Full wwPDB X-ray Structure Validation Report ⓘ

Nov 1, 2023 – 07:43 AM EDT

PDB ID	:	3QOF
Title	:	Crystal structure of the cytosolic domain of human atlastin-1 in complex with GDP, orthorhombic form
Authors	:	Liu, X.
Deposited on	:	2011-02-09
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:

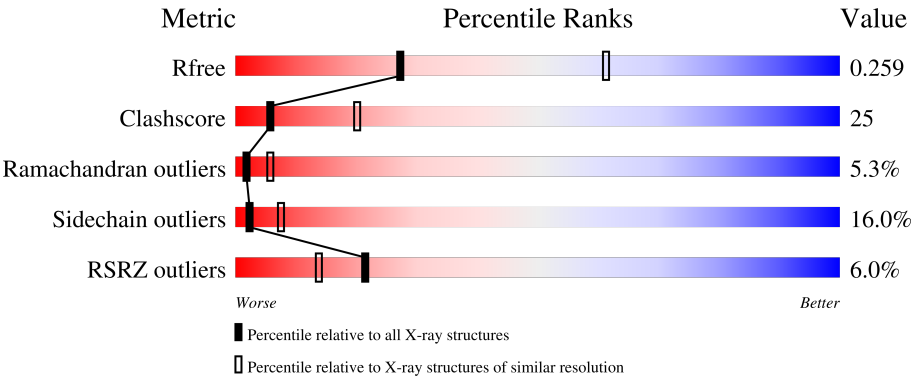
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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 <=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	459	4% 49% 31% 8% · 12%
1	B	459	6% 42% 33% 11% · 14%
1	C	459	3% 47% 31% 10% 12%
1	D	459	8% 46% 31% 9% · 13%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 12574 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 Atlastin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	404	Total	C	N	O	S	0	0	0
			3108	1994	518	583	13			
1	B	397	Total	C	N	O	S	0	0	0
			3079	1979	509	578	13			
1	C	405	Total	C	N	O	S	0	0	0
			3116	2003	518	582	13			
1	D	398	Total	C	N	O	S	0	0	0
			3029	1948	508	561	12			

There are 116 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	expression tag	UNP Q8WXF7
A	-10	HIS	-	expression tag	UNP Q8WXF7
A	-9	HIS	-	expression tag	UNP Q8WXF7
A	-8	HIS	-	expression tag	UNP Q8WXF7
A	-7	HIS	-	expression tag	UNP Q8WXF7
A	-6	HIS	-	expression tag	UNP Q8WXF7
A	-5	HIS	-	expression tag	UNP Q8WXF7
A	-4	GLY	-	expression tag	UNP Q8WXF7
A	-3	SER	-	expression tag	UNP Q8WXF7
A	-2	HIS	-	expression tag	UNP Q8WXF7
A	-1	MET	-	expression tag	UNP Q8WXF7
A	0	ALA	-	expression tag	UNP Q8WXF7
A	1	SER	-	expression tag	UNP Q8WXF7
A	2	ALA	-	expression tag	UNP Q8WXF7
A	3	LYS	-	expression tag	UNP Q8WXF7
A	4	ASN	-	expression tag	UNP Q8WXF7
A	5	ARG	-	expression tag	UNP Q8WXF7
A	6	ARG	-	expression tag	UNP Q8WXF7
A	7	ASP	-	expression tag	UNP Q8WXF7
A	8	ARG	-	expression tag	UNP Q8WXF7
A	9	ASN	-	expression tag	UNP Q8WXF7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	10	SER	-	expression tag	UNP Q8WXF7
A	11	TRP	-	expression tag	UNP Q8WXF7
A	12	GLY	-	expression tag	UNP Q8WXF7
A	13	GLY	-	expression tag	UNP Q8WXF7
A	14	PHE	-	expression tag	UNP Q8WXF7
A	15	SER	-	expression tag	UNP Q8WXF7
A	16	GLU	-	expression tag	UNP Q8WXF7
A	17	LYS	-	expression tag	UNP Q8WXF7
B	-11	MET	-	expression tag	UNP Q8WXF7
B	-10	HIS	-	expression tag	UNP Q8WXF7
B	-9	HIS	-	expression tag	UNP Q8WXF7
B	-8	HIS	-	expression tag	UNP Q8WXF7
B	-7	HIS	-	expression tag	UNP Q8WXF7
B	-6	HIS	-	expression tag	UNP Q8WXF7
B	-5	HIS	-	expression tag	UNP Q8WXF7
B	-4	GLY	-	expression tag	UNP Q8WXF7
B	-3	SER	-	expression tag	UNP Q8WXF7
B	-2	HIS	-	expression tag	UNP Q8WXF7
B	-1	MET	-	expression tag	UNP Q8WXF7
B	0	ALA	-	expression tag	UNP Q8WXF7
B	1	SER	-	expression tag	UNP Q8WXF7
B	2	ALA	-	expression tag	UNP Q8WXF7
B	3	LYS	-	expression tag	UNP Q8WXF7
B	4	ASN	-	expression tag	UNP Q8WXF7
B	5	ARG	-	expression tag	UNP Q8WXF7
B	6	ARG	-	expression tag	UNP Q8WXF7
B	7	ASP	-	expression tag	UNP Q8WXF7
B	8	ARG	-	expression tag	UNP Q8WXF7
B	9	ASN	-	expression tag	UNP Q8WXF7
B	10	SER	-	expression tag	UNP Q8WXF7
B	11	TRP	-	expression tag	UNP Q8WXF7
B	12	GLY	-	expression tag	UNP Q8WXF7
B	13	GLY	-	expression tag	UNP Q8WXF7
B	14	PHE	-	expression tag	UNP Q8WXF7
B	15	SER	-	expression tag	UNP Q8WXF7
B	16	GLU	-	expression tag	UNP Q8WXF7
B	17	LYS	-	expression tag	UNP Q8WXF7
C	-11	MET	-	expression tag	UNP Q8WXF7
C	-10	HIS	-	expression tag	UNP Q8WXF7
C	-9	HIS	-	expression tag	UNP Q8WXF7
C	-8	HIS	-	expression tag	UNP Q8WXF7
C	-7	HIS	-	expression tag	UNP Q8WXF7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-6	HIS	-	expression tag	UNP Q8WXF7
C	-5	HIS	-	expression tag	UNP Q8WXF7
C	-4	GLY	-	expression tag	UNP Q8WXF7
C	-3	SER	-	expression tag	UNP Q8WXF7
C	-2	HIS	-	expression tag	UNP Q8WXF7
C	-1	MET	-	expression tag	UNP Q8WXF7
C	0	ALA	-	expression tag	UNP Q8WXF7
C	1	SER	-	expression tag	UNP Q8WXF7
C	2	ALA	-	expression tag	UNP Q8WXF7
C	3	LYS	-	expression tag	UNP Q8WXF7
C	4	ASN	-	expression tag	UNP Q8WXF7
C	5	ARG	-	expression tag	UNP Q8WXF7
C	6	ARG	-	expression tag	UNP Q8WXF7
C	7	ASP	-	expression tag	UNP Q8WXF7
C	8	ARG	-	expression tag	UNP Q8WXF7
C	9	ASN	-	expression tag	UNP Q8WXF7
C	10	SER	-	expression tag	UNP Q8WXF7
C	11	TRP	-	expression tag	UNP Q8WXF7
C	12	GLY	-	expression tag	UNP Q8WXF7
C	13	GLY	-	expression tag	UNP Q8WXF7
C	14	PHE	-	expression tag	UNP Q8WXF7
C	15	SER	-	expression tag	UNP Q8WXF7
C	16	GLU	-	expression tag	UNP Q8WXF7
C	17	LYS	-	expression tag	UNP Q8WXF7
D	-11	MET	-	expression tag	UNP Q8WXF7
D	-10	HIS	-	expression tag	UNP Q8WXF7
D	-9	HIS	-	expression tag	UNP Q8WXF7
D	-8	HIS	-	expression tag	UNP Q8WXF7
D	-7	HIS	-	expression tag	UNP Q8WXF7
D	-6	HIS	-	expression tag	UNP Q8WXF7
D	-5	HIS	-	expression tag	UNP Q8WXF7
D	-4	GLY	-	expression tag	UNP Q8WXF7
D	-3	SER	-	expression tag	UNP Q8WXF7
D	-2	HIS	-	expression tag	UNP Q8WXF7
D	-1	MET	-	expression tag	UNP Q8WXF7
D	0	ALA	-	expression tag	UNP Q8WXF7
D	1	SER	-	expression tag	UNP Q8WXF7
D	2	ALA	-	expression tag	UNP Q8WXF7
D	3	LYS	-	expression tag	UNP Q8WXF7
D	4	ASN	-	expression tag	UNP Q8WXF7
D	5	ARG	-	expression tag	UNP Q8WXF7
D	6	ARG	-	expression tag	UNP Q8WXF7

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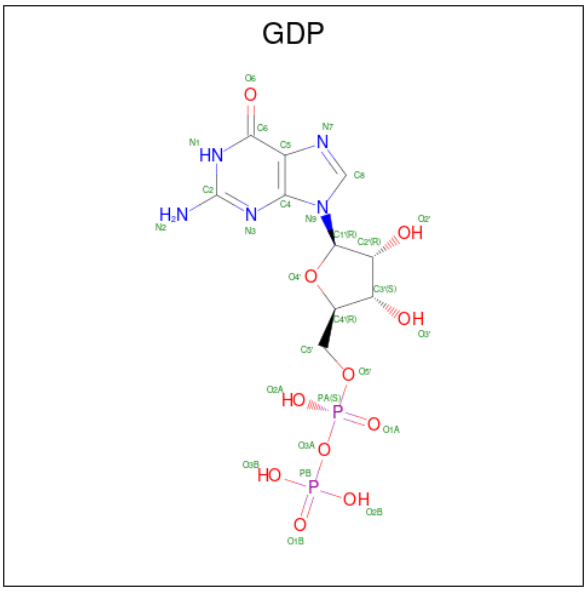
Chain	Residue	Modelled	Actual	Comment	Reference
D	7	ASP	-	expression tag	UNP Q8WXF7
D	8	ARG	-	expression tag	UNP Q8WXF7
D	9	ASN	-	expression tag	UNP Q8WXF7
D	10	SER	-	expression tag	UNP Q8WXF7
D	11	TRP	-	expression tag	UNP Q8WXF7
D	12	GLY	-	expression tag	UNP Q8WXF7
D	13	GLY	-	expression tag	UNP Q8WXF7
D	14	PHE	-	expression tag	UNP Q8WXF7
D	15	SER	-	expression tag	UNP Q8WXF7
D	16	GLU	-	expression tag	UNP Q8WXF7
D	17	LYS	-	expression tag	UNP Q8WXF7

- Molecule 2 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



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

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

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

- Molecule 4 is water.

