.79	0.64
1:A:168:TYR:CE2	1:A:436:ARG:HG3	2.32	0.64
1:B:592:ARG:HH21	1:B:594:LEU:HD21	1.62	0.64
1:B:587:PRO:HG3	1:B:612:PRO:HG3	1.79	0.64
1:B:243:ASN:HA	1:B:245:TYR:CZ	2.33	0.64
1:E:347:LEU:HD23	1:E:387:LYS:HD3	1.78	0.64
1:A:8:GLU:HB2	1:A:44:HIS:O	1.98	0.64
1:B:240:ARG:NH2	1:B:242:ASP:OD1	2.31	0.64
1:B:71:ALA:N	3:B:821:HOH:O	2.29	0.63
1:A:320:PHE:CZ	1:B:528:TYR:CD1	2.86	0.63
1:B:205:LYS:HG2	1:B:206:ASN:N	2.14	0.63
1:B:508:LEU:HD12	1:B:528:TYR:CD2	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:HIS:HB3	1:A:270:GLN:HE21	1.64	0.63
1:B:615:VAL:HG12	1:B:616:ALA:N	2.13	0.63
1:B:310:ASN:ND2	1:B:312:LEU:O	2.32	0.63
1:E:387:LYS:HG3	1:E:388:TYR:CE2	2.33	0.62
1:E:624:VAL:HB	1:E:652:MET:HE2	1.81	0.62
1:B:467:GLU:HG2	1:B:468:LYS:N	2.15	0.62
1:E:305:HIS:C	1:E:307:GLN:H	2.07	0.62
1:E:305:HIS:O	1:E:307:GLN:N	2.32	0.62
1:B:320:PHE:CE1	1:B:528:TYR:CE2	2.87	0.62
1:B:222:ARG:HB2	1:B:373:PRO:HD3	1.79	0.62
1:E:167:ILE:HD12	1:E:297:VAL:HG11	1.81	0.62
1:A:347:LEU:HD12	1:A:347:LEU:N	2.14	0.62
1:B:144:PRO:HA	1:B:149:TYR:CD1	2.35	0.62
1:B:320:PHE:HD1	1:B:528:TYR:HH	1.46	0.62
1:E:32:VAL:HG22	1:E:136:ILE:HG13	1.81	0.62
1:E:88:TRP:CZ3	1:E:106:THR:HG22	2.33	0.62
1:A:255:ILE:HB	1:A:665:VAL:CG2	2.30	0.61
1:B:344:ARG:NH2	1:B:387:LYS:NZ	2.48	0.61
1:E:177:ASN:HD22	1:E:177:ASN:H	1.48	0.61
1:B:311:LEU:HD23	1:B:461:HIS:CD2	2.35	0.61
1:B:320:PHE:HD1	1:B:528:TYR:OH	1.84	0.61
1:B:229:ASN:ND2	1:B:237:LEU:O	2.32	0.61
1:A:17:ASN:O	1:A:21:HIS:N	2.31	0.61
1:A:344:ARG:CZ	1:A:387:LYS:HZ1	2.13	0.61
1:A:78:PRO:HG2	1:A:80:ARG:HH11	1.65	0.60
1:A:463:ASN:O	1:A:464:LYS:CG	2.42	0.60
1:A:552:ARG:HH21	1:A:672:LYS:HE2	1.64	0.60
1:B:85:GLU:CD	1:B:86:GLY:H	2.09	0.60
1:E:250:SER:HB3	1:E:253:SER:OG	2.01	0.60
1:A:364:LYS:C	1:A:366:GLU:H	2.09	0.60
1:E:615:VAL:CG1	1:E:616:ALA:H	2.15	0.60
1:B:235:GLY:O	1:B:264:TRP:NE1	2.34	0.60
1:E:347:LEU:HD21	1:E:387:LYS:NZ	2.16	0.60
1:A:307:GLN:HA	1:A:307:GLN:NE2	2.16	0.59
1:B:387:LYS:NZ	1:B:387:LYS:O	2.35	0.59
1:E:491:VAL:HG22	1:E:546:ILE:HD11	1.85	0.59
1:E:663:LYS:NZ	1:E:681:ASN:OD1	2.31	0.59
1:E:242:ASP:O	1:E:243:ASN:CB	2.51	0.59
1:E:598:LYS:HB2	1:E:601:ARG:HG2	1.84	0.59
1:A:293:ILE:HG22	1:A:340:SER:HB3	1.84	0.59
1:A:493:ALA:HB2	1:A:509:LEU:HD21	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:241:TRP:HD1	1:B:517:ASN:ND2	1.99	0.59
1:E:406:GLN:O	1:E:406:GLN:HG2	2.03	0.58
1:E:13:GLU:HB2	1:E:31:LEU:HD22	1.84	0.58
1:E:107:PRO:HG2	1:E:110:ALA:HB2	1.86	0.58
1:B:43:LEU:O	1:B:99:THR:HA	2.04	0.58
1:A:319:GLU:OE1	1:B:527:LYS:HA	2.03	0.58
1:E:599:GLN:HB3	1:E:687:ALA:HB2	1.86	0.58
1:E:326:ASP:C	1:E:328:SER:H	2.12	0.57
1:A:17:ASN:H	1:A:17:ASN:HD22	1.49	0.57
1:E:252:MET:HE3	1:E:558:SER:HA	1.86	0.57
1:A:35:ARG:HA	1:A:137:LEU:HD11	1.86	0.57
1:A:514:VAL:O	1:A:556:THR:HG21	2.04	0.57
1:E:242:ASP:O	1:E:243:ASN:HB3	2.05	0.57
1:E:321:GLY:O	1:E:564:ARG:HD2	2.05	0.57
1:E:48:ARG:NH2	1:E:55:ASP:OD2	2.38	0.57
1:E:317:ARG:NH1	1:E:403:ASP:OD1	2.38	0.57
1:B:109:ASN:O	1:B:215:SER:HB2	2.05	0.56
1:A:48:ARG:NH2	1:A:55:ASP:OD2	2.38	0.56
1:B:107:PRO:C	1:B:109:ASN:H	2.13	0.56
1:B:548:TYR:HA	1:B:551:TYR:CE2	2.40	0.56
1:E:121:ALA:HB3	1:E:128:SER:HB3	1.86	0.56
1:A:508:LEU:O	1:A:565:ALA:HA	2.05	0.56
1:E:634:LYS:HE3	1:E:653:ASP:O	2.06	0.56
1:B:17:ASN:HD21	1:B:40:TRP:N	2.02	0.56
1:B:344:ARG:NH2	1:B:387:LYS:HZ3	2.03	0.56
1:A:530:LEU:HD11	1:B:320:PHE:CZ	2.40	0.56
1:E:7:LEU:HD13	1:E:46:GLU:HB2	1.87	0.56
1:B:34:ARG:HB2	1:B:140:ASN:ND2	2.20	0.56
1:E:216:SER:OG	1:E:218:VAL:HG13	2.06	0.56
1:B:5:LEU:HD11	1:B:128:SER:HB2	1.86	0.56
1:B:213:ARG:C	1:B:215:SER:H	2.14	0.56
1:A:650:VAL:HG22	1:A:651:ARG:N	2.18	0.56
1:B:281:ALA:O	1:B:284:ALA:HB3	2.06	0.56
1:A:364:LYS:O	1:A:366:GLU:N	2.38	0.55
1:E:109:ASN:O	1:E:215:SER:HB2	2.05	0.55
1:E:373:PRO:O	1:E:388:TYR:HB2	2.06	0.55
1:A:230:CYS:HB2	1:A:361:PRO:HB3	1.87	0.55
1:E:121:ALA:HB1	1:E:123:THR:HG22	1.88	0.55
1:A:195:ILE:O	1:A:199:VAL:HB	2.06	0.55
1:B:118:SER:HB3	1:B:131:VAL:HG22	1.88	0.55
1:B:121:ALA:O	1:B:122:SER:HB2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:564:ARG:HB2	1:B:579:GLU:HG2	1.87	0.55
1:B:661:LEU:HD12	1:B:662:HIS:N	2.22	0.55
1:E:470:GLU:C	1:E:472:GLY:H	2.15	0.55
1:A:81:ASP:O	1:A:82:ALA:CB	2.54	0.55
1:B:232:ASP:O	1:B:271:ARG:NH1	2.40	0.55
1:B:85:GLU:C	1:B:87:ASP:H	2.14	0.55
1:E:86:GLY:O	1:E:87:ASP:HB2	2.07	0.55
1:E:344:ARG:HB3	1:E:347:LEU:HD12	1.88	0.55
1:E:358:ASP:HB3	1:E:371:CYS:HB2	1.88	0.55
1:E:56:SER:O	1:E:121:ALA:O	2.25	0.55
1:A:168:TYR:CE2	1:A:177:ASN:HB3	2.42	0.54
1:B:462:LEU:O	1:B:464:LYS:N	2.40	0.54
1:B:508:LEU:HB3	1:B:528:TYR:HE2	1.71	0.54
1:E:95:GLN:HG2	1:E:100:LEU:HD13	1.89	0.54
1:E:169:GLN:HB2	1:E:178:ILE:HD12	1.89	0.54
1:E:51:GLU:O	1:E:55:ASP:HB2	2.08	0.54
1:B:14:LEU:HD13	1:B:40:TRP:HB3	1.88	0.54
1:B:320:PHE:CD1	1:B:528:TYR:OH	2.60	0.54