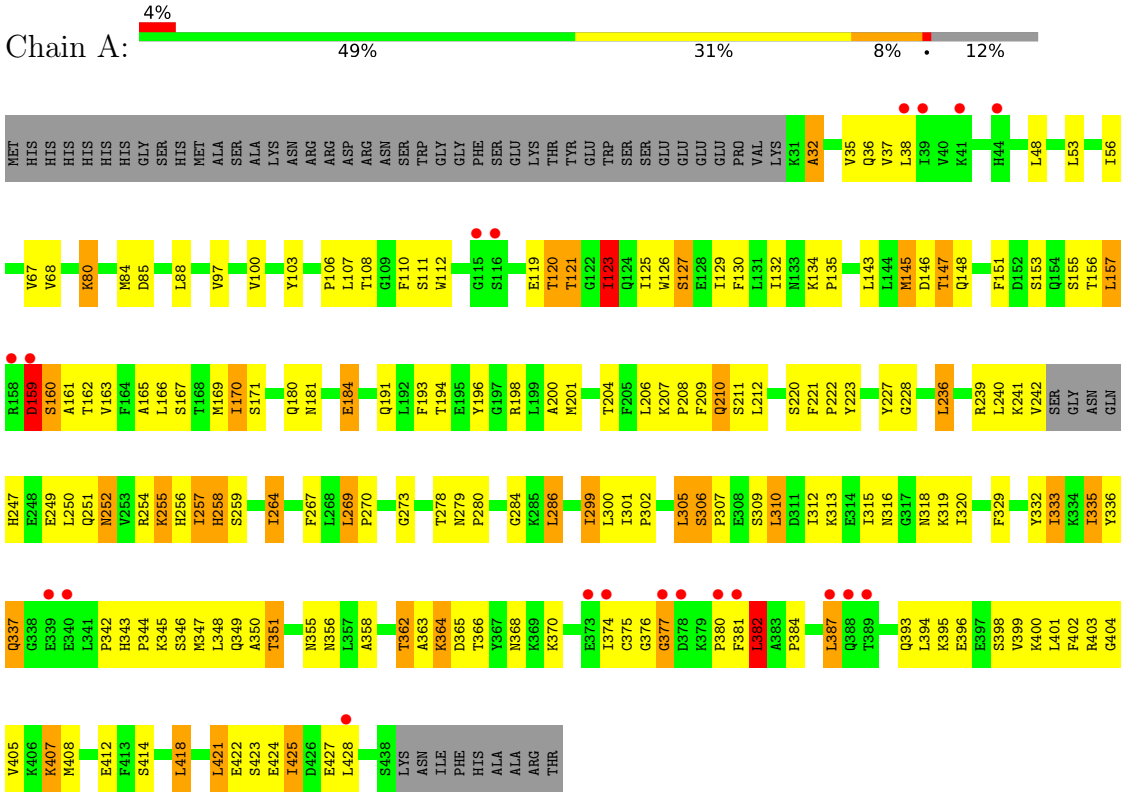
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	37	Total O 37 37	0	0
4	B	29	Total O 29 29	0	0
4	C	37	Total O 37 37	0	0
4	D	23	Total O 23 23	0	0

3 Residue-property plots (i)

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

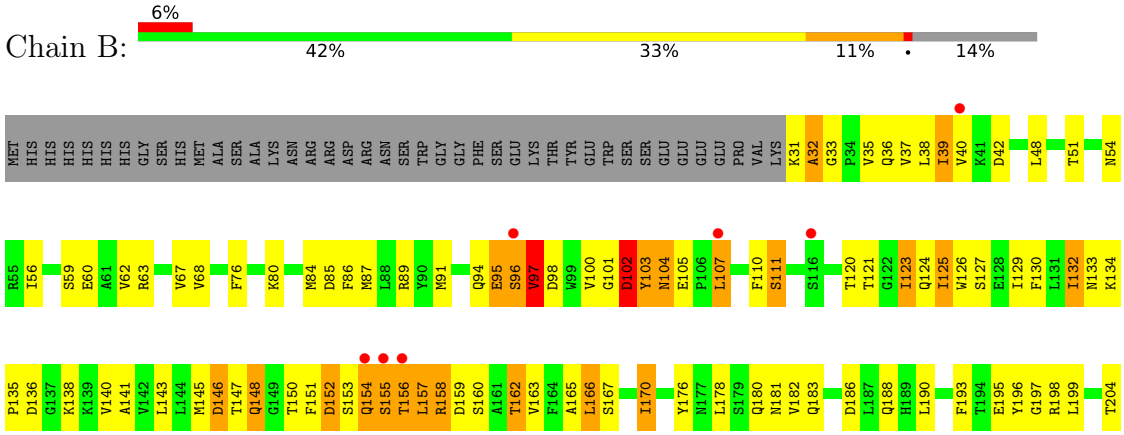
• Molecule 1: Atlastin-1

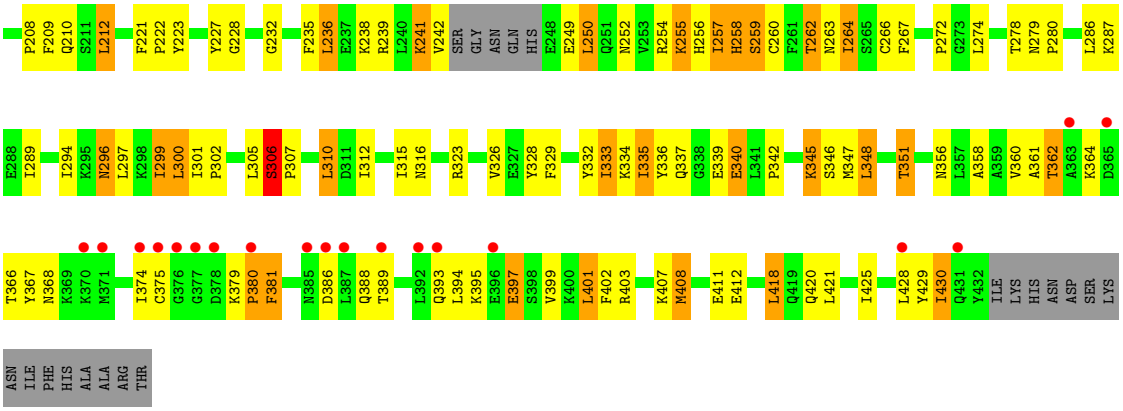
Chain A:



• Molecule 1: Atlastin-1

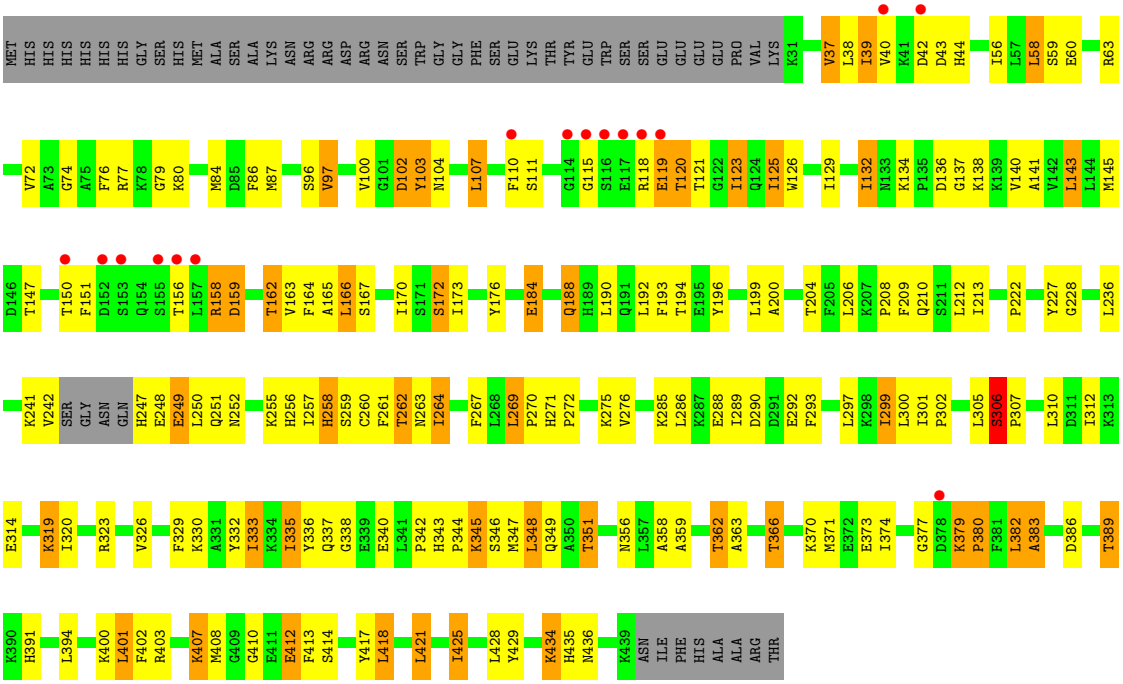
Chain B:





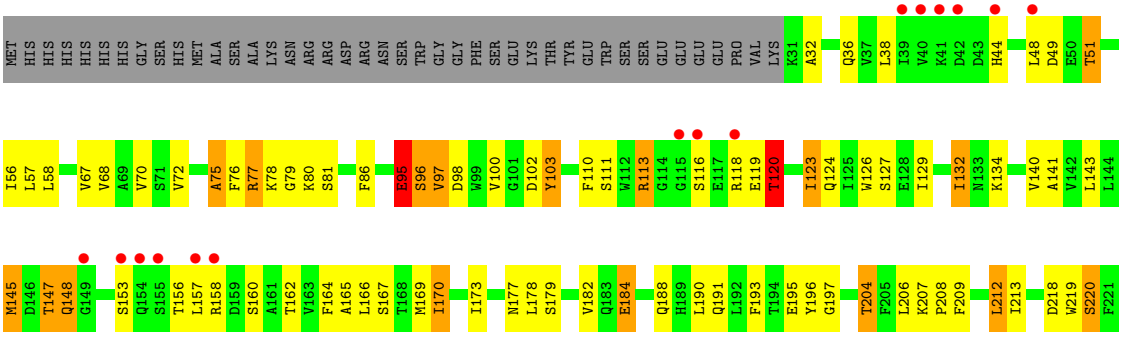
• Molecule 1: Atlastin-1

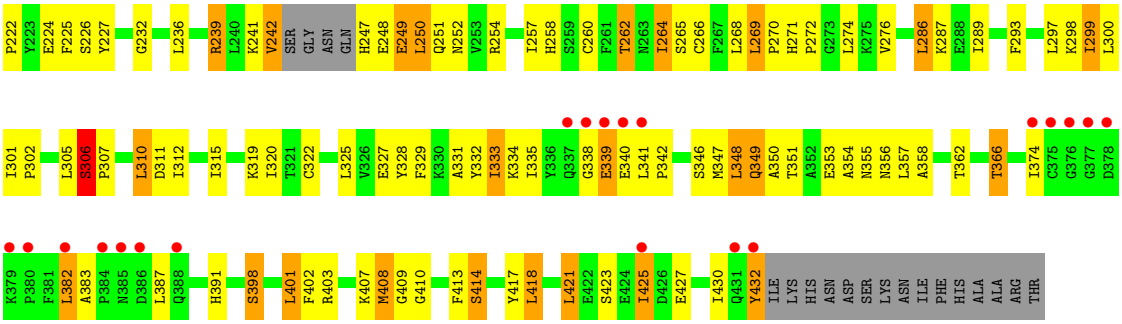
Chain C:



• Molecule 1: Atlastin-1

Chain D:




P222 Y223 E224 F225 S226 Y227 G232 L236 R239 L240 K241 V242 SER GLY ASN GLN H247 E248 E249 L250 Q251 N252 V253 R254 I257 H258 S259 C260 F261 T262 N263 I264 S265 C266 F267 L268 L269 P270 H271 P272 G273 L274 K275 V276 L286 K287 E288 I289 F293 L297 K298 I299 L300
I301 P302 L305 S306 P307 L310 D311 I312 I315 K319 I320 T321 C322 L325 V326 E327 Y328 F329 K330 A331 Y332 I333 K334 I335 Y336 Q337 G338 E339 E340 L341 P342 S346 M347 L348 Q349 A350 T351 A352 E353 A354 N355 N356 L357 A358 T362 T366 I374 C375 G376 G377 D378
K379 P380 F381 L382 A383 P384 N385 D386 L387 Q388 H391 S398 L401 F402 R403 K407 M408 G409 G410 F413 S414 Y417 L418 L421 E422 S423 E424 I425 D426 E427 I430 Q431 Y432 ILE LYS HIS ASN ASP SER LYS ASN ILE PHE HIS ALA ALA ARG THR

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	104.74Å 133.44Å 176.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.80 48.75 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.8 (40.00-2.80) 98.9 (48.75-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	5.25 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.225 , 0.267 0.218 , 0.259	Depositor DCC
R_{free} test set	3079 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	56.5	Xtriage
Anisotropy	0.688	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 55.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	12574	wwPDB-VP
Average B, all atoms (Å^2)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.42	0/3173	0.61	1/4301 (0.0%)
1	B	0.42	0/3142	0.61	1/4252 (0.0%)
1	C	0.46	0/3180	0.65	0/4307
1	D	0.41	0/3092	0.62	0/4195
All	All	0.43	0/12587	0.62	2/17055 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	D	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	305	LEU	CA-CB-CG	-5.65	102.30	115.30
1	B	300	LEU	CA-CB-CG	5.29	127.48	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	252	ASN	Peptide
1	D	95	GLU	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3108	0	2980	145	0
1	B	3079	0	2997	171	0
1	C	3116	0	3007	161	0
1	D	3029	0	2899	146	0
2	A	28	0	12	0	0
2	B	28	0	12	2	0
2	C	28	0	12	3	0
2	D	28	0	12	4	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	37	0	0	2	0
4	B	29	0	0	1	0
4	C	37	0	0	3	0
4	D	23	0	0	1	0
All	All	12574	0	11931	618	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 25.