1:B:347:LEU:HD23	1:B:387:LYS:HE3	1.90	0.54
1:E:279:VAL:O	1:E:283:VAL:HG23	2.07	0.54
1:A:421:ILE:HG13	1:A:424:LEU:HD21	1.89	0.54
1:B:40:TRP:HD1	1:B:103:GLN:HE21	1.56	0.54
1:E:347:LEU:HD22	1:E:386:THR:HG23	1.90	0.54
1:A:636:VAL:HG11	1:A:650:VAL:HG21	1.89	0.54
1:A:144:PRO:HA	1:A:149:TYR:CD1	2.43	0.53
1:B:148:VAL:HB	1:B:294:PRO:HD2	1.91	0.53
1:A:341:TRP:CZ3	1:A:353:GLY:HA2	2.43	0.53
1:B:217:PRO:HB2	1:B:342:MET:SD	2.48	0.53
1:B:357:LEU:HA	1:B:372:GLY:HA3	1.90	0.53
1:B:421:ILE:HG13	1:B:424:LEU:HD11	1.89	0.53
1:E:175:ILE:HG21	1:E:436:ARG:HD2	1.89	0.53
1:A:14:LEU:HD11	1:A:42:THR:HG22	1.90	0.53
1:B:121:ALA:HB1	1:B:123:THR:HG22	1.90	0.53
1:B:508:LEU:HB2	1:B:566:LEU:HB3	1.91	0.53
1:E:552:ARG:HH21	1:E:672:LYS:HE2	1.73	0.53
1:A:81:ASP:O	1:A:82:ALA:HB2	2.09	0.53
1:A:168:TYR:CZ	1:A:436:ARG:HG3	2.43	0.53
1:B:320:PHE:CD1	1:B:528:TYR:CE2	2.97	0.53
1:B:502:GLU:HG3	1:B:535:GLU:HG3	1.91	0.53
1:B:600:LYS:HG2	1:B:600:LYS:O	2.08	0.53
1:E:344:ARG:NH2	1:E:387:LYS:NZ	2.51	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:344:ARG:NH1	1:E:355:GLN:OE1	2.42	0.53
1:A:83:VAL:HG12	1:A:84:GLU:N	2.24	0.53
1:B:107:PRO:HB2	1:B:109:ASN:OD1	2.08	0.53
1:A:384:LEU:O	1:A:390:ALA:HB3	2.09	0.53
1:B:452:GLU:HG2	1:B:456:PHE:HE1	1.72	0.53
2:B:701:GTP:O1G	1:E:478:ARG:NH1	2.37	0.53
1:E:111:PRO:HA	1:E:215:SER:HA	1.91	0.53
1:A:169:GLN:OE1	1:A:178:ILE:HD13	2.09	0.52
1:A:514:VAL:HG22	1:A:515:SER:N	2.23	0.52
1:B:636:VAL:CG1	1:B:650:VAL:HG21	2.39	0.52
1:E:242:ASP:OD2	1:E:243:ASN:N	2.42	0.52
1:A:624:VAL:HB	1:A:652:MET:HE2	1.91	0.52
1:A:14:LEU:HB2	1:A:17:ASN:ND2	2.16	0.52
1:A:475:MET:HA	1:A:494:HIS:O	2.09	0.52
1:B:643:GLU:HB2	1:B:646:GLU:HG2	1.91	0.52
1:A:240:ARG:NH2	1:A:242:ASP:OD1	2.43	0.52
1:B:369:TYR:CG	1:B:370:CYS:N	2.78	0.52
1:B:499:THR:HG22	1:B:500:ALA:N	2.24	0.52
1:B:515:SER:OG	1:B:519:ILE:HB	2.10	0.52
1:E:167:ILE:HG21	1:E:278:TRP:HB2	1.91	0.52
1:B:402:VAL:HG13	1:B:414:LYS:HE3	1.91	0.52
1:E:249:VAL:HG11	1:E:254:TRP:CH2	2.45	0.52
1:E:615:VAL:CG1	1:E:616:ALA:N	2.72	0.52
1:A:61:VAL:HG21	1:A:88:TRP:CZ3	2.45	0.52
1:A:107:PRO:HG2	1:A:110:ALA:HB2	1.92	0.52
1:B:502:GLU:HG3	1:B:535:GLU:HA	1.92	0.52
1:E:344:ARG:HE	1:E:387:LYS:HZ1	1.58	0.52
1:E:347:LEU:CD2	1:E:387:LYS:HD3	2.40	0.52
1:E:326:ASP:C	1:E:328:SER:N	2.68	0.51
1:E:365:SER:HB2	1:E:366:GLU:OE2	2.10	0.51
1:A:13:GLU:H	1:A:13:GLU:CD	2.19	0.51
1:B:227:MET:O	1:B:236:VAL:HG23	2.10	0.51
1:B:476:ARG:HH22	1:B:494:HIS:CD2	2.28	0.51
1:B:343:THR:O	1:B:345:PRO:HD3	2.10	0.51
1:A:530:LEU:HD22	1:B:530:LEU:HD11	1.92	0.51
1:A:311:LEU:CD2	1:A:461:HIS:HD2	2.22	0.51
1:B:307:GLN:O	1:B:308:ASN:C	2.54	0.51
1:E:163:GLN:HA	1:E:184:GLN:HE22	1.76	0.51
1:E:236:VAL:HA	1:E:264:TRP:CD1	2.46	0.51
1:A:587:PRO:HD3	1:A:612:PRO:HG3	1.91	0.50
1:B:401:VAL:HG21	1:B:420:LEU:HD21	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:167:ILE:HG21	1:B:278:TRP:HB2	1.92	0.50
1:B:317:ARG:HA	1:B:322:GLU:O	2.12	0.50
1:B:316:PHE:CE2	1:B:404:TRP:CD1	3.00	0.50
1:E:87:ASP:HB3	1:E:107:PRO:CB	2.36	0.50
1:A:433:ARG:HB3	1:A:435:GLU:OE1	2.11	0.50
1:B:364:LYS:HE2	1:B:369:TYR:O	2.12	0.50
1:E:74:LYS:CE	1:E:76:ARG:HD2	2.37	0.50
1:E:344:ARG:HE	1:E:387:LYS:NZ	2.08	0.50
1:B:168:TYR:CE2	1:B:177:ASN:HB3	2.47	0.50
1:B:615:VAL:CG1	1:B:616:ALA:H	2.21	0.50
1:E:552:ARG:HH22	1:E:615:VAL:HG21	1.77	0.50
1:B:624:VAL:HB	1:B:652:MET:HE2	1.92	0.49
1:E:346:ASP:OD1	1:E:387:LYS:HE2	2.12	0.49
1:B:68:SER:C	3:B:821:HOH:O	2.54	0.49
1:A:48:ARG:HH21	1:A:55:ASP:CG	2.19	0.49
1:A:125:TYR:HD2	1:A:126:GLN:H	1.58	0.49
1:B:48:ARG:HG2	1:B:49:ASN:N	2.26	0.49
1:A:320:PHE:CZ	1:B:528:TYR:HE1	2.31	0.49
1:A:496:THR:HG23	1:A:539:GLU:HG2	1.94	0.49
1:E:51:GLU:N	1:E:55:ASP:OD1	2.38	0.49
1:A:8:GLU:HA	1:A:45:PHE:HA	1.93	0.49
1:B:238:LEU:HD12	1:B:239:GLY:H	1.75	0.49
1:A:293:ILE:CG2	1:A:340:SER:HB3	2.42	0.49
1:B:257:SER:HB3	1:B:283:VAL:HG22	1.94	0.48
1:E:267:HIS:O	1:E:270:GLN:CG	2.57	0.48
1:A:369:TYR:CG	1:A:370:CYS:N	2.81	0.48
1:B:83:VAL:O	1:B:84:GLU:HB2	2.13	0.48
1:B:289:ARG:O	1:B:290:CYS:C	2.56	0.48
1:B:503:TYR:HB2	1:B:534:LEU:HB2	1.95	0.48
1:A:13:GLU:CD	1:A:13:GLU:N	2.71	0.48
1:B:107:PRO:HD2	1:B:110:ALA:HB2	1.95	0.48
1:B:242:ASP:OD2	1:B:242:ASP:C	2.56	0.48
1:B:320:PHE:HE1	1:B:528:TYR:CE1	2.30	0.48
1:A:8:GLU:HB3	1:A:45:PHE:CD1	2.49	0.48
1:B:252:MET:O	1:B:677:LYS:NZ	2.47	0.48
1:E:647:GLU:HG3	1:E:648:VAL:N	2.27	0.48
1:E:630:THR:HG21	1:E:634:LYS:HE2	1.95	0.48
1:E:343:THR:HA	1:E:352:GLU:HB3	1.95	0.48
1:B:176:LYS:NZ	1:B:585:GLU:OE1	2.47	0.48
1:E:255:ILE:HG22	1:E:677:LYS:HE2	1.95	0.48
1:B:362:GLN:HB3	1:B:364:LYS:HG3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:636:VAL:HG11	1:B:650:VAL:CG2	2.43	0.48
1:A:242:ASP:O	1:A:243:ASN:HB3	2.13	0.47
1:E:6:VAL:HG12	1:E:123:THR:HG21	1.96	0.47
1:A:528:TYR:HB2	1:B:320:PHE:CZ	2.49	0.47
1:E:79:LEU:HD11	1:E:92:VAL:HG12	1.96	0.47
1:E:169:GLN:OE1	1:E:252:MET:HE1	2.14	0.47
1:B:277:CYS:HA	1:B:280:PHE:CD2	2.49	0.47
1:B:394:PHE:O	1:B:398:ASN:HB2	2.14	0.47
1:B:624:VAL:HG13	1:B:664:LEU:HD11	1.95	0.47
1:E:481:GLN:H	1:E:481:GLN:NE2	2.12	0.47
1:A:548:TYR:HA	1:A:551:TYR:CE2	2.50	0.47
1:B:87:ASP:HB3	1:B:107:PRO:HB3	1.96	0.47
2:A:701:GTP:O2G	2:A:701:GTP:O1A	2.32	0.47
1:E:33:VAL:HG23	1:E:137:LEU:CD1	2.44	0.47
1:E:305:HIS:O	1:E:307:GLN:HG2	2.13	0.47
1:E:471:THR:O	1:E:471:THR:HG22	2.14	0.47
1:B:600:LYS:O	1:B:600:LYS:CG	2.63	0.47
1:B:238:LEU:HD12	1:B:239:GLY:N	2.28	0.47
1:B:374:VAL:HB	1:B:388:TYR:O	2.15	0.47
1:E:206:ASN:O	1:E:208:GLY:N	2.47	0.47
1:E:647:GLU:HG3	1:E:648:VAL:H	1.79	0.47
1:B:344:ARG:HH21	1:B:387:LYS:NZ	2.13	0.47
1:A:586:ASN:HB3	1:A:587:PRO:HD2	1.96	0.47
1:B:344:ARG:NH1	1:B:355:GLN:OE1	2.48	0.47
1:E:365:SER:C	1:E:366:GLU:HG3	2.39	0.47
1:E:501:GLU:H	1:E:501:GLU:HG2	1.57	0.47
1:A:227:MET:HE1	1:A:234:GLN:HG2	1.96	0.47
1:B:499:THR:HG21	1:B:501:GLU:HG2	1.97	0.47
1:E:259:ASP:O	1:E:260:ILE:C	2.58	0.47
1:E:471:THR:O	1:E:471:THR:CG2	2.63	0.47
1:E:572:ILE:O	1:E:573:ASN:CB	2.63	0.47
1:B:172:ALA:HB2	1:B:301:TYR:HB3	1.97	0.46
1:E:508:LEU:HD23	1:E:566:LEU:HD23	1.96	0.46
1:A:13:GLU:HB2	1:A:31:LEU:HD22	1.97	0.46
1:E:122:SER:CA	1:E:127:GLY:HA2	2.45	0.46
1:B:13:GLU:CD	1:B:13:GLU:N	2.71	0.46
1:E:634:LYS:HB2	1:E:652:MET:HE3	1.98	0.46
1:E:386:THR:HG22	1:E:387:LYS:H	1.81	0.46
1:B:8:GLU:HA	1:B:45:PHE:HA	1.97	0.46
1:B:57:LEU:HD22	1:B:119:LEU:HD11	1.96	0.46
1:B:186:GLU:OE1	1:B:627:ALA:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:624:VAL:CG1	1:E:664:LEU:HD11	2.45	0.46
1:A:252:MET:HE3	1:A:558:SER:HG	1.78	0.46
1:E:163:GLN:HG2	1:E:184:GLN:NE2	2.31	0.46
1:E:249:VAL:O	1:E:274:TYR:HB2	2.15	0.46
1:E:493:ALA:HB2	1:E:509:LEU:HD21	1.97	0.46
1:B:205:LYS:NZ	1:B:205:LYS:HB3	2.31	0.46
1:B:255:ILE:HB	1:B:665:VAL:HG22	1.97	0.46
1:A:296:ARG:O	1:A:296:ARG:CG	2.64	0.46
1:A:374:VAL:HG11	1:A:393:VAL:HG21	1.98	0.46
1:E:464:LYS:HA	1:E:465:LEU:HA	1.73	0.46
1:A:175:ILE:HG21	1:A:436:ARG:HD2	1.98	0.45
1:B:467:GLU:HG2	1:B:468:LYS:H	1.81	0.45
1:A:555:LEU:HD21	1:A:559:ASN:HA	1.98	0.45
1:A:629:LEU:HA	1:A:656:PRO:HB3	1.97	0.45
1:A:14:LEU:HD13	1:A:40:TRP:HB3	1.98	0.45
1:B:134:HIS:N	3:B:828:HOH:O	2.49	0.45
1:B:143:CYS:HA	1:B:144:PRO:HD3	1.77	0.45
1:B:499:THR:CG2	1:B:501:GLU:HG2	2.46	0.45
1:E:596:GLU:HA	1:E:597:PRO:HD3	1.83	0.45
1:A:54:VAL:HG13	1:A:55:ASP:H	1.82	0.45
1:A:121:ALA:O	1:A:122:SER:CB	2.65	0.45
1:A:242:ASP:O	1:A:243:ASN:CB	2.64	0.45
1:A:262:ARG:O	1:A:266:ASN:HB2	2.16	0.45
1:A:657:LEU:HD12	1:A:657:LEU:N	2.31	0.45
1:A:241:TRP:CD1	1:A:517:ASN:ND2	2.85	0.45
1:B:344:ARG:HD2	1:B:344:ARG:HA	1.77	0.45
1:B:475:MET:HG3	1:B:494:HIS:O	2.16	0.45
1:E:12:LEU:HD22	1:E:14:LEU:HG	1.98	0.45
1:E:60:SER:HA	1:E:75:ALA:O	2.17	0.45
1:B:8:GLU:OE2	1:B:130:PHE:CE1	2.70	0.45
1:B:183:GLY:O	1:B:186:GLU:HB2	2.17	0.45
1:B:660:GLY:O	1:B:662:HIS:CD2	2.70	0.45
1:E:387:LYS:HG3	1:E:388:TYR:CD2	2.51	0.45
1:E:650:VAL:HG22	1:E:651:ARG:H	1.82	0.45
1:B:320:PHE:HD1	1:B:528:TYR:CZ	2.30	0.45
1:B:373:PRO:O	1:B:388:TYR:CB	2.64	0.45
1:A:240:ARG:HG3	1:A:274:TYR:CE1	2.52	0.44
1:B:164:GLN:HG3	1:B:663:LYS:CB	2.38	0.44
1:B:199:VAL:O	1:B:199:VAL:HG13	2.17	0.44
1:E:8:GLU:HA	1:E:45:PHE:HA	1.99	0.44
1:E:9:ARG:HE	1:E:44:HIS:HB3	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:ASN:C	1:A:320:PHE:H	2.25	0.44
1:B:86:GLY:C	1:B:88:TRP:H	2.25	0.44
1:B:347:LEU:HD23	1:B:387:LYS:CE	2.47	0.44
1:A:140:ASN:OD1	1:A:142:TRP:HB2	2.18	0.44
1:A:344:ARG:NE	1:A:387:LYS:HZ1	2.15	0.44
1:A:380:LYS:HE2	1:A:445:TYR:CE1	2.53	0.44
1:A:462:LEU:O	1:A:463:ASN:C	2.60	0.44
1:E:647:GLU:CG	1:E:648:VAL:N	2.81	0.44
1:A:347:LEU:HD12	1:A:347:LEU:H	1.81	0.44
1:A:514:VAL:HG22	1:A:515:SER:O	2.18	0.44
1:B:408:ASP:OD1	1:B:409:ASP:N	2.49	0.44
1:E:95:GLN:HG2	1:E:100:LEU:CD1	2.48	0.44
1:E:252:MET:O	1:E:677:LYS:NZ	2.50	0.44
1:A:249:VAL:HG22	1:A:254:TRP:CE2	2.53	0.44
1:A:267:HIS:O	1:A:270:GLN:HG2	2.17	0.44
1:A:307:GLN:HG3	1:A:313:ILE:HD11	2.00	0.44
1:E:97:ASP:HB3	1:E:98:CYS:H	1.64	0.44
1:A:364:LYS:C	1:A:366:GLU:N	2.76	0.44
1:A:387:LYS:HE2	1:A:388:TYR:CE2	2.52	0.44
1:A:49:ASN:OD1	1:A:50:TYR:N	2.48	0.43
1:E:58:THR:HG23	1:E:120:GLU:HG3	2.00	0.43
1:E:330:MET:HB2	1:E:518:GLY:HA3	2.00	0.43
1:E:33:VAL:HG23	1:E:137:LEU:HD12	2.01	0.43
1:E:341:TRP:CZ3	1:E:353:GLY:HA2	2.53	0.43
1:A:491:VAL:HG11	1:A:582:LEU:HD11	2.00	0.43
1:B:348:GLN:HA	1:B:349:PRO:HD3	1.80	0.43
1:A:153:GLU:HA	1:A:153:GLU:OE1	2.17	0.43
1:B:342:MET:CG	1:B:355:GLN:HG3	2.49	0.43
1:A:552:ARG:HH21	1:A:672:LYS:CE	2.31	0.43
1:B:267:HIS:O	1:B:270:GLN:HG2	2.19	0.43
1:E:406:GLN:O	1:E:406:GLN:CG	2.66	0.43
1:A:121:ALA:O	1:A:122:SER:HB2	2.18	0.43
1:A:629:LEU:HD12	1:A:656:PRO:HB3	2.01	0.43
1:B:26:LEU:HD11	1:B:190:LEU:HB2	2.00	0.43