All (618) 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:B:403:ARG:HH21	1:B:418:LEU:HD11	1.21	0.98
1:B:196:TYR:HB2	1:B:347:MET:HE3	1.47	0.95
1:B:402:PHE:O	1:B:407:LYS:HE3	1.65	0.95
1:A:165:ALA:HA	1:A:193:PHE:HE2	1.33	0.92
1:D:102:ASP:O	1:D:103:TYR:HB2	1.69	0.92
1:A:400:LYS:HZ3	1:A:403:ARG:HH11	1.16	0.92
1:A:165:ALA:HA	1:A:193:PHE:CE2	2.05	0.91
1:B:48:LEU:HB2	1:B:333:ILE:HG13	1.56	0.88
1:C:356:ASN:ND2	1:C:414:SER:HB2	1.88	0.88
1:D:250:LEU:H	1:D:250:LEU:HD23	1.39	0.87
1:D:48:LEU:HB2	1:D:333:ILE:HG13	1.56	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:LYS:NZ	1:A:403:ARG:HH11	1.73	0.86
1:C:305:LEU:O	1:C:306:SER:HB3	1.73	0.86
1:C:196:TYR:HB2	1:C:347:MET:HE3	1.59	0.84
1:C:252:ASN:HB3	1:C:255:LYS:HE2	1.60	0.83
1:B:38:LEU:HB3	1:B:123:ILE:HG23	1.62	0.81
1:C:335:ILE:HD11	1:C:346:SER:O	1.80	0.81
1:D:191:GLN:HE22	1:D:250:LEU:HD12	1.45	0.81
1:A:200:ALA:O	1:A:204:THR:HG22	1.81	0.81
1:C:199:LEU:HD13	1:C:345:LYS:HE3	1.61	0.81
1:D:191:GLN:NE2	1:D:250:LEU:HD12	1.95	0.81
1:A:335:ILE:HD12	1:A:350:ALA:HB2	1.63	0.81
1:C:209:PHE:O	1:C:262:THR:HG22	1.82	0.80
1:D:95:GLU:O	1:D:96:SER:HB2	1.80	0.79
1:A:257:ILE:O	1:A:258:HIS:HB2	1.82	0.79
1:D:209:PHE:O	1:D:262:THR:HG22	1.81	0.79
1:D:407:LYS:HB2	1:D:407:LYS:NZ	1.97	0.79
1:B:102:ASP:HA	1:B:286:LEU:HD12	1.66	0.78
1:C:414:SER:HA	1:C:417:TYR:HD1	1.50	0.77
1:B:196:TYR:HB2	1:B:347:MET:CE	2.15	0.77
1:D:204:THR:HG22	1:D:206:LEU:H	1.48	0.76
1:C:103:TYR:HA	1:C:286:LEU:HB3	1.66	0.76
1:A:194:THR:O	1:A:198:ARG:HG3	1.86	0.76
1:C:402:PHE:O	1:C:407:LYS:HE3	1.85	0.75
1:B:335:ILE:HD11	1:B:346:SER:O	1.87	0.74
1:C:60:GLU:HA	1:C:63:ARG:HH21	1.53	0.74
1:C:343:HIS:ND1	1:C:344:PRO:HD2	2.02	0.74
1:A:387:LEU:HG	1:A:387:LEU:O	1.88	0.74
1:B:157:LEU:HD22	1:B:159:ASP:HB3	1.69	0.74
1:C:210:GLN:HA	1:C:262:THR:HG23	1.69	0.74
1:A:38:LEU:HB3	1:A:123:ILE:HG23	1.70	0.73
1:A:332:TYR:OH	1:A:351:THR:HB	1.87	0.73
1:A:264:ILE:HD13	1:A:264:ILE:O	1.87	0.73
1:B:305:LEU:O	1:B:306:SER:HB3	1.88	0.73
1:C:258:HIS:HB3	1:C:264:ILE:HG23	1.69	0.73
1:B:210:GLN:HA	1:B:262:THR:HG23	1.71	0.72
1:D:264:ILE:HD13	1:D:264:ILE:O	1.88	0.72
1:C:407:LYS:O	1:C:408:MET:HB2	1.87	0.72
1:A:204:THR:HG23	1:A:206:LEU:H	1.54	0.72
1:D:178:LEU:HD12	1:D:182:VAL:HG22	1.71	0.72
1:D:78:LYS:HD2	1:D:179:SER:HB2	1.71	0.71
1:C:358:ALA:O	1:C:362:THR:HG22	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:GLN:HA	1:B:262:THR:CG2	2.21	0.71
1:A:165:ALA:O	1:A:169:MET:HG2	1.91	0.71
1:D:299:ILE:O	1:D:299:ILE:HG13	1.91	0.70
1:B:364:LYS:HE3	1:B:428:LEU:HD11	1.72	0.70
1:C:72:VAL:HG12	1:C:80:LYS:HG2	1.71	0.70
1:C:103:TYR:HA	1:C:286:LEU:HD12	1.72	0.70
1:C:258:HIS:HB3	1:C:264:ILE:CG2	2.21	0.70
1:D:44:HIS:HB3	1:D:339:GLU:HB3	1.74	0.70
1:D:80:LYS:HG3	1:D:177:ASN:HD22	1.57	0.70
1:B:250:LEU:O	1:B:250:LEU:HG	1.92	0.69
1:C:312:ILE:HG21	1:C:319:LYS:HG3	1.73	0.69
1:A:337:GLN:HE21	1:A:337:GLN:HA	1.58	0.69
1:D:56:ILE:HD13	1:D:127:SER:HA	1.73	0.69
1:C:356:ASN:ND2	1:C:414:SER:CB	2.56	0.69
1:A:85:ASP:OD1	1:A:111:SER:HA	1.92	0.68
1:A:401:LEU:O	1:A:405:VAL:HG23	1.93	0.68
1:D:332:TYR:O	1:D:335:ILE:HG22	1.93	0.68
1:D:402:PHE:O	1:D:407:LYS:HE3	1.94	0.68
1:A:110:PHE:HB3	1:A:126:TRP:HH2	1.59	0.67
1:D:327:GLU:OE1	1:D:357:LEU:HB3	1.94	0.67
1:D:335:ILE:HD12	1:D:350:ALA:HB2	1.75	0.67
1:B:104:ASN:O	1:B:105:GLU:HG3	1.95	0.67
1:C:151:PHE:HA	1:C:156:THR:HB	1.77	0.67
1:D:315:ILE:HD13	1:D:328:TYR:CE2	2.30	0.67
1:D:409:GLY:O	1:D:413:PHE:HB3	1.94	0.67
1:B:198:ARG:HD2	1:B:256:HIS:CG	2.30	0.66
1:C:301:ILE:HB	1:C:302:PRO:HD3	1.77	0.66
1:B:59:SER:O	1:B:63:ARG:HB2	1.95	0.66
1:B:395:LYS:HG3	1:B:425:ILE:HD11	1.78	0.66
1:D:38:LEU:HB3	1:D:123:ILE:HG23	1.76	0.66
1:B:286:LEU:HD22	1:B:294:ILE:HD11	1.77	0.66
1:D:356:ASN:HD21	1:D:414:SER:HB3	1.59	0.66
1:D:286:LEU:HD23	1:D:289:ILE:HD12	1.78	0.65
1:D:70:VAL:HG22	1:D:173:ILE:HD12	1.79	0.65
1:C:332:TYR:OH	1:C:351:THR:HB	1.96	0.65
1:D:347:MET:C	1:D:349:GLN:H	2.00	0.65
1:B:236:LEU:HG	1:B:266:CYS:HB2	1.77	0.65
1:A:250:LEU:HD23	1:A:250:LEU:H	1.60	0.65
1:A:156:THR:HA	1:A:160:SER:HB2	1.79	0.65
1:D:156:THR:OG1	1:D:160:SER:HB2	1.97	0.65
1:C:210:GLN:HA	1:C:262:THR:CG2	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:412:GLU:CD	1:C:412:GLU:H	2.00	0.64
1:B:107:LEU:HD22	1:B:107:LEU:O	1.97	0.64
1:A:403:ARG:HH21	1:A:418:LEU:HD11	1.61	0.64
1:D:103:TYR:HA	1:D:286:LEU:HB3	1.78	0.64
1:D:301:ILE:HB	1:D:302:PRO:HD3	1.79	0.64
1:B:165:ALA:HA	1:B:193:PHE:CE2	2.33	0.64
1:D:222:PRO:HG3	1:D:227:TYR:CZ	2.33	0.64
1:A:316:ASN:ND2	1:A:408:MET:HG3	2.13	0.64
1:C:272:PRO:HG3	2:C:593:GDP:C6	2.32	0.64
1:B:136:ASP:OD1	1:B:138:LYS:HG2	1.97	0.63
1:C:371:MET:C	1:C:373:GLU:H	2.02	0.63
1:B:315:ILE:HD13	1:B:328:TYR:CE2	2.33	0.63
1:C:204:THR:HG22	1:C:206:LEU:H	1.64	0.63
1:D:96:SER:O	1:D:97:VAL:O	2.16	0.63
1:B:85:ASP:OD1	1:B:111:SER:HA	1.98	0.63
1:B:296:ASN:N	1:B:296:ASN:HD22	1.97	0.63
1:C:386:ASP:O	1:C:389:THR:HG22	1.99	0.63
1:C:407:LYS:HB2	1:C:407:LYS:NZ	2.14	0.62
1:A:155:SER:O	1:A:159:ASP:HB3	1.98	0.62
1:A:407:LYS:O	1:A:408:MET:HB2	1.98	0.62
1:B:386:ASP:HA	1:B:389:THR:HG22	1.81	0.62
1:B:255:LYS:HE3	1:B:256:HIS:CE1	2.34	0.62
1:C:348:LEU:O	1:C:348:LEU:HD22	1.98	0.62
1:C:84:MET:HG2	1:C:87:MET:HE2	1.81	0.62
1:B:195:GLU:OE2	1:B:195:GLU:HA	1.98	0.62
1:A:257:ILE:O	1:A:258:HIS:CB	2.48	0.62
1:A:241:LYS:O	1:A:242:VAL:HB	1.99	0.61
1:D:335:ILE:HD11	1:D:346:SER:O	2.00	0.61
1:D:356:ASN:ND2	1:D:414:SER:HB3	2.15	0.61
1:A:48:LEU:HB2	1:A:333:ILE:HG13	1.82	0.61
1:C:170:ILE:HD12	1:C:329:PHE:CZ	2.35	0.61
1:C:251:GLN:OE1	1:C:251:GLN:HA	2.00	0.61
1:D:305:LEU:O	1:D:306:SER:HB3	1.99	0.61
1:A:103:TYR:HA	1:A:286:LEU:HB3	1.81	0.61
1:A:160:SER:C	1:A:162:THR:H	2.03	0.61
1:D:48:LEU:HD12	1:D:49:ASP:N	2.15	0.61
1:C:172:SER:HA	4:C:456:HOH:O	2.00	0.61
1:C:356:ASN:HD21	1:C:414:SER:CB	2.14	0.61
1:C:38:LEU:HB3	1:C:123:ILE:HG23	1.82	0.60
1:C:343:HIS:CE1	1:C:344:PRO:HD2	2.36	0.60
1:D:36:GLN:HE22	1:D:124:GLN:NE2	1.99	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:209:PHE:HB2	1:D:260:CYS:O	2.00	0.60
1:C:143:LEU:HD23	4:C:452:HOH:O	2.01	0.60
1:C:199:LEU:CD1	1:C:345:LYS:HE3	2.30	0.60
1:B:147:THR:HG21	1:B:167:SER:CB	2.32	0.60
1:C:84:MET:HG2	1:C:87:MET:CE	2.32	0.60
1:B:35:VAL:HG21	1:B:56:ILE:HD11	1.83	0.60
1:B:182:VAL:HB	1:B:239:ARG:HG3	1.82	0.60
1:B:299:ILE:HD12	1:B:299:ILE:O	2.00	0.60
1:A:110:PHE:HB3	1:A:126:TRP:CH2	2.37	0.59
1:A:162:THR:HG23	1:A:163:VAL:H	1.66	0.59
1:D:353:GLU:HG3	1:D:417:TYR:OH	2.02	0.59
1:D:358:ALA:O	1:D:362:THR:HG23	2.02	0.59
1:C:196:TYR:HB2	1:C:347:MET:CE	2.32	0.59
1:D:147:THR:HG21	1:D:167:SER:HB2	1.84	0.59
1:A:252:ASN:N	1:A:252:ASN:HD22	2.00	0.59
1:A:423:SER:O	1:A:427:GLU:HG2	2.02	0.59
1:D:272:PRO:HG3	2:D:593:GDP:C6	2.38	0.59
1:C:63:ARG:HD2	1:C:323:ARG:NH2	2.18	0.58
1:C:256:HIS:O	1:C:259:SER:HB3	2.03	0.58
1:B:162:THR:HG22	1:B:163:VAL:N	2.18	0.58
1:A:80:LYS:O	1:A:84:MET:HG3	2.04	0.58
1:A:236:LEU:HD22	1:A:240:LEU:HG	1.86	0.58
1:D:102:ASP:O	1:D:103:TYR:CB	2.49	0.58
1:C:119:GLU:OE1	1:C:150:THR:HG22	2.04	0.58
1:C:345:LYS:HB2	1:C:345:LYS:NZ	2.18	0.58
1:D:119:GLU:O	1:D:120:THR:C	2.41	0.58
1:D:407:LYS:HB2	1:D:407:LYS:HZ3	1.65	0.58
1:C:305:LEU:O	1:C:306:SER:CB	2.46	0.58
1:A:85:ASP:CG	1:A:111:SER:HA	2.25	0.58
1:B:430:ILE:HG13	1:B:430:ILE:O	2.04	0.58
1:C:299:ILE:O	1:C:299:ILE:HG13	1.99	0.58
1:B:32:ALA:HB3	1:B:110:PHE:CE2	2.39	0.58
1:C:103:TYR:CA	1:C:286:LEU:HB3	2.35	0.57
1:A:162:THR:HG23	1:A:163:VAL:N	2.20	0.57
1:C:151:PHE:HZ	1:C:164:PHE:HB2	1.68	0.57
1:B:165:ALA:HA	1:B:193:PHE:HE2	1.67	0.57
1:B:196:TYR:OH	1:B:351:THR:HG21	2.05	0.57
1:D:72:VAL:HG12	1:D:80:LYS:HG2	1.85	0.57
1:D:204:THR:CG2	1:D:206:LEU:H	2.17	0.57
1:C:228:GLY:HA2	1:C:267:PHE:CZ	2.40	0.57
1:A:335:ILE:CD1	1:A:350:ALA:HB2	2.33	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:ASN:HD22	1:A:408:MET:HB2	1.69	0.56
1:D:239:ARG:HG2	1:D:239:ARG:HH11	1.69	0.56
1:A:160:SER:N	1:A:162:THR:HG22	2.20	0.56
1:C:356:ASN:HD22	1:C:414:SER:HB2	1.71	0.56
1:D:103:TYR:O	1:D:287:LYS:HG2	2.06	0.56
1:D:382:LEU:HD21	1:D:432:TYR:HB2	1.86	0.56
1:C:147:THR:HG21	1:C:167:SER:CB	2.35	0.56
1:C:102:ASP:O	1:C:103:TYR:CB	2.54	0.56
1:D:49:ASP:OD2	1:D:51:THR:HG23	2.06	0.56
1:B:102:ASP:O	1:B:103:TYR:O	2.23	0.56
1:C:40:VAL:HB	1:C:121:THR:HG23	1.88	0.56
1:C:107:LEU:O	1:C:107:LEU:HD22	2.06	0.56
1:B:305:LEU:O	1:B:306:SER:CB	2.54	0.56
1:B:86:PHE:CG	1:B:297:LEU:HD21	2.40	0.56
1:B:37:VAL:HG12	1:B:38:LEU:N	2.21	0.56
1:B:190:LEU:HD13	1:B:257:ILE:CD1	2.36	0.55
1:C:118:ARG:C	1:C:120:THR:H	2.10	0.55
1:D:355:ASN:HD22	1:D:408:MET:HB2	1.69	0.55
1:B:358:ALA:O	1:B:362:THR:HG22	2.06	0.55
1:C:190:LEU:HD13	1:C:257:ILE:HD11	1.88	0.55
1:C:407:LYS:HB2	1:C:407:LYS:HZ3	1.71	0.55
1:D:252:ASN:C	1:D:254:ARG:H	2.09	0.55
1:D:305:LEU:O	1:D:306:SER:CB	2.54	0.55
1:A:278:THR:CG2	1:A:278:THR:O	2.54	0.55
1:B:241:LYS:O	1:B:254:ARG:HD3	2.06	0.55
1:C:173:ILE:HD13	4:C:448:HOH:O	2.06	0.55
1:C:242:VAL:HG11	1:C:247:HIS:CB	2.36	0.55
1:D:68:VAL:HG13	1:D:311:ASP:O	2.07	0.55
1:D:148:GLN:CA	1:D:148:GLN:HE21	2.20	0.55
1:B:96:SER:O	1:B:97:VAL:O	2.23	0.55
1:D:421:LEU:O	1:D:425:ILE:HG12	2.07	0.55
1:A:201:MET:HE1	1:A:259:SER:HB3	1.89	0.55
1:B:228:GLY:HA2	1:B:267:PHE:CZ	2.42	0.55
1:B:31:LYS:O	1:B:32:ALA:HB3	2.07	0.55
1:C:86:PHE:CG	1:C:297:LEU:HD21	2.41	0.55
1:A:32:ALA:HA	1:A:127:SER:OG	2.07	0.55
1:A:196:TYR:OH	1:A:351:THR:HG21	2.06	0.55
1:A:301:ILE:HB	1:A:302:PRO:HD3	1.89	0.55
1:A:364:LYS:O	1:A:364:LYS:HG2	2.06	0.54
1:B:154:GLN:HG2	1:B:155:SER:OG	2.06	0.54
1:B:86:PHE:CD2	1:B:297:LEU:HD21	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:158:ARG:O	1:C:159:ASP:CB	2.56	0.54
1:C:258:HIS:CD2	1:C:264:ILE:HD12	2.43	0.54
1:A:400:LYS:HZ3	1:A:403:ARG:HD2	1.72	0.54
1:B:54:ASN:HD21	1:B:326:VAL:HG11	1.72	0.54
1:C:421:LEU:O	1:C:425:ILE:HG12	2.08	0.54
1:A:318:ASN:O	1:A:320:ILE:HD12	2.07	0.54
1:D:407:LYS:HB2	1:D:407:LYS:HZ2	1.71	0.54
1:A:358:ALA:O	1:A:362:THR:HG22	2.08	0.54
1:B:232:GLY:O	1:B:266:CYS:HB3	2.08	0.54
1:A:364:LYS:HD2	1:A:424:GLU:OE1	2.08	0.54
1:B:162:THR:CG2	1:B:163:VAL:N	2.70	0.54
1:A:169:MET:HE2	1:A:332:TYR:CE1	2.43	0.54
1:C:413:PHE:O	1:C:414:SER:CB	2.55	0.54
1:C:356:ASN:HD21	1:C:414:SER:HB2	1.67	0.53
1:D:148:GLN:HE21	1:D:148:GLN:HA	1.73	0.53
1:B:335:ILE:HG22	1:B:336:TYR:CD1	2.42	0.53
1:B:339:GLU:O	1:B:340:GLU:HB2	2.08	0.53
1:C:264:ILE:O	1:C:264:ILE:HD13	2.08	0.53
1:C:335:ILE:HG23	1:C:342:PRO:HB3	1.90	0.53
1:B:238:LYS:HB2	1:B:238:LYS:NZ	2.23	0.53
1:A:108:THR:O	1:A:108:THR:HG23	2.09	0.53
1:B:267:PHE:CG	1:B:300:LEU:HD23	2.44	0.53
1:D:170:ILE:HD13	1:D:329:PHE:CZ	2.43	0.53
1:D:75:ALA:HB3	1:D:78:LYS:HG3	1.91	0.53
1:D:156:THR:OG1	1:D:157:LEU:N	2.40	0.53
1:D:165:ALA:O	1:D:169:MET:HG2	2.08	0.53
1:D:76:PHE:CG	1:D:77:ARG:N	2.77	0.53
1:A:278:THR:O	1:A:278:THR:HG22	2.09	0.53
1:C:222:PRO:HG3	1:C:227:TYR:CZ	2.44	0.53
1:A:228:GLY:HA2	1:A:267:PHE:CZ	2.43	0.53
1:B:362:THR:O	1:B:366:THR:HG22	2.09	0.53
1:D:347:MET:C	1:D:349:GLN:N	2.60	0.53
1:D:209:PHE:O	1:D:262:THR:CG2	2.54	0.53
1:C:79:GLY:HA2	2:C:593:GDP:O1A	2.09	0.52
1:B:209:PHE:O	1:B:262:THR:HG22	2.10	0.52
1:A:123:ILE:HD11	1:A:145:MET:HE3	1.91	0.52
1:B:154:GLN:HG2	1:B:155:SER:N	2.24	0.52
1:C:269:LEU:HD23	1:C:270:PRO:HD2	1.90	0.52
1:D:97:VAL:HG12	1:D:98:ASP:OD2	2.08	0.52
1:B:222:PRO:HG3	1:B:227:TYR:CZ	2.44	0.52
1:B:274:LEU:O	1:B:278:THR:HB	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:208:PRO:HD2	1:C:260:CYS:O	2.09	0.52
1:D:212:LEU:HD12	1:D:264:ILE:HB	1.92	0.52
1:B:38:LEU:HB3	1:B:123:ILE:CG2	2.36	0.52
1:C:379:LYS:CB	1:C:380:PRO:HD3	2.39	0.52
1:A:269:LEU:CD2	1:A:270:PRO:HD2	2.39	0.52
1:C:190:LEU:HD13	1:C:257:ILE:CD1	2.40	0.52
1:D:178:LEU:CD1	1:D:182:VAL:HG22	2.38	0.52
1:A:280:PRO:HG3	1:B:223:TYR:CE1	2.45	0.52
1:A:160:SER:C	1:A:162:THR:N	2.63	0.52
1:A:400:LYS:HZ3	1:A:403:ARG:NH1	1.98	0.52
1:A:335:ILE:HD11	1:A:346:SER:O	2.10	0.51
1:B:166:LEU:O	1:B:170:ILE:HG23	2.10	0.51
1:D:362:THR:O	1:D:366:THR:HG22	2.10	0.51
1:B:157:LEU:HD22	1:B:159:ASP:CB	2.38	0.51
1:C:241:LYS:O	1:C:242:VAL:HB	2.10	0.51
1:D:251:GLN:HA	1:D:251:GLN:OE1	2.09	0.51
1:B:94:GLN:HE22	1:B:132:ILE:HD12	1.74	0.51
1:A:400:LYS:NZ	1:A:403:ARG:NH1	2.51	0.51
1:B:356:ASN:ND2	1:B:407:LYS:HD2	2.26	0.51
1:D:333:ILE:HG22	1:D:334:LYS:N	2.26	0.51
1:A:134:LYS:HB3	1:A:135:PRO:CD	2.40	0.51
1:A:316:ASN:HD22	1:A:408:MET:HG3	1.75	0.51
1:B:129:ILE:HG21	1:B:141:ALA:HB1	1.91	0.51
1:A:302:PRO:O	1:A:305:LEU:O	2.28	0.51
1:B:59:SER:OG	1:B:62:VAL:HG22	2.11	0.51
1:C:76:PHE:CE2	1:C:77:ARG:HG2	2.46	0.51
1:A:134:LYS:HB3	1:A:135:PRO:HD2	1.93	0.51
1:B:54:ASN:ND2	1:B:326:VAL:HG11	2.26	0.51
1:D:147:THR:HG21	1:D:167:SER:CB	2.40	0.51
1:D:156:THR:CB	1:D:160:SER:HB2	2.41	0.51
1:A:68:VAL:HG11	1:A:310:LEU:HG	1.92	0.50
1:B:91:MET:HB3	1:B:130:PHE:CE2	2.46	0.50
1:A:299:ILE:O	1:A:299:ILE:HG13	2.09	0.50
1:B:170:ILE:HD13	1:B:329:PHE:CE2	2.47	0.50
1:C:151:PHE:CZ	1:C:164:PHE:HB2	2.46	0.50
1:A:422:GLU:HA	1:A:425:ILE:HG13	1.92	0.50
1:B:399:VAL:O	1:B:403:ARG:HB2	2.12	0.50
1:A:223:TYR:CD1	1:B:280:PRO:HG3	2.46	0.50
1:D:407:LYS:O	1:D:408:MET:O	2.29	0.50
1:A:421:LEU:O	1:A:425:ILE:HG12	2.10	0.50
1:B:147:THR:HG21	1:B:167:SER:HB2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:LEU:O	1:B:289:ILE:HB	2.11	0.50
1:C:204:THR:HG22	1:C:206:LEU:N	2.25	0.50
1:C:37:VAL:HG21	1:C:125:ILE:HD13	1.92	0.50
1:C:269:LEU:CD2	1:C:270:PRO:HD2	2.41	0.50
1:D:226:SER:O	1:D:268:LEU:HD12	2.11	0.50
1:D:272:PRO:HB2	1:D:276:VAL:HB	1.93	0.50
1:C:252:ASN:CB	1:C:255:LYS:HE2	2.37	0.50
1:A:88:LEU:HD11	1:A:112:TRP:NE1	2.26	0.49
1:A:191:GLN:HE22	1:A:250:LEU:HD12	1.76	0.49
1:A:363:ALA:C	1:A:365:ASP:H	2.15	0.49
1:B:335:ILE:HD11	1:B:346:SER:C	2.31	0.49
1:D:190:LEU:HD13	1:D:257:ILE:HD11	1.93	0.49
1:A:273:GLY:HA2	1:B:274:LEU:HD11	1.94	0.49
1:B:101:GLY:O	1:B:102:ASP:O	2.30	0.49
1:C:165:ALA:HA	1:C:193:PHE:HZ	1.76	0.49
1:C:222:PRO:HG3	1:C:227:TYR:CE1	2.47	0.49
1:B:274:LEU:HG	4:B:448:HOH:O	2.13	0.49
1:C:212:LEU:HB2	1:C:261:PHE:CD2	2.47	0.49
1:D:262:THR:HA	4:D:452:HOH:O	2.13	0.49
1:A:368:ASN:HB2	1:A:428:LEU:HD21	1.93	0.49
1:D:110:PHE:HB3	1:D:126:TRP:CZ2	2.48	0.49
1:D:145:MET:SD	1:D:170:ILE:HD11	2.52	0.49
1:C:250:LEU:C	1:C:252:ASN:H	2.16	0.49
1:C:118:ARG:O	1:C:120:THR:HG22	2.13	0.49
1:A:165:ALA:HA	1:A:193:PHE:CZ	2.47	0.48
1:B:241:LYS:HG2	1:B:242:VAL:H	1.77	0.48
1:B:36:GLN:HE22	1:B:124:GLN:NE2	2.11	0.48
1:B:190:LEU:HD13	1:B:257:ILE:HD12	1.95	0.48
1:C:269:LEU:HD13	1:C:293:PHE:HE2	1.76	0.48
1:C:196:TYR:OH	1:C:351:THR:HG21	2.13	0.48
1:D:197:GLY:HA2	1:D:208:PRO:HG2	1.94	0.48
1:A:184:GLU:HG3	1:A:251:GLN:HG3	1.95	0.48
1:B:335:ILE:HG23	1:B:342:PRO:CG	2.43	0.48
1:C:403:ARG:HH21	1:C:418:LEU:HD11	1.79	0.48
1:D:213:ILE:CD1	1:D:265:SER:OG	2.61	0.48
1:B:296:ASN:N	1:B:296:ASN:ND2	2.61	0.48
1:C:335:ILE:HG22	1:C:336:TYR:CD1	2.48	0.48
1:B:358:ALA:O	1:B:361:ALA:HB3	2.14	0.48
1:D:250:LEU:H	1:D:250:LEU:CD2	2.15	0.48
1:B:267:PHE:CD1	1:B:300:LEU:HD23	2.49	0.48
1:A:395:LYS:HG3	1:A:425:ILE:HD12	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:333:ILE:HD13	1:C:333:ILE:O	2.14	0.48
1:D:156:THR:HG23	1:D:157:LEU:N	2.28	0.48
1:D:252:ASN:C	1:D:254:ARG:N	2.68	0.48
1:D:347:MET:O	1:D:351:THR:HG22	2.14	0.48
1:A:337:GLN:HE21	1:A:337:GLN:CA	2.24	0.48
1:B:272:PRO:HG3	2:B:593:GDP:C6	2.49	0.48
1:C:347:MET:O	1:C:351:THR:HG22	2.13	0.48
1:C:363:ALA:HA	1:C:366:THR:CG2	2.43	0.48
1:D:67:VAL:HG11	1:D:325:LEU:HD22	1.95	0.48
1:D:271:HIS:ND1	1:D:272:PRO:HD2	2.29	0.48
1:B:332:TYR:OH	1:B:351:THR:HB	2.12	0.47
1:C:136:ASP:OD1	1:C:138:LYS:HG2	2.14	0.47
1:A:221:PHE:N	1:A:222:PRO:HD3	2.29	0.47
1:A:241:LYS:O	1:A:254:ARG:HD3	2.13	0.47
1:A:252:ASN:N	1:A:252:ASN:ND2	2.62	0.47
1:B:150:THR:C	1:B:152:ASP:H	2.17	0.47
1:B:183:GLN:O	1:B:186:ASP:HB2	2.14	0.47
1:C:110:PHE:HB3	1:C:126:TRP:HH2	1.79	0.47
1:A:156:THR:O	1:A:157:LEU:C	2.52	0.47
1:B:425:ILE:HA	1:B:428:LEU:HB2	1.97	0.47
1:C:302:PRO:O	1:C:306:SER:HB3	2.13	0.47
1:A:335:ILE:HG22	1:A:336:TYR:CD1	2.49	0.47
1:B:107:LEU:HD13	1:B:107:LEU:H	1.80	0.47
1:A:269:LEU:HD23	1:A:270:PRO:HD2	1.97	0.47
1:B:147:THR:HG21	1:B:167:SER:HB3	1.95	0.47
1:B:379:LYS:CB	1:B:380:PRO:HD2	2.45	0.47
1:D:38:LEU:HD13	1:D:333:ILE:HD11	1.95	0.47
1:C:248:GLU:O	1:C:249:GLU:O	2.33	0.47
1:D:129:ILE:HG21	1:D:141:ALA:HB1	1.96	0.47
1:D:218:ASP:OD2	2:D:593:GDP:N2	2.41	0.47
1:D:355:ASN:ND2	1:D:408:MET:HB2	2.28	0.47
1:A:208:PRO:HB2	1:A:209:PHE:CD1	2.50	0.47
1:B:31:LYS:O	1:B:32:ALA:CB	2.63	0.47
1:B:60:GLU:HA	1:B:63:ARG:HH21	1.79	0.47
1:D:403:ARG:HH21	1:D:418:LEU:HD11	1.80	0.47
1:A:38:LEU:HB3	1:A:123:ILE:CG2	2.42	0.46
1:C:166:LEU:HD22	1:C:336:TYR:CD1	2.50	0.46
1:D:398:SER:HA	1:D:401:LEU:HB2	1.97	0.46
1:C:434:LYS:O	1:C:436:ASN:N	2.49	0.46
1:D:224:GLU:HG2	1:D:225:PHE:CD1	2.51	0.46
1:A:35:VAL:O	1:A:37:VAL:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:316:ASN:ND2	1:B:408:MET:HG3	2.30	0.46
1:C:165:ALA:O	1:C:166:LEU:C	2.54	0.46
1:D:156:THR:C	1:D:158:ARG:H	2.18	0.46
1:C:194:THR:HA	1:C:260:CYS:SG	2.56	0.46
1:A:48:LEU:HD11	1:A:53:LEU:HD22	1.96	0.46
1:B:407:LYS:O	1:B:408:MET:O	2.33	0.46
1:A:400:LYS:HD3	1:A:400:LYS:HA	1.60	0.46
1:C:382:LEU:HA	1:C:436:ASN:OD1	2.15	0.46
1:D:196:TYR:HE2	1:D:348:LEU:HA	1.81	0.46
1:A:180:GLN:O	1:A:181:ASN:HB2	2.15	0.46
1:A:381:PHE:O	1:A:382:LEU:HB2	2.15	0.46
1:C:371:MET:C	1:C:373:GLU:N	2.69	0.46
1:D:196:TYR:OH	1:D:351:THR:HG21	2.14	0.46
1:D:232:GLY:O	1:D:266:CYS:HB3	2.16	0.46
1:D:341:LEU:HA	1:D:342:PRO:HD3	1.76	0.46
1:C:285:LYS:O	1:C:288:GLU:HB2	2.16	0.46
1:D:423:SER:O	1:D:427:GLU:HG3	2.15	0.46
1:A:161:ALA:O	1:A:165:ALA:HB2	2.16	0.46
1:B:89:ARG:NH2	1:B:107:LEU:HB2	2.30	0.46
1:B:208:PRO:HD2	1:B:260:CYS:O	2.16	0.46
1:C:305:LEU:N	1:C:305:LEU:HD23	2.31	0.46
1:D:118:ARG:O	1:D:120:THR:HG22	2.16	0.46
1:B:123:ILE:HD12	1:B:147:THR:HG22	1.98	0.45
1:A:247:HIS:N	4:A:483:HOH:O	2.49	0.45
1:B:199:LEU:HD13	1:B:345:LYS:HD3	1.98	0.45
1:C:72:VAL:CG1	1:C:80:LYS:HG2	2.44	0.45
1:D:241:LYS:O	1:D:242:VAL:HB	2.16	0.45
1:A:222:PRO:HG3	1:A:227:TYR:CZ	2.51	0.45
1:B:32:ALA:HA	1:B:127:SER:OG	2.16	0.45
1:B:84:MET:HA	1:B:87:MET:HE2	1.97	0.45
1:B:258:HIS:HD1	1:B:258:HIS:C	2.20	0.45
1:B:339:GLU:O	1:B:340:GLU:CB	2.63	0.45
1:C:414:SER:HA	1:C:417:TYR:CD1	2.39	0.45
1:A:382:LEU:HD23	1:A:384:PRO:HD3	1.98	0.45
1:B:407:LYS:NZ	1:B:407:LYS:HB2	2.32	0.45