1:B:152:SER:HB2	1:E:592:ARG:HH21	1.84	0.43
1:B:462:LEU:HB3	1:B:463:ASN:H	1.65	0.43
1:E:152:SER:OG	1:E:155:GLU:HG3	2.18	0.43
1:A:11:ASP:OD1	1:A:41:LEU:HD21	2.18	0.43
1:A:22:HIS:CE1	1:A:142:TRP:CD1	3.07	0.43
1:A:638:ILE:HD12	1:A:638:ILE:N	2.33	0.43
1:B:187:ASP:OD1	1:B:187:ASP:C	2.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:471:THR:HG22	1:B:471:THR:O	2.19	0.43
1:E:307:GLN:O	1:E:310:ASN:HB2	2.18	0.43
1:E:337:TRP:HB2	1:E:357:LEU:O	2.18	0.43
1:A:318:ASN:OD1	1:A:320:PHE:HB2	2.18	0.42
1:B:560:LEU:HA	1:B:582:LEU:O	2.19	0.42
1:E:178:ILE:HA	1:E:179:PRO:HD2	1.81	0.42
1:A:47:GLY:O	1:A:98:CYS:SG	2.76	0.42
1:A:613:LEU:HD12	1:A:617:LEU:CD1	2.49	0.42
1:B:445:TYR:O	1:B:446:PRO:O	2.36	0.42
1:E:192:ILE:HG23	1:E:264:TRP:HZ3	1.84	0.42
1:E:403:ASP:O	1:E:415:SER:HB3	2.19	0.42
1:A:542:VAL:HA	1:A:543:PRO:HD3	1.79	0.42
1:A:335:HIS:CD2	1:A:337:TRP:CE3	3.07	0.42
1:B:424:LEU:HD23	1:B:424:LEU:HA	1.79	0.42
1:B:464:LYS:HA	1:B:465:LEU:HA	1.67	0.42
1:E:255:ILE:CG2	1:E:677:LYS:HE2	2.50	0.42
1:E:408:ASP:C	1:E:410:GLY:H	2.25	0.42
1:E:470:GLU:C	1:E:472:GLY:N	2.76	0.42
1:B:48:ARG:HG2	1:B:49:ASN:O	2.20	0.42
1:B:426:ILE:HG13	1:B:440:THR:HA	2.01	0.42
1:B:506:ARG:HB3	1:B:530:LEU:HD23	2.01	0.42
1:B:527:LYS:NZ	1:B:543:PRO:O	2.34	0.42
1:B:652:MET:HE3	1:B:652:MET:HB3	1.91	0.42
1:A:548:TYR:HA	1:A:551:TYR:CZ	2.54	0.42
1:B:57:LEU:O	1:B:79:LEU:N	2.46	0.42
1:B:108:ALA:HB1	1:B:146:ASP:HA	2.01	0.42
1:A:143:CYS:O	1:A:145:ALA:N	2.53	0.42
1:A:236:VAL:HA	1:A:264:TRP:CD1	2.55	0.42
1:A:535:GLU:HG3	1:A:536:PRO:HD3	2.02	0.42
1:B:593:ILE:O	1:E:154:GLU:HG3	2.20	0.42
1:E:362:GLN:O	1:E:364:LYS:N	2.51	0.42
1:A:607:VAL:HG11	1:A:666:VAL:HG21	2.01	0.42
1:B:421:ILE:CG1	1:B:424:LEU:HD11	2.49	0.42
1:E:86:GLY:O	1:E:87:ASP:CB	2.68	0.42
1:E:628:GLY:HA2	1:E:658:HIS:ND1	2.34	0.42
1:B:56:SER:O	1:B:57:LEU:HD23	2.19	0.42
1:B:318:ASN:C	1:B:320:PHE:H	2.28	0.42
1:E:177:ASN:H	1:E:177:ASN:ND2	2.15	0.42
1:A:296:ARG:O	1:A:296:ARG:HG2	2.20	0.41
1:A:320:PHE:HZ	1:B:528:TYR:CD1	2.30	0.41
1:A:332:TRP:O	1:A:333:ASN:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:337:TRP:CZ3	1:E:396:GLU:HG2	2.55	0.41
1:E:405:ILE:O	1:E:412:VAL:HA	2.19	0.41
1:A:48:ARG:NH2	1:A:55:ASP:CG	2.78	0.41
1:A:13:GLU:HG2	3:A:826:HOH:O	2.20	0.41
1:A:233:ASP:O	1:A:271:ARG:NH1	2.53	0.41
1:A:530:LEU:CD1	1:B:506:ARG:HH21	2.33	0.41
1:B:413:HIS:CE1	1:B:573:ASN:HD22	2.37	0.41
1:E:264:TRP:HB2	1:E:272:VAL:HG23	2.01	0.41
1:E:306:ASP:C	1:E:308:ASN:H	2.28	0.41
1:E:364:LYS:HB3	1:E:365:SER:H	1.54	0.41
1:A:132:LEU:HD12	1:A:132:LEU:HA	1.93	0.41
1:B:344:ARG:CG	1:B:344:ARG:HH11	2.33	0.41
1:B:630:THR:C	1:B:632:GLU:H	2.28	0.41
1:E:79:LEU:HD13	1:E:102:LEU:HD22	2.02	0.41
1:E:621:THR:HG23	1:E:637:GLU:HG3	2.02	0.41
1:A:230:CYS:CB	1:A:361:PRO:HB3	2.50	0.41
1:B:213:ARG:C	1:B:215:SER:N	2.77	0.41
1:B:233:ASP:HB2	1:B:234:GLN:H	1.68	0.41
1:A:57:LEU:HB3	1:A:119:LEU:HD11	2.03	0.41
1:E:184:GLN:CD	1:E:184:GLN:H	2.28	0.41
1:A:119:LEU:HB3	1:A:132:LEU:HD13	2.02	0.41
1:A:317:ARG:NH1	1:A:403:ASP:OD1	2.52	0.41
1:A:319:GLU:OE2	1:B:528:TYR:O	2.38	0.41
1:B:294:PRO:HG2	1:B:341:TRP:HB3	2.01	0.41
1:B:366:GLU:HB2	1:B:367:GLY:H	1.73	0.41
1:B:119:LEU:HB3	1:B:132:LEU:CD1	2.48	0.41
1:E:83:VAL:HG12	1:E:89:THR:HG21	2.02	0.41
1:E:492:PHE:CD1	1:E:492:PHE:N	2.88	0.41
1:E:548:TYR:HA	1:E:551:TYR:CE2	2.56	0.41
1:A:187:ASP:O	1:A:262:ARG:NH2	2.54	0.41
1:A:589:ILE:HD13	1:A:666:VAL:HG22	2.03	0.41
1:B:88:TRP:CZ3	1:B:106:THR:HG22	2.56	0.41
1:B:236:VAL:HA	1:B:264:TRP:CD1	2.56	0.41
1:B:316:PHE:O	1:B:324:GLN:HB2	2.21	0.41
1:E:169:GLN:OE1	1:E:178:ILE:HD13	2.21	0.41
1:E:375:PRO:O	1:E:376:VAL:C	2.61	0.41
1:E:462:LEU:HB3	1:E:463:ASN:H	1.70	0.41
1:E:486:GLY:HA2	1:E:548:TYR:CD1	2.56	0.41
1:E:617:LEU:HB3	1:E:620:CYS:SG	2.60	0.41
1:B:362:GLN:HB3	1:B:364:LYS:CG	2.51	0.41
1:B:629:LEU:HD22	1:B:662:HIS:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:305:HIS:HA	1:E:396:GLU:OE1	2.21	0.41
1:A:143:CYS:O	1:A:144:PRO:C	2.64	0.40
1:A:506:ARG:CZ	1:A:568:VAL:HG11	2.50	0.40
1:E:83:VAL:CG1	1:E:89:THR:HG21	2.50	0.40
1:E:164:GLN:HG3	1:E:663:LYS:H	1.85	0.40
1:E:635:THR:O	1:E:636:VAL:HG23	2.21	0.40
1:A:335:HIS:CD2	1:A:337:TRP:HE3	2.39	0.40
1:E:131:VAL:HG12	1:E:133:GLY:H	1.86	0.40
1:A:154:GLU:HG2	1:A:431:VAL:CG2	2.51	0.40
1:A:247:ASP:OD1	1:A:247:ASP:N	2.48	0.40
1:A:387:LYS:HG3	1:A:388:TYR:CG	2.56	0.40
1:A:154:GLU:HG2	1:A:431:VAL:HG23	2.03	0.40
1:B:48:ARG:NH2	1:B:55:ASP:OD1	2.55	0.40
1:B:64:GLY:C	3:B:831:HOH:O	2.64	0.40
1:B:252:MET:HG2	1:B:278:TRP:CZ2	2.57	0.40
1:E:346:ASP:OD1	1:E:387:LYS:CE	2.69	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	683/695 (98%)	605 (89%)	54 (8%)	24 (4%)	3	10
1	B	683/695 (98%)	582 (85%)	81 (12%)	20 (3%)	3	13
1	E	683/695 (98%)	595 (87%)	69 (10%)	19 (3%)	4	14
All	All	2049/2085 (98%)	1782 (87%)	204 (10%)	63 (3%)	3	12