1:D:249:GLU:CB	1:D:250:LEU:HD23	2.47	0.45
1:A:67:VAL:HG22	1:A:68:VAL:N	2.32	0.45
1:B:132:ILE:HG13	1:B:133:ASN:N	2.30	0.45
1:D:298:LYS:O	1:D:302:PRO:HD2	2.17	0.45
1:B:257:ILE:O	1:B:258:HIS:CG	2.69	0.45
1:D:269:LEU:HD13	1:D:293:PHE:CE2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:ILE:HD12	1:B:125:ILE:HD11	1.99	0.45
1:C:110:PHE:HB3	1:C:126:TRP:CH2	2.52	0.45
1:A:207:LYS:HA	1:A:208:PRO:HD3	1.71	0.45
1:B:134:LYS:HB3	1:B:134:LYS:HE2	1.57	0.45
1:B:347:MET:O	1:B:351:THR:HG22	2.15	0.45
1:D:132:ILE:CD1	1:D:307:PRO:HG3	2.47	0.45
1:B:272:PRO:CG	2:B:593:GDP:C6	2.99	0.45
1:D:156:THR:HG23	1:D:157:LEU:H	1.81	0.45
1:D:432:TYR:N	1:D:432:TYR:CD1	2.85	0.45
1:A:119:GLU:O	1:A:121:THR:N	2.50	0.45
1:A:280:PRO:HD3	1:B:223:TYR:CE2	2.52	0.45
1:B:198:ARG:HD2	1:B:256:HIS:CD2	2.52	0.45
1:B:238:LYS:HB2	1:B:238:LYS:HZ3	1.80	0.45
1:C:56:ILE:HD12	1:C:125:ILE:HD11	1.98	0.45
1:C:134:LYS:HB3	1:C:134:LYS:HE2	1.78	0.45
1:C:162:THR:CG2	1:C:163:VAL:N	2.80	0.45
1:C:272:PRO:HB2	1:C:276:VAL:HB	1.98	0.45
1:A:207:LYS:HG2	1:A:259:SER:O	2.17	0.44
1:B:151:PHE:O	1:B:152:ASP:C	2.55	0.44
1:B:33:GLY:O	1:B:127:SER:HB3	2.17	0.44
1:C:39:ILE:HD12	1:C:39:ILE:HA	1.62	0.44
1:D:81:SER:HB2	2:D:593:GDP:O2A	2.18	0.44
1:D:232:GLY:O	1:D:236:LEU:HB2	2.18	0.44
1:D:239:ARG:HG2	1:D:239:ARG:NH1	2.31	0.44
1:D:242:VAL:HG11	1:D:247:HIS:N	2.33	0.44
1:A:356:ASN:HD21	1:A:414:SER:HB3	1.82	0.44
1:B:95:GLU:O	1:B:96:SER:O	2.35	0.44
1:C:343:HIS:CG	1:C:344:PRO:HD2	2.52	0.44
1:A:343:HIS:O	1:A:344:PRO:C	2.54	0.44
1:B:107:LEU:H	1:B:107:LEU:CD1	2.30	0.44
1:B:155:SER:O	1:B:156:THR:CB	2.66	0.44
1:B:301:ILE:HB	1:B:302:PRO:HD3	2.00	0.44
1:B:399:VAL:HG13	1:B:418:LEU:HD21	2.00	0.44
1:C:212:LEU:HB2	1:C:261:PHE:CE2	2.53	0.44
1:B:257:ILE:C	1:B:259:SER:H	2.21	0.44
1:C:129:ILE:HG21	1:C:141:ALA:HB1	1.98	0.44
1:D:178:LEU:HD13	1:D:182:VAL:HA	1.99	0.44
1:C:60:GLU:CA	1:C:63:ARG:HH21	2.27	0.44
1:C:162:THR:HG22	1:C:163:VAL:N	2.33	0.44
1:C:382:LEU:O	1:C:383:ALA:HB3	2.17	0.44
1:D:76:PHE:CE2	1:D:77:ARG:HG3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:134:LYS:HE3	1:D:310:LEU:O	2.17	0.44
1:A:422:GLU:HA	1:A:425:ILE:HD11	2.00	0.44
1:B:279:ASN:HA	1:B:280:PRO:HD3	1.74	0.44
1:B:63:ARG:HD2	1:B:323:ARG:HH21	1.83	0.44
1:B:267:PHE:HE1	1:B:299:ILE:HD11	1.82	0.44
1:C:269:LEU:HD13	1:C:293:PHE:CE2	2.52	0.44
1:A:80:LYS:HB2	1:A:80:LYS:NZ	2.33	0.44
1:C:410:GLY:O	1:C:413:PHE:O	2.35	0.44
1:D:184:GLU:HG3	1:D:251:GLN:HG3	2.00	0.43
1:A:255:LYS:HG3	1:A:256:HIS:CD2	2.53	0.43
1:A:313:LYS:HE3	1:A:315:ILE:HD11	1.99	0.43
1:B:190:LEU:HD13	1:B:257:ILE:HD11	2.00	0.43
1:B:380:PRO:HB2	1:B:381:PHE:H	1.50	0.43
1:C:184:GLU:O	1:C:188:GLN:HB2	2.18	0.43
1:C:363:ALA:HA	1:C:366:THR:HG22	2.00	0.43
1:B:367:TYR:O	1:B:367:TYR:CG	2.71	0.43
1:A:279:ASN:HA	1:A:280:PRO:HD3	1.75	0.43
1:A:344:PRO:HA	1:A:347:MET:CE	2.49	0.43
1:A:356:ASN:ND2	1:A:414:SER:HB3	2.34	0.43
1:A:402:PHE:O	1:A:407:LYS:HE3	2.18	0.43
1:C:391:HIS:CE1	1:C:429:TYR:HB2	2.53	0.43
1:D:80:LYS:HB2	1:D:80:LYS:NZ	2.34	0.43
1:D:79:GLY:CA	2:D:593:GDP:O1A	2.67	0.43
1:D:86:PHE:CG	1:D:297:LEU:HD21	2.53	0.43
1:D:258:HIS:HB3	1:D:264:ILE:CG2	2.48	0.43
1:B:176:TYR:CZ	1:B:178:LEU:HD21	2.53	0.43
1:B:302:PRO:O	1:B:305:LEU:O	2.37	0.43
1:C:60:GLU:HA	1:C:63:ARG:NH2	2.28	0.43
1:C:209:PHE:O	1:C:262:THR:CG2	2.59	0.43
1:C:258:HIS:CD2	1:C:264:ILE:CD1	3.02	0.43
1:C:319:LYS:HA	1:C:319:LYS:HD2	1.86	0.43
1:A:404:GLY:O	1:A:405:VAL:C	2.55	0.43
1:B:134:LYS:HE3	1:B:307:PRO:O	2.19	0.43
1:C:428:LEU:HD23	1:C:428:LEU:HA	1.81	0.43
1:D:271:HIS:CG	1:D:272:PRO:HD2	2.54	0.43
1:A:335:ILE:HG23	1:A:342:PRO:CG	2.49	0.43
1:B:162:THR:HG22	1:B:163:VAL:H	1.80	0.43
1:B:241:LYS:HG2	1:B:242:VAL:N	2.33	0.43
1:B:360:VAL:HG23	1:B:402:PHE:CE1	2.54	0.43
1:B:388:GLN:HA	1:B:429:TYR:OH	2.18	0.43
1:C:402:PHE:CE2	1:C:407:LYS:HE2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:ASP:C	1:A:146:ASP:OD1	2.56	0.42
1:C:314:GLU:HG3	1:C:319:LYS:HD2	2.01	0.42
1:C:370:LYS:HD3	1:C:394:LEU:CD2	2.49	0.42
1:D:57:LEU:HD23	1:D:57:LEU:HA	1.81	0.42
1:D:227:TYR:CG	1:D:270:PRO:HG3	2.53	0.42
1:B:316:ASN:HD22	1:B:408:MET:HG3	1.84	0.42
1:D:207:LYS:HA	1:D:208:PRO:HD3	1.81	0.42
1:C:136:ASP:OD1	1:C:137:GLY:N	2.52	0.42
1:D:248:GLU:O	1:D:249:GLU:O	2.38	0.42
1:A:343:HIS:O	1:A:345:LYS:N	2.53	0.42
1:B:38:LEU:CD1	1:B:333:ILE:HD11	2.49	0.42
1:B:39:ILE:HG13	1:B:40:VAL:N	2.32	0.42
1:C:196:TYR:CE2	1:C:351:THR:HG21	2.55	0.42
1:C:362:THR:O	1:C:366:THR:HG22	2.20	0.42
1:D:193:PHE:O	1:D:195:GLU:N	2.52	0.42
1:A:220:SER:O	1:A:221:PHE:CD2	2.72	0.42
1:B:348:LEU:HD23	1:B:348:LEU:HA	1.85	0.42
1:D:421:LEU:HD22	1:D:425:ILE:CD1	2.49	0.42
1:A:129:ILE:HG22	1:A:130:PHE:N	2.35	0.42
1:C:59:SER:O	1:C:63:ARG:HB2	2.20	0.42
1:C:271:HIS:ND1	1:C:272:PRO:HD2	2.35	0.42
1:C:359:ALA:O	1:C:362:THR:HG23	2.20	0.42
1:A:374:ILE:HD11	1:A:394:LEU:HD11	2.02	0.42
1:B:120:THR:HG23	1:B:120:THR:O	2.19	0.42
1:C:74:GLY:O	1:C:80:LYS:HE2	2.19	0.42
1:C:200:ALA:O	1:C:204:THR:HB	2.19	0.42
1:C:343:HIS:O	1:C:344:PRO:C	2.57	0.42
1:A:35:VAL:HG21	1:A:56:ILE:HD11	2.01	0.42
1:B:212:LEU:HB3	1:B:264:ILE:HB	2.01	0.42
1:A:147:THR:O	1:A:147:THR:OG1	2.32	0.42
1:A:250:LEU:C	1:A:252:ASN:H	2.23	0.42
1:A:422:GLU:HA	1:A:425:ILE:CG1	2.49	0.42
1:B:68:VAL:HG11	1:B:310:LEU:HG	2.00	0.42
1:B:153:SER:O	1:B:154:GLN:C	2.57	0.42
1:B:228:GLY:HA2	1:B:267:PHE:CE2	2.55	0.42
1:A:269:LEU:HD22	1:A:270:PRO:HD2	2.02	0.42
1:C:132:ILE:HD11	1:C:307:PRO:HA	2.01	0.42
1:C:228:GLY:HA2	1:C:267:PHE:CE2	2.54	0.42
1:C:252:ASN:N	1:C:252:ASN:ND2	2.65	0.42
1:D:188:GLN:O	1:D:191:GLN:HB3	2.19	0.42
1:A:332:TYR:HH	1:A:351:THR:HB	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:HIS:C	1:A:345:LYS:N	2.74	0.41
1:B:94:GLN:NE2	1:B:307:PRO:HD3	2.35	0.41
1:B:366:THR:C	1:B:368:ASN:H	2.22	0.41
1:B:401:LEU:HD22	1:B:401:LEU:HA	1.82	0.41
1:B:110:PHE:HB3	1:B:126:TRP:CH2	2.55	0.41
1:B:181:ASN:OD1	1:B:235:PHE:HZ	2.04	0.41
1:D:113:ARG:HD2	1:D:113:ARG:HA	1.91	0.41
1:D:129:ILE:CG2	1:D:141:ALA:HB1	2.50	0.41
1:B:333:ILE:HG22	1:B:334:LYS:N	2.35	0.41
1:B:394:LEU:HA	1:B:397:GLU:CD	2.41	0.41
1:A:344:PRO:HA	1:A:347:MET:HE3	2.02	0.41
1:B:134:LYS:HB3	1:B:135:PRO:CD	2.50	0.41
1:B:158:ARG:O	1:B:162:THR:HB	2.21	0.41
1:B:238:LYS:NZ	1:B:238:LYS:CB	2.83	0.41
1:B:239:ARG:HD3	1:B:239:ARG:HA	1.85	0.41
1:B:264:ILE:HD13	1:B:264:ILE:O	2.21	0.41
1:B:286:LEU:HD22	1:B:294:ILE:CD1	2.47	0.41
1:C:326:VAL:CG1	1:C:330:LYS:HE3	2.50	0.41
1:D:57:LEU:HD22	1:D:322:CYS:HB3	2.02	0.41
1:D:220:SER:C	1:D:222:PRO:HD3	2.40	0.41
1:D:271:HIS:HA	1:D:272:PRO:HD3	1.87	0.41
1:D:421:LEU:HD22	1:D:425:ILE:HD13	2.02	0.41
1:A:305:LEU:HA	1:A:305:LEU:HD23	1.73	0.41
1:A:370:LYS:HB3	1:A:394:LEU:HD13	2.03	0.41
1:B:76:PHE:HD1	1:B:148:GLN:OE1	2.03	0.41
1:B:84:MET:SD	1:B:146:ASP:HB2	2.60	0.41
1:B:393:GLN:O	1:B:397:GLU:HG3	2.20	0.41
1:A:123:ILE:O	1:A:123:ILE:HG12	2.20	0.41
1:A:170:ILE:HD13	1:A:329:PHE:CZ	2.55	0.41
1:A:221:PHE:HA	1:A:223:TYR:CE2	2.56	0.41
1:A:228:GLY:HA2	1:A:267:PHE:CE1	2.56	0.41
1:A:242:VAL:HG22	1:C:401:LEU:HD22	2.02	0.41
1:A:422:GLU:HA	1:A:425:ILE:CD1	2.50	0.41
1:C:42:ASP:C	1:C:44:HIS:H	2.23	0.41
1:C:118:ARG:C	1:C:120:THR:N	2.74	0.41
1:D:312:ILE:HG21	1:D:319:LYS:CG	2.51	0.41
1:A:167:SER:O	1:A:171:SER:HB3	2.21	0.41
1:A:210:GLN:HB3	1:A:211:SER:H	1.53	0.41
1:C:107:LEU:HD22	1:C:107:LEU:C	2.41	0.41
1:C:276:VAL:CG2	1:C:289:ILE:HG12	2.51	0.41
1:A:206:LEU:HD12	1:A:316:ASN:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:LYS:HG3	1:A:320:ILE:HD13	2.03	0.41
1:A:402:PHE:CE2	1:A:407:LYS:HE2	2.56	0.41
1:B:374:ILE:HG22	1:B:374:ILE:O	2.21	0.41
1:D:338:GLY:O	1:D:340:GLU:N	2.54	0.41
1:B:193:PHE:O	1:B:197:GLY:N	2.43	0.41
1:C:192:LEU:HG	1:C:347:MET:HE2	2.02	0.41
1:C:258:HIS:HD2	1:C:264:ILE:CD1	2.34	0.41
1:D:56:ILE:CD1	1:D:127:SER:HA	2.46	0.41
1:D:80:LYS:HG3	1:D:177:ASN:ND2	2.31	0.41
1:D:219:TRP:HD1	1:D:227:TYR:CE2	2.39	0.41
1:D:333:ILE:CG2	1:D:334:LYS:N	2.81	0.41
1:A:151:PHE:N	1:A:160:SER:OG	2.44	0.41
1:B:221:PHE:N	1:B:222:PRO:HD3	2.36	0.41
1:D:331:ALA:HB3	1:D:354:ALA:HB2	2.03	0.41
1:A:84:MET:SD	1:A:146:ASP:HB2	2.61	0.40
1:A:106:PRO:O	1:A:107:LEU:C	2.59	0.40
1:C:58:LEU:HD12	1:C:58:LEU:HA	1.85	0.40
1:C:80:LYS:HB2	1:C:80:LYS:NZ	2.36	0.40
1:C:165:ALA:HA	1:C:193:PHE:CZ	2.55	0.40
1:D:425:ILE:HG12	1:D:425:ILE:H	1.67	0.40
1:A:126:TRP:HB3	4:A:452:HOH:O	2.19	0.40
1:B:360:VAL:HG23	1:B:402:PHE:HE1	1.86	0.40
1:D:315:ILE:HB	1:D:320:ILE:HD11	2.02	0.40
1:A:376:GLY:O	1:A:377:GLY:C	2.59	0.40
1:C:79:GLY:CA	2:C:593:GDP:O1A	2.69	0.40
1:C:290:ASP:OD2	1:C:292:GLU:N	2.54	0.40
1:D:274:LEU:HA	1:D:274:LEU:HD23	1.82	0.40
1:B:59:SER:O	1:B:63:ARG:CB	2.68	0.40
1:B:212:LEU:HD23	1:B:212:LEU:HA	1.91	0.40
1:C:184:GLU:HG3	1:C:251:GLN:HG3	2.03	0.40
1:C:335:ILE:HD13	1:C:335:ILE:HG21	1.81	0.40
1:A:364:LYS:O	1:A:364:LYS:CG	2.70	0.40
1:B:103:TYR:O	1:B:105:GLU:N	2.55	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	400/459 (87%)	323 (81%)	57 (14%)	20 (5%)	2	6
1	B	393/459 (86%)	333 (85%)	37 (9%)	23 (6%)	1	4
1	C	401/459 (87%)	337 (84%)	43 (11%)	21 (5%)	2	6
1	D	394/459 (86%)	312 (79%)	62 (16%)	20 (5%)	2	6
All	All	1588/1836 (86%)	1305 (82%)	199 (12%)	84 (5%)	2	6

All (84) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	123	ILE
1	A	249	GLU
1	A	258	HIS
1	A	307	PRO
1	A	382	LEU
1	B	96	SER
1	B	97	VAL
1	B	102	ASP
1	B	103	TYR
1	B	104	ASN
1	B	111	SER
1	B	154	GLN
1	B	249	GLU
1	B	306	SER
1	B	380	PRO
1	B	381	PHE
1	B	408	MET
1	C	96	SER
1	C	97	VAL
1	C	249	GLU
1	C	382	LEU
1	D	96	SER

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Mol	Chain	Res	Type
1	D	97	VAL
1	D	120	THR
1	D	249	GLU
1	D	374	ILE
1	D	408	MET
1	A	97	VAL
1	A	120	THR
1	A	153	SER
1	A	284	GLY
1	A	377	GLY
1	A	393	GLN
1	B	156	THR
1	B	241	LYS
1	C	102	ASP
1	C	103	TYR
1	C	159	ASP
1	C	377	GLY
1	D	75	ALA
1	D	103	TYR
1	D	111	SER
1	D	153	SER
1	D	410	GLY
1	A	127	SER
1	A	157	LEU
1	A	159	ASP
1	A	375	CYS
1	A	380	PRO
1	B	32	ALA
1	B	158	ARG
1	C	111	SER
1	C	115	GLY
1	C	119	GLU
1	C	338	GLY
1	C	379	LYS
1	C	434	LYS
1	C	435	HIS
1	D	164	PHE
1	A	36	GLN
1	B	152	ASP
1	B	155	SER
1	B	340	GLU
1	C	158	ARG