All (63) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	VAL

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Mol	Chain	Res	Type
1	A	82	ALA
1	A	122	SER
1	A	233	ASP
1	A	274	TYR
1	A	365	SER
1	A	464	LYS
1	A	470	GLU
1	A	600	LYS
1	B	233	ASP
1	B	399	ALA
1	B	463	ASN
1	E	230	CYS
1	E	243	ASN
1	E	274	TYR
1	E	306	ASP
1	E	573	ASN
1	A	9	ARG
1	A	83	VAL
1	A	84	GLU
1	A	183	GLY
1	A	325	GLY
1	B	108	ALA
1	B	122	SER
1	B	208	GLY
1	B	214	ARG
1	B	232	ASP
1	B	446	PRO
1	B	462	LEU
1	B	519	ILE
1	E	14	LEU
1	E	327	LYS
1	E	364	LYS
1	E	571	VAL
1	A	16	THR
1	A	28	ARG
1	A	121	ALA
1	A	243	ASN
1	A	383	ASP
1	B	84	GLU
1	B	85	GLU
1	B	121	ALA
1	E	97	ASP

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Mol	Chain	Res	Type
1	E	121	ALA
1	E	232	ASP
1	E	233	ASP
1	E	396	GLU
1	A	388	TYR
1	B	40	TRP
1	B	388	TYR
1	B	396	GLU
1	E	207	ALA
1	A	366	GLU
1	A	385	SER
1	B	14	LEU
1	B	217	PRO
1	B	363	GLU
1	E	84	GLU
1	E	363	GLU
1	A	97	ASP
1	A	430	SER
1	E	615	VAL
1	E	47	GLY

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	595/605 (98%)	509 (86%)	86 (14%)	3	11
1	B	595/605 (98%)	501 (84%)	94 (16%)	2	9
1	E	595/605 (98%)	511 (86%)	84 (14%)	3	12
All	All	1785/1815 (98%)	1521 (85%)	264 (15%)	3	10

All (264) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	11	ASP

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Mol	Chain	Res	Type
1	A	13	GLU
1	A	14	LEU
1	A	15	GLU
1	A	17	ASN
1	A	25	ASP
1	A	28	ARG
1	A	41	LEU
1	A	42	THR
1	A	48	ARG
1	A	53	SER
1	A	56	SER
1	A	58	THR
1	A	62	VAL
1	A	63	THR
1	A	68	SER
1	A	84	GLU
1	A	85	GLU
1	A	91	THR
1	A	97	ASP
1	A	101	SER
1	A	118	SER
1	A	123	THR
1	A	125	TYR
1	A	128	SER
1	A	130	PHE
1	A	132	LEU
1	A	136	ILE
1	A	148	VAL
1	A	151	ASP
1	A	164	GLN
1	A	167	ILE
1	A	176	LYS
1	A	178	ILE
1	A	199	VAL
1	A	200	ASN
1	A	205	LYS
1	A	218	VAL
1	A	231	ASN
1	A	234	GLN
1	A	240	ARG
1	A	244	ASN
1	A	247	ASP

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Mol	Chain	Res	Type
1	A	249	VAL
1	A	257	SER
1	A	261	LEU
1	A	262	ARG
1	A	273	LYS
1	A	291	LEU
1	A	307	GLN
1	A	319	GLU
1	A	346	ASP
1	A	347	LEU
1	A	385	SER
1	A	386	THR
1	A	387	LYS
1	A	400	ASP
1	A	411	SER
1	A	421	ILE
1	A	431	VAL
1	A	452	GLU
1	A	454	GLU
1	A	460	ASN
1	A	465	LEU
1	A	468	LYS
1	A	478	ARG
1	A	499	THR
1	A	526	THR
1	A	535	GLU
1	A	541	SER
1	A	549	GLU
1	A	550	LYS
1	A	556	THR
1	A	562	LYS
1	A	600	LYS
1	A	617	LEU
1	A	621	THR
1	A	624	VAL
1	A	629	LEU
1	A	630	THR
1	A	648	VAL
1	A	652	MET
1	A	665	VAL
1	A	666	VAL
1	A	683	ILE

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Mol	Chain	Res	Type
1	B	4	GLU
1	B	9	ARG
1	B	12	LEU
1	B	13	GLU
1	B	15	GLU
1	B	19	ARG
1	B	29	GLU
1	B	30	LYS
1	B	40	TRP
1	B	42	THR
1	B	48	ARG
1	B	58	THR
1	B	70	GLU
1	B	76	ARG
1	B	85	GLU
1	B	91	THR
1	B	92	VAL
1	B	100	LEU
1	B	102	LEU
1	B	118	SER
1	B	119	LEU
1	B	123	THR
1	B	136	ILE
1	B	164	GLN
1	B	167	ILE
1	B	176	LYS
1	B	178	ILE
1	B	186	GLU
1	B	187	ASP
1	B	199	VAL
1	B	200	ASN
1	B	205	LYS
1	B	206	ASN
1	B	225	SER
1	B	234	GLN
1	B	236	VAL
1	B	240	ARG
1	B	249	VAL
1	B	253	SER
1	B	257	SER
1	B	261	LEU
1	B	271	ARG

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Mol	Chain	Res	Type
1	B	273	LYS
1	B	291	LEU
1	B	309	SER
1	B	313	ILE
1	B	319	GLU
1	B	344	ARG
1	B	346	ASP
1	B	347	LEU
1	B	365	SER
1	B	366	GLU
1	B	387	LYS
1	B	389	ASP
1	B	396	GLU
1	B	397	VAL
1	B	400	ASP
1	B	415	SER
1	B	416	ILE
1	B	418	ARG
1	B	421	ILE
1	B	426	ILE
1	B	431	VAL
1	B	468	LYS
1	B	473	MET
1	B	485	MET
1	B	498	ASN
1	B	508	LEU
1	B	530	LEU
1	B	535	GLU
1	B	541	SER
1	B	549	GLU
1	B	550	LYS
1	B	562	LYS
1	B	564	ARG
1	B	574	SER
1	B	576	LEU
1	B	585	GLU
1	B	600	LYS
1	B	601	ARG
1	B	602	LYS
1	B	607	VAL
1	B	617	LEU
1	B	621	THR

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Mol	Chain	Res	Type
1	B	624	VAL
1	B	629	LEU
1	B	630	THR
1	B	632	GLU
1	B	650	VAL
1	B	652	MET
1	B	657	LEU
1	B	665	VAL
1	B	666	VAL
1	B	688	LEU
1	E	7	LEU
1	E	8	GLU
1	E	12	LEU
1	E	15	GLU
1	E	16	THR
1	E	29	GLU
1	E	41	LEU
1	E	42	THR
1	E	54	VAL
1	E	58	THR
1	E	76	ARG
1	E	80	ARG
1	E	85	GLU
1	E	91	THR
1	E	92	VAL
1	E	96	GLN
1	E	97	ASP
1	E	102	LEU
1	E	103	GLN
1	E	130	PHE
1	E	132	LEU
1	E	136	ILE
1	E	157	GLN
1	E	164	GLN
1	E	176	LYS
1	E	177	ASN
1	E	200	ASN
1	E	209	ARG
1	E	218	VAL
1	E	231	ASN
1	E	233	ASP
1	E	234	GLN