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Mol	Chain	Res	Type
1	C	306	SER
1	D	95	GLU
1	D	306	SER
1	D	339	GLU
1	A	32	ALA
1	A	364	LYS
1	B	180	GLN
1	C	43	ASP
1	C	383	ALA
1	D	32	ALA
1	D	113	ARG
1	D	116	SER
1	A	306	SER
1	B	95	GLU
1	B	375	CYS
1	B	430	ILE
1	D	430	ILE
1	C	380	PRO
1	D	383	ALA
1	C	374	ILE

5.3.2 Protein sidechains (i)

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	320/405 (79%)	270 (84%)	50 (16%)	2 8
1	B	323/405 (80%)	266 (82%)	57 (18%)	2 5
1	C	321/405 (79%)	269 (84%)	52 (16%)	2 7
1	D	306/405 (76%)	262 (86%)	44 (14%)	3 10
All	All	1270/1620 (78%)	1067 (84%)	203 (16%)	2 7

All (203) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	LYS

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Mol	Chain	Res	Type
1	A	100	VAL
1	A	120	THR
1	A	121	THR
1	A	123	ILE
1	A	125	ILE
1	A	132	ILE
1	A	143	LEU
1	A	145	MET
1	A	147	THR
1	A	148	GLN
1	A	159	ASP
1	A	160	SER
1	A	166	LEU
1	A	170	ILE
1	A	184	GLU
1	A	210	GLN
1	A	212	LEU
1	A	236	LEU
1	A	239	ARG
1	A	255	LYS
1	A	257	ILE
1	A	264	ILE
1	A	269	LEU
1	A	286	LEU
1	A	299	ILE
1	A	300	LEU
1	A	306	SER
1	A	309	SER
1	A	310	LEU
1	A	312	ILE
1	A	319	LYS
1	A	333	ILE
1	A	335	ILE
1	A	337	GLN
1	A	348	LEU
1	A	349	GLN
1	A	351	THR
1	A	362	THR
1	A	366	THR
1	A	382	LEU
1	A	387	LEU
1	A	396	GLU

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Mol	Chain	Res	Type
1	A	398	SER
1	A	399	VAL
1	A	407	LYS
1	A	412	GLU
1	A	418	LEU
1	A	421	LEU
1	A	425	ILE
1	B	39	ILE
1	B	42	ASP
1	B	51	THR
1	B	67	VAL
1	B	80	LYS
1	B	97	VAL
1	B	98	ASP
1	B	100	VAL
1	B	102	ASP
1	B	107	LEU
1	B	121	THR
1	B	123	ILE
1	B	125	ILE
1	B	132	ILE
1	B	140	VAL
1	B	143	LEU
1	B	145	MET
1	B	146	ASP
1	B	148	GLN
1	B	157	LEU
1	B	160	SER
1	B	162	THR
1	B	166	LEU
1	B	170	ILE
1	B	188	GLN
1	B	204	THR
1	B	212	LEU
1	B	236	LEU
1	B	250	LEU
1	B	252	ASN
1	B	255	LYS
1	B	257	ILE
1	B	258	HIS
1	B	259	SER
1	B	262	THR

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Mol	Chain	Res	Type
1	B	263	ASN
1	B	264	ILE
1	B	287	LYS
1	B	296	ASN
1	B	299	ILE
1	B	306	SER
1	B	310	LEU
1	B	312	ILE
1	B	333	ILE
1	B	335	ILE
1	B	337	GLN
1	B	345	LYS
1	B	348	LEU
1	B	351	THR
1	B	362	THR
1	B	397	GLU
1	B	401	LEU
1	B	411	GLU
1	B	412	GLU
1	B	418	LEU
1	B	420	GLN
1	B	421	LEU
1	C	37	VAL
1	C	39	ILE
1	C	58	LEU
1	C	97	VAL
1	C	100	VAL
1	C	104	ASN
1	C	107	LEU
1	C	120	THR
1	C	123	ILE
1	C	125	ILE
1	C	132	ILE
1	C	140	VAL
1	C	143	LEU
1	C	145	MET
1	C	162	THR
1	C	166	LEU
1	C	172	SER
1	C	176	TYR
1	C	184	GLU
1	C	188	GLN

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Mol	Chain	Res	Type
1	C	213	ILE
1	C	236	LEU
1	C	258	HIS
1	C	262	THR
1	C	263	ASN
1	C	264	ILE
1	C	269	LEU
1	C	275	LYS
1	C	299	ILE
1	C	300	LEU
1	C	306	SER
1	C	310	LEU
1	C	319	LYS
1	C	320	ILE
1	C	333	ILE
1	C	335	ILE
1	C	337	GLN
1	C	340	GLU
1	C	345	LYS
1	C	348	LEU
1	C	349	GLN
1	C	351	THR
1	C	362	THR
1	C	366	THR
1	C	389	THR
1	C	400	LYS
1	C	401	LEU
1	C	407	LYS
1	C	412	GLU
1	C	418	LEU
1	C	421	LEU
1	C	425	ILE
1	D	51	THR
1	D	58	LEU
1	D	77	ARG
1	D	100	VAL
1	D	120	THR
1	D	123	ILE
1	D	132	ILE
1	D	140	VAL
1	D	143	LEU
1	D	145	MET

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Mol	Chain	Res	Type
1	D	147	THR
1	D	148	GLN
1	D	162	THR
1	D	166	LEU
1	D	170	ILE
1	D	184	GLU
1	D	204	THR
1	D	212	LEU
1	D	220	SER
1	D	239	ARG
1	D	242	VAL
1	D	250	LEU
1	D	262	THR
1	D	264	ILE
1	D	269	LEU
1	D	286	LEU
1	D	299	ILE
1	D	300	LEU
1	D	306	SER
1	D	310	LEU
1	D	333	ILE
1	D	348	LEU
1	D	349	GLN
1	D	366	THR
1	D	382	LEU
1	D	387	LEU
1	D	391	HIS
1	D	398	SER
1	D	401	LEU
1	D	414	SER
1	D	418	LEU
1	D	421	LEU
1	D	425	ILE
1	D	432	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	GLN
1	A	44	HIS
1	A	188	GLN
1	A	191	GLN

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Mol	Chain	Res	Type
1	A	252	ASN
1	A	337	GLN
1	A	355	ASN
1	A	356	ASN
1	A	368	ASN
1	A	420	GLN
1	B	36	GLN
1	B	54	ASN
1	B	94	GLN
1	B	252	ASN
1	B	296	ASN
1	B	355	ASN
1	B	356	ASN
1	B	420	GLN
1	C	36	GLN
1	C	54	ASN
1	C	133	ASN
1	C	252	ASN
1	C	318	ASN
1	C	356	ASN
1	C	420	GLN
1	D	54	ASN
1	D	124	GLN
1	D	148	GLN
1	D	177	ASN
1	D	191	GLN
1	D	318	ASN
1	D	355	ASN
1	D	356	ASN
1	D	393	GLN
1	D	431	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
2	GDP	B	593	3	24,30,30	1.00	2 (8%)	30,47,47	1.29	5 (16%)
2	GDP	D	593	3	24,30,30	1.06	2 (8%)	30,47,47	1.00	3 (10%)
2	GDP	C	593	3	24,30,30	1.03	1 (4%)	30,47,47	1.47	4 (13%)
2	GDP	A	593	3	24,30,30	1.01	1 (4%)	30,47,47	1.45	6 (20%)

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	GDP	B	593	3	-	7/12/32/32	0/3/3/3
2	GDP	D	593	3	-	5/12/32/32	0/3/3/3
2	GDP	C	593	3	-	4/12/32/32	0/3/3/3
2	GDP	A	593	3	-	4/12/32/32	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	593	GDP	C6-N1	-3.23	1.33	1.37
2	C	593	GDP	C6-N1	-2.97	1.33	1.37
2	B	593	GDP	C6-N1	-2.55	1.34	1.37
2	D	593	GDP	C6-N1	-2.54	1.34	1.37
2	B	593	GDP	C5-C4	2.20	1.48	1.43
2	D	593	GDP	O4'-C1'	2.14	1.44	1.41

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	593	GDP	PA-O3A-PB	-5.10	115.34	132.83
2	A	593	GDP	PA-O3A-PB	-3.73	120.02	132.83
2	C	593	GDP	O3B-PB-O3A	2.89	114.34	104.64
2	B	593	GDP	C5-C6-N1	2.62	118.57	113.95
2	D	593	GDP	C8-N7-C5	2.59	107.93	102.99
2	A	593	GDP	C5-C6-N1	2.56	118.47	113.95
2	B	593	GDP	C3'-C2'-C1'	2.55	104.82	100.98
2	B	593	GDP	PA-O3A-PB	-2.48	124.30	132.83
2	A	593	GDP	C8-N7-C5	2.47	107.70	102.99
2	C	593	GDP	C3'-C2'-C1'	2.35	104.51	100.98
2	B	593	GDP	C8-N7-C5	2.33	107.42	102.99
2	D	593	GDP	PA-O3A-PB	-2.23	125.17	132.83
2	C	593	GDP	C8-N7-C5	2.17	107.12	102.99
2	A	593	GDP	O5'-PA-O1A	2.09	117.22	109.07
2	A	593	GDP	C3'-C2'-C1'	2.07	104.09	100.98
2	D	593	GDP	C5-C6-N1	2.06	117.58	113.95
2	A	593	GDP	O6-C6-N1	-2.05	118.22	120.65
2	B	593	GDP	C2-N1-C6	-2.02	121.38	125.10