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Mol	Chain	Res	Type
1	E	240	ARG
1	E	244	ASN
1	E	249	VAL
1	E	261	LEU
1	E	262	ARG
1	E	273	LYS
1	E	276	GLN
1	E	291	LEU
1	E	311	LEU
1	E	327	LYS
1	E	347	LEU
1	E	366	GLU
1	E	387	LYS
1	E	389	ASP
1	E	396	GLU
1	E	400	ASP
1	E	408	ASP
1	E	409	ASP
1	E	411	SER
1	E	418	ARG
1	E	421	ILE
1	E	426	ILE
1	E	431	VAL
1	E	453	ARG
1	E	454	GLU
1	E	468	LYS
1	E	470	GLU
1	E	481	GLN
1	E	499	THR
1	E	501	GLU
1	E	523	GLU
1	E	526	THR
1	E	535	GLU
1	E	550	LYS
1	E	569	GLU
1	E	576	LEU
1	E	577	LEU
1	E	582	LEU
1	E	584	LEU
1	E	601	ARG
1	E	617	LEU
1	E	621	THR

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Mol	Chain	Res	Type
1	E	624	VAL
1	E	629	LEU
1	E	630	THR
1	E	637	GLU
1	E	640	ASP
1	E	647	GLU
1	E	653	ASP
1	E	665	VAL
1	E	666	VAL
1	E	677	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	ASN
1	A	22	HIS
1	A	177	ASN
1	A	270	GLN
1	A	276	GLN
1	A	307	GLN
1	A	407	GLN
1	A	441	HIS
1	B	17	ASN
1	B	22	HIS
1	B	177	ASN
1	B	206	ASN
1	B	243	ASN
1	B	276	GLN
1	B	461	HIS
1	B	573	ASN
1	E	17	ASN
1	E	95	GLN
1	E	164	GLN
1	E	177	ASN
1	E	206	ASN
1	E	231	ASN
1	E	234	GLN
1	E	276	GLN
1	E	413	HIS
1	E	481	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 ⓘ

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	GTP	A	701	-	33,34,34	1.38	3 (9%)	50,54,54	1.81	12 (24%)
2	GTP	E	701	-	33,34,34	1.38	4 (12%)	50,54,54	1.88	13 (26%)
2	GTP	B	701	-	33,34,34	1.30	4 (12%)	50,54,54	1.96	17 (34%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GTP	A	701	-	-	3/22/38/38	0/3/3/3
2	GTP	E	701	-	-	3/22/38/38	0/3/3/3
2	GTP	B	701	-	-	1/22/38/38	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	GTP	PB-O3A	-3.98	1.55	1.59
2	B	701	GTP	C2'-C3'	-3.10	1.45	1.53
2	B	701	GTP	C5-N7	-2.90	1.33	1.39
2	B	701	GTP	C5-C6	-2.76	1.34	1.44
2	E	701	GTP	PB-O3A	-2.73	1.56	1.59
2	E	701	GTP	C5-C6	-2.73	1.34	1.44
2	A	701	GTP	C5-C6	-2.70	1.34	1.44
2	A	701	GTP	C5-N7	-2.62	1.33	1.39
2	E	701	GTP	C5-N7	-2.52	1.34	1.39
2	B	701	GTP	C8-N9	-2.17	1.32	1.37
2	E	701	GTP	PG-O2G	-2.05	1.47	1.54

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	GTP	C2-N3-C4	5.32	121.47	112.30
2	B	701	GTP	C2-N3-C4	4.98	120.88	112.30
2	E	701	GTP	C2-N3-C4	4.65	120.30	112.30
2	A	701	GTP	C5-C4-N3	-4.61	121.05	128.39
2	E	701	GTP	C5-C4-N3	-4.43	121.34	128.39
2	B	701	GTP	C5-C4-N3	-4.42	121.36	128.39
2	E	701	GTP	O2A-PA-O3A	3.77	117.45	107.27
2	E	701	GTP	C2-N1-C6	-3.72	118.36	125.11
2	B	701	GTP	O3A-PB-O1B	-3.55	100.02	110.70
2	A	701	GTP	O3B-PG-O1G	-3.48	92.71	111.04
2	A	701	GTP	C2-N1-C6	-3.26	119.20	125.11
2	B	701	GTP	O2A-PA-O3A	3.12	115.71	107.27
2	B	701	GTP	N9-C8-N7	-3.01	107.82	113.40
2	A	701	GTP	N9-C4-N3	2.83	131.60	125.95
2	B	701	GTP	O3'-C3'-C2'	-2.82	102.79	111.82
2	B	701	GTP	N1-C2-N3	-2.78	118.22	123.32
2	B	701	GTP	O3B-PG-O1G	-2.78	96.42	111.04
2	A	701	GTP	N9-C8-N7	-2.71	108.37	113.40
2	E	701	GTP	O2B-PB-O3A	-2.68	100.02	107.27
2	B	701	GTP	C8-N7-C5	2.68	109.04	104.26
2	E	701	GTP	N2-C2-N1	2.66	122.37	116.76
2	B	701	GTP	C2-N1-C6	-2.65	120.30	125.11
2	A	701	GTP	O2A-PA-O3A	2.61	114.34	107.27
2	A	701	GTP	N1-C2-N3	-2.61	118.54	123.32
2	E	701	GTP	O3B-PG-O1G	-2.57	97.52	111.04
2	A	701	GTP	C5-C6-N1	2.44	119.46	113.25
2	B	701	GTP	N9-C4-N3	2.37	130.69	125.95
2	A	701	GTP	O4'-C1'-N9	-2.32	103.09	108.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	701	GTP	N9-C8-N7	-2.29	109.15	113.40
2	B	701	GTP	C5-C6-N1	2.28	119.06	113.25
2	E	701	GTP	O3A-PA-O1A	-2.27	103.87	110.70
2	B	701	GTP	C4-C5-N7	-2.27	107.07	110.67
2	E	701	GTP	C5-C4-N9	2.25	109.69	105.66
2	E	701	GTP	C5-C6-N1	2.25	118.97	113.25
2	E	701	GTP	C4-C5-N7	-2.23	107.14	110.67
2	B	701	GTP	O2B-PB-O3A	2.22	113.28	107.27
2	B	701	GTP	O3G-PG-O2G	2.19	116.01	107.80
2	B	701	GTP	O2'-C2'-C3'	-2.16	104.89	111.82
2	A	701	GTP	O3G-PG-O2G	2.16	115.90	107.80
2	B	701	GTP	O3G-PG-O3B	2.16	111.87	104.64
2	A	701	GTP	C8-N7-C5	2.03	107.87	104.26
2	E	701	GTP	C3'-C2'-C1'	2.01	105.26	101.46

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	GTP	C5'-O5'-PA-O1A
2	E	701	GTP	C5'-O5'-PA-O1A
2	A	701	GTP	C5'-O5'-PA-O3A
2	A	701	GTP	C5'-O5'-PA-O2A
2	E	701	GTP	C5'-O5'-PA-O3A
2	E	701	GTP	C5'-O5'-PA-O2A
2	B	701	GTP	PB-O3B-PG-O1G

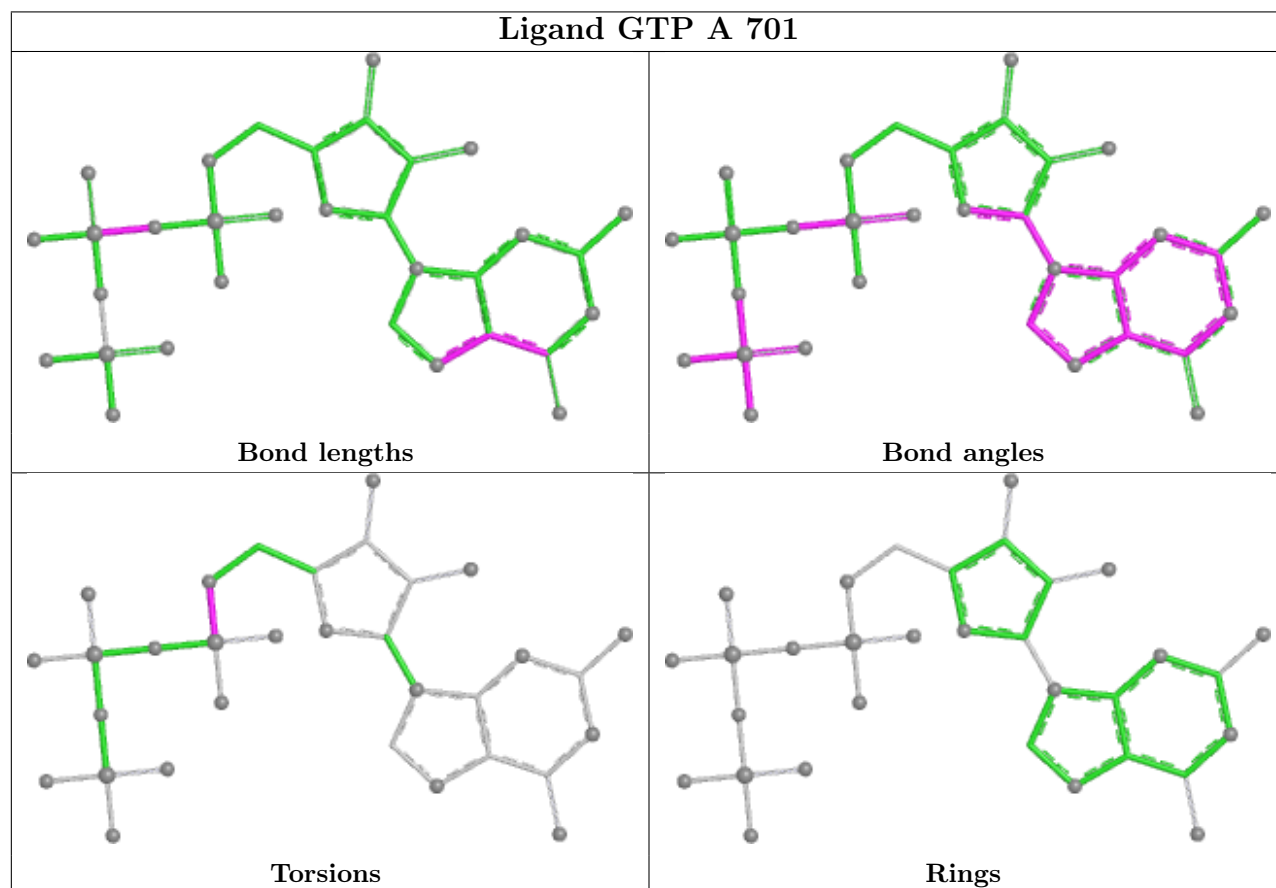
There are no ring outliers.

2 monomers are involved in 2 short contacts:

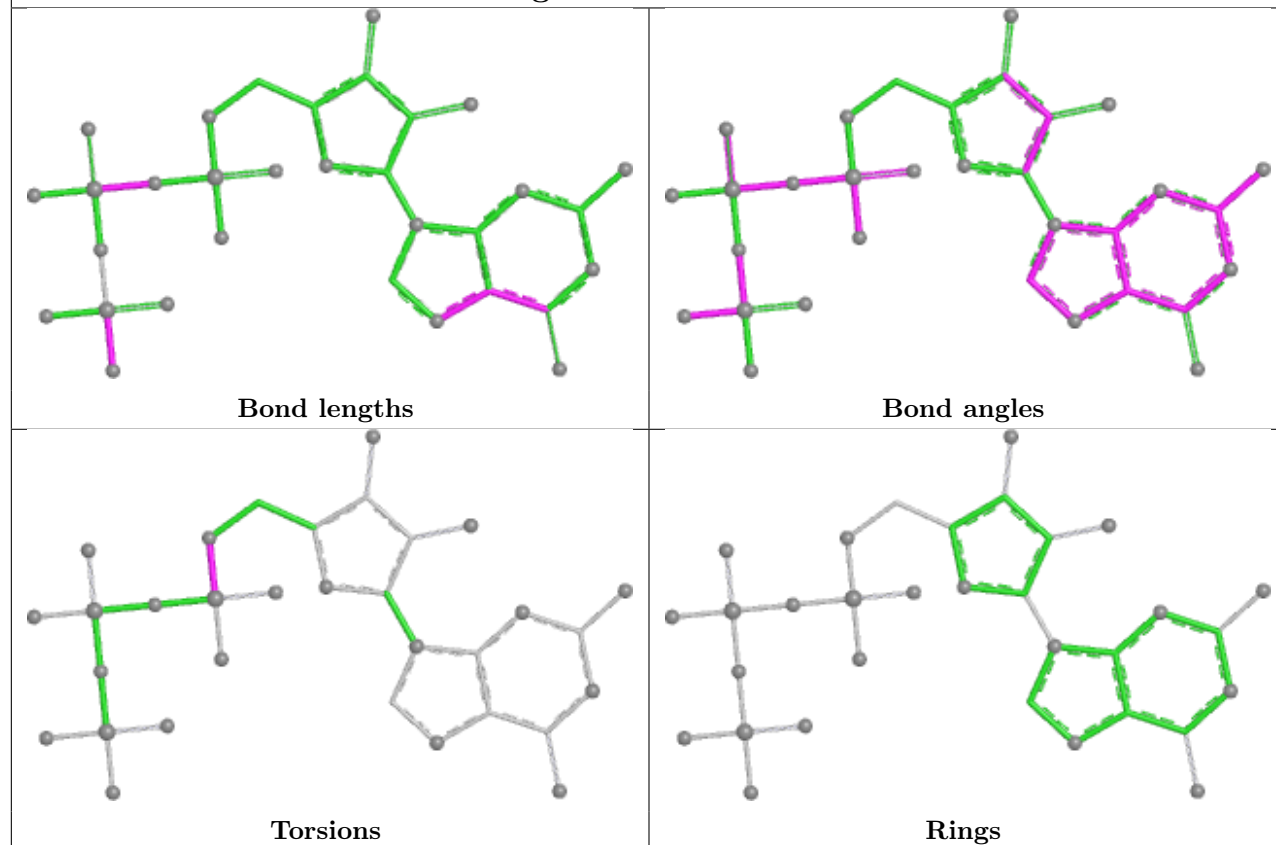
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	GTP	1	0
2	B	701	GTP	1	0

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

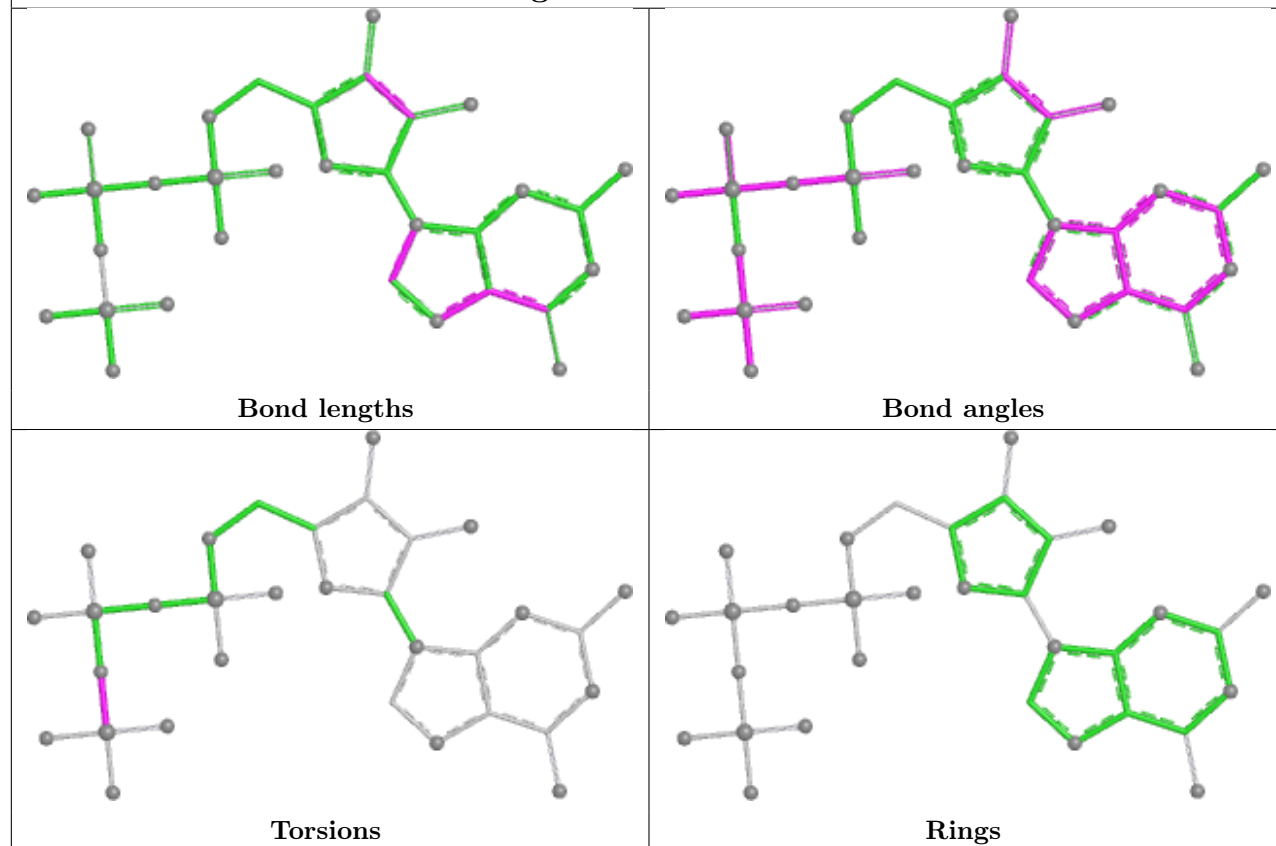
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



Ligand GTP E 701



Ligand GTP B 701



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	685/695 (98%)	-0.08	12 (1%) 67 58	41, 66, 99, 121	0
1	B	685/695 (98%)	0.13	13 (1%) 66 57	44, 78, 119, 135	0
1	E	685/695 (98%)	0.12	12 (1%) 67 58	43, 77, 106, 126	0
All	All	2055/2085 (98%)	0.05	37 (1%) 67 58	41, 73, 113, 135	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	528	TYR	4.5
1	E	688	LEU	4.3
1	A	465	LEU	3.6
1	A	121	ALA	3.6
1	E	230	CYS	3.4
1	E	121	ALA	3.4
1	A	231	ASN	3.1
1	E	368	THR	3.0
1	B	6	VAL	3.0
1	B	688	LEU	3.0
1	E	14	LEU	2.9
1	E	128	SER	2.8
1	B	72	GLY	2.8
1	A	492	PHE	2.7
1	B	123	THR	2.7
1	B	101	SER	2.7
1	A	12	LEU	2.5
1	E	462	LEU	2.4
1	B	231	ASN	2.4
1	B	5	LEU	2.4
1	A	688	LEU	2.3
1	E	125	TYR	2.3
1	B	343	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	367	GLY	2.3
1	B	320	PHE	2.2
1	E	83	VAL	2.2
1	A	13	GLU	2.2
1	A	14	LEU	2.2
1	A	5	LEU	2.1
1	B	462	LEU	2.1
1	B	12	LEU	2.1
1	E	465	LEU	2.1
1	A	471	THR	2.1
1	A	466	ALA	2.1
1	A	234	GLN	2.0
1	E	6	VAL	2.0
1	E	241	TRP	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](#)

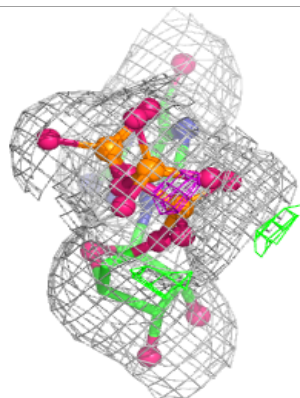
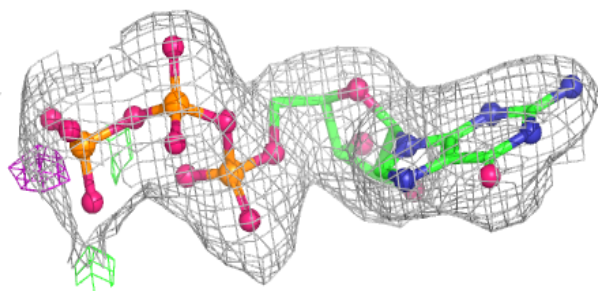
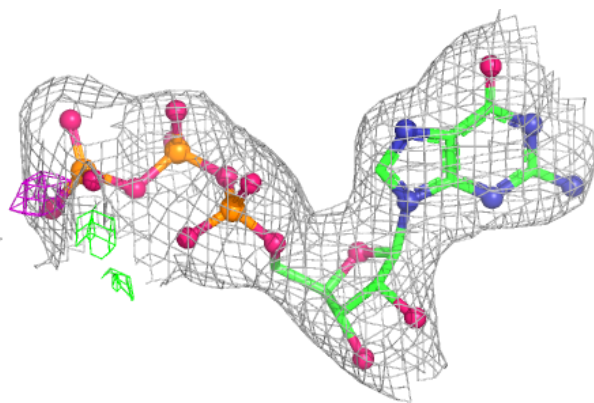
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	GTP	B	701	32/32	0.92	0.07	63,67,79,80	0
2	GTP	A	701	32/32	0.93	0.06	45,53,80,81	0
2	GTP	E	701	32/32	0.94	0.06	45,63,75,75	0

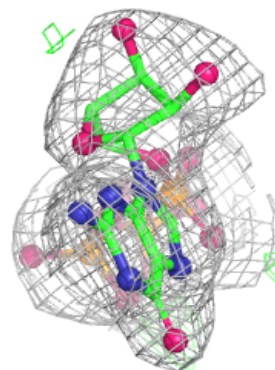
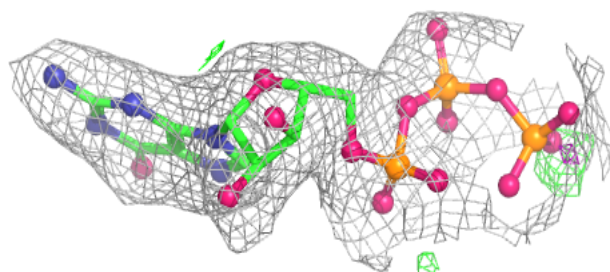
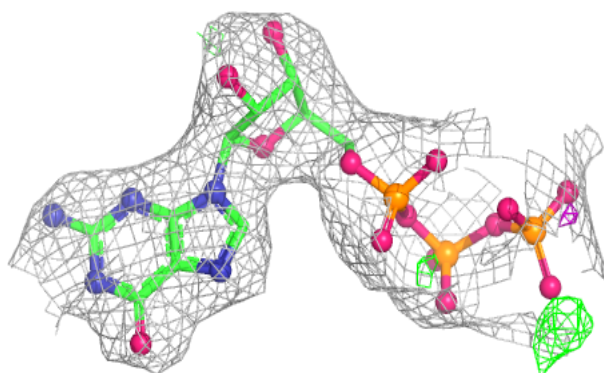
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

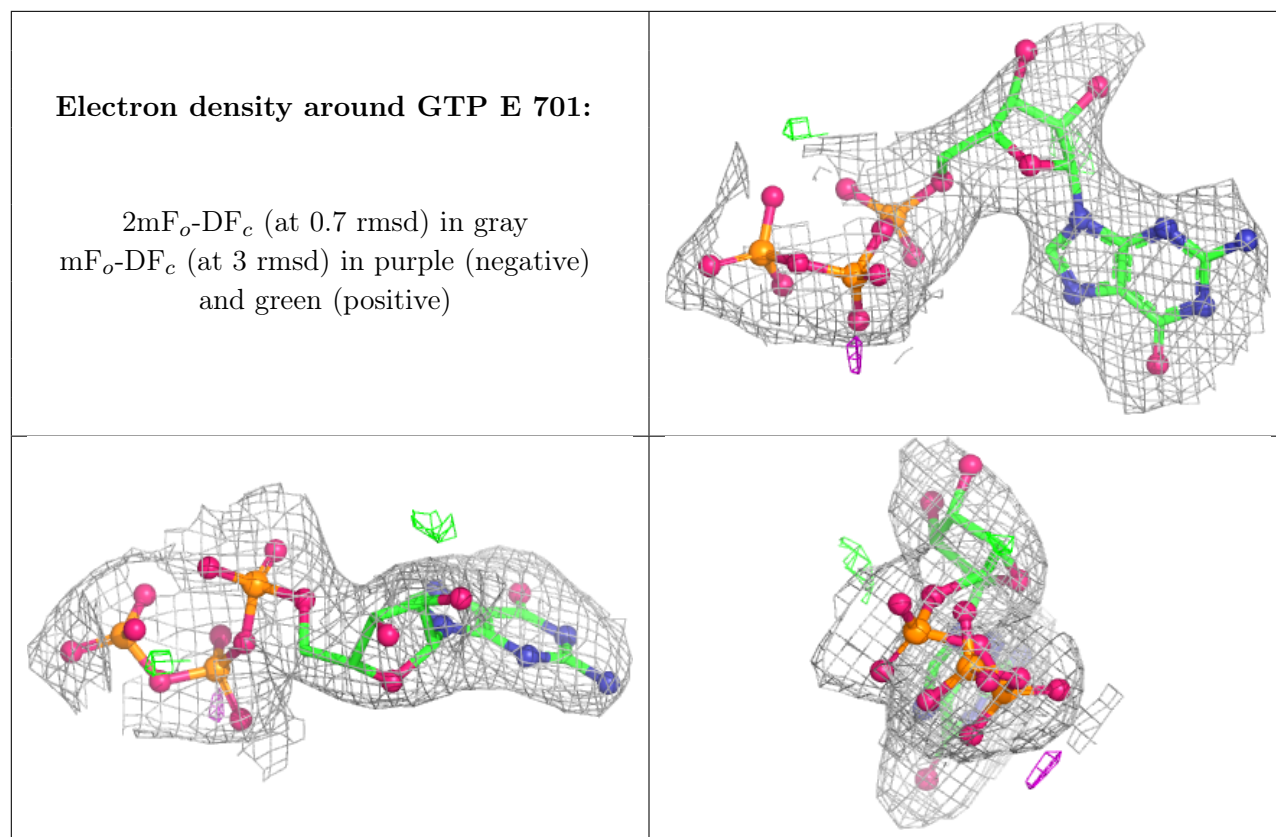
Electron density around GTP B 701:

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

**Electron density around GTP A 701:**

$2mF_o-DF_c$ (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.