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	593	GDP	C5'-O5'-PA-O3A
2	A	593	GDP	C5'-O5'-PA-O1A
2	B	593	GDP	C5'-O5'-PA-O1A
2	B	593	GDP	C5'-O5'-PA-O2A
2	C	593	GDP	C5'-O5'-PA-O1A
2	D	593	GDP	C5'-O5'-PA-O1A
2	A	593	GDP	O4'-C4'-C5'-O5'
2	B	593	GDP	O4'-C4'-C5'-O5'
2	D	593	GDP	O4'-C4'-C5'-O5'
2	B	593	GDP	C3'-C4'-C5'-O5'
2	A	593	GDP	C3'-C4'-C5'-O5'
2	B	593	GDP	PA-O3A-PB-O3B
2	C	593	GDP	C5'-O5'-PA-O3A
2	D	593	GDP	C5'-O5'-PA-O3A
2	D	593	GDP	PB-O3A-PA-O1A
2	C	593	GDP	C5'-O5'-PA-O2A
2	D	593	GDP	C5'-O5'-PA-O2A
2	B	593	GDP	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
2	C	593	GDP	O4'-C4'-C5'-O5'
2	B	593	GDP	PB-O3A-PA-O1A

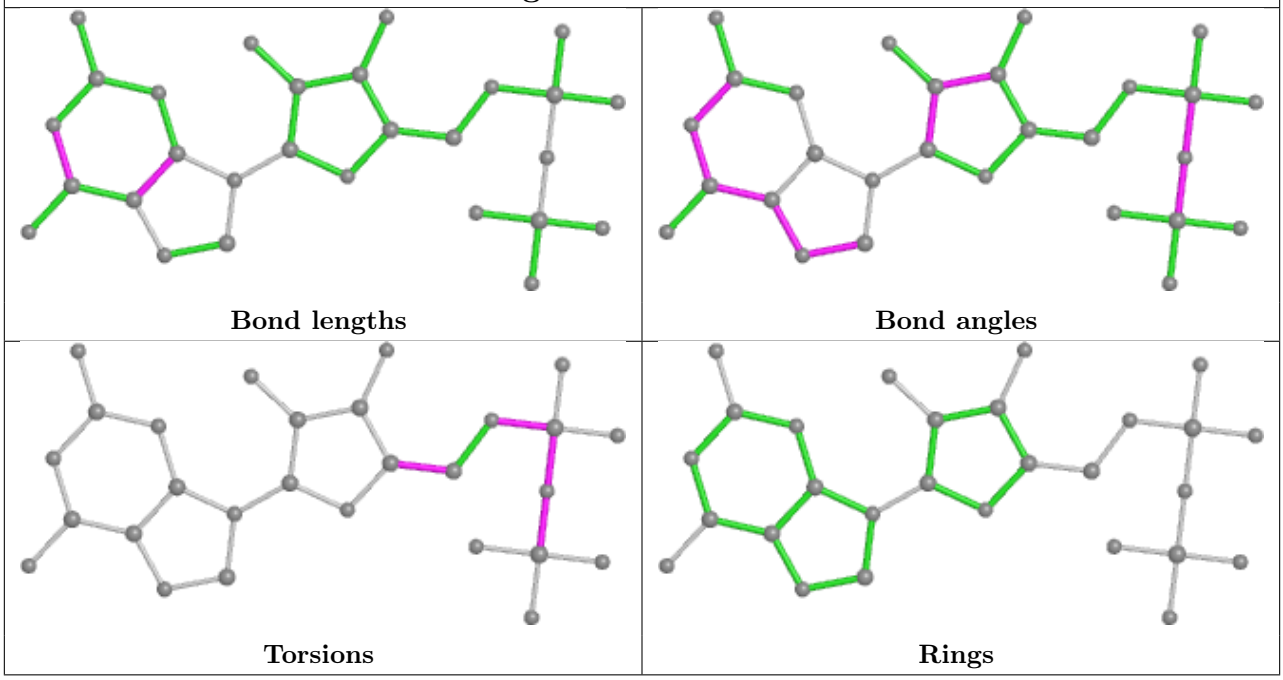
There are no ring outliers.

3 monomers are involved in 9 short contacts:

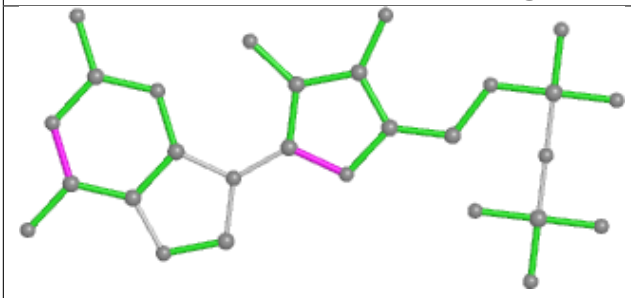
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	593	GDP	2	0
2	D	593	GDP	4	0
2	C	593	GDP	3	0

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 then 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.

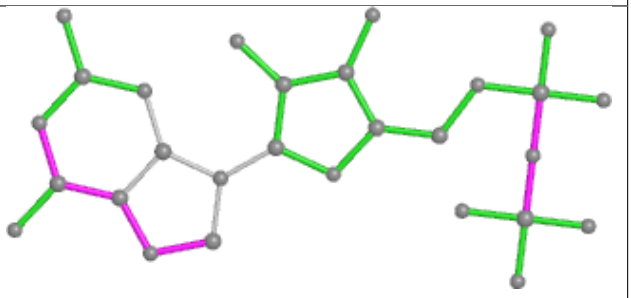
Ligand GDP B 593



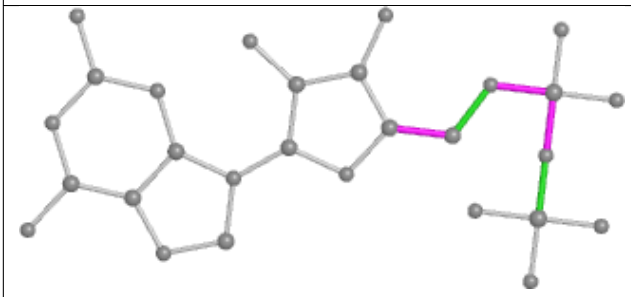
Ligand GDP D 593



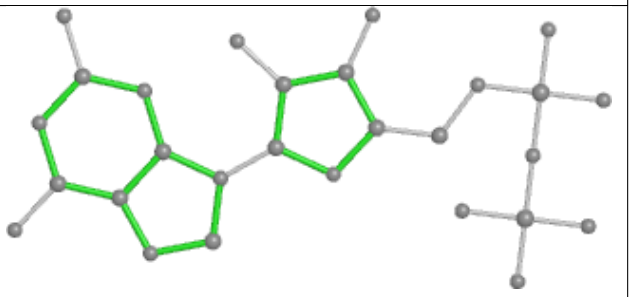
Bond lengths



Bond angles

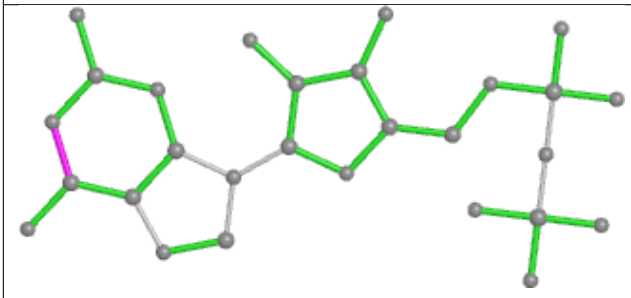


Torsions

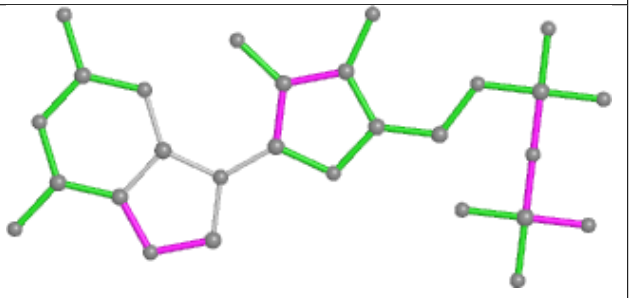


Rings

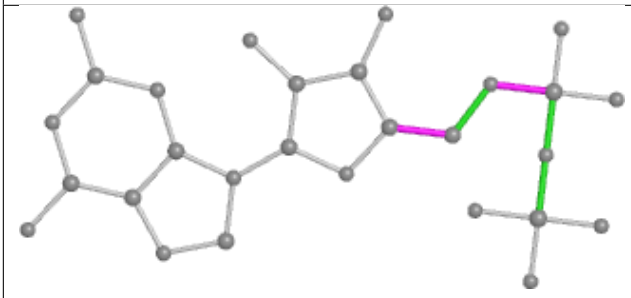
Ligand GDP C 593



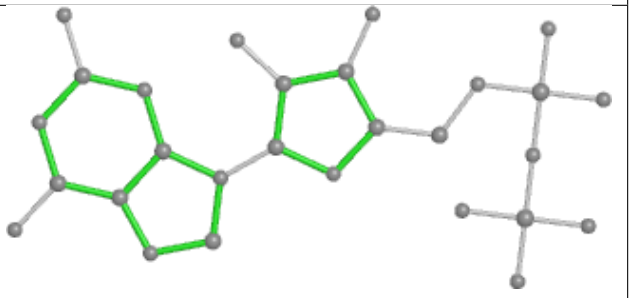
Bond lengths



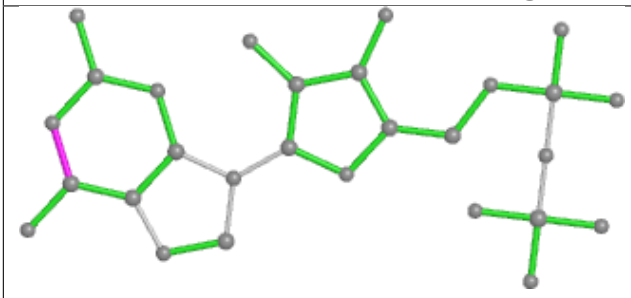
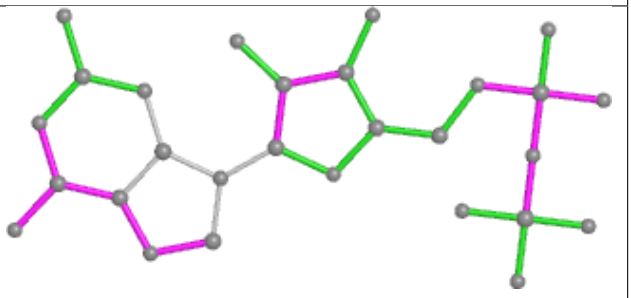
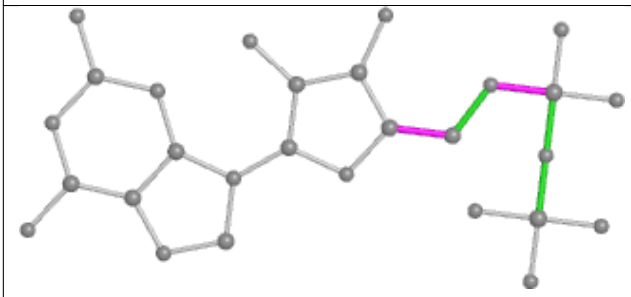
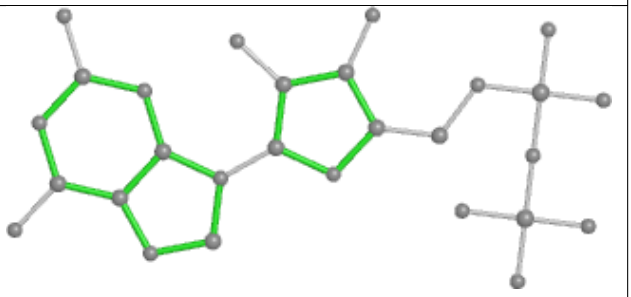
Bond angles



Torsions



Rings

Ligand GDP A 593	
 Bond lengths	 Bond angles
 Torsions	 Rings

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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	404/459 (88%)	0.25	20 (4%)	28	19	27, 71, 119, 147	0
1	B	397/459 (86%)	0.25	26 (6%)	18	11	31, 68, 138, 152	0
1	C	405/459 (88%)	0.14	16 (3%)	38	28	32, 53, 106, 158	0
1	D	398/459 (86%)	0.24	35 (8%)	10	5	34, 69, 140, 159	0
All	All	1604/1836 (87%)	0.22	97 (6%)	21	14	27, 65, 132, 159	0

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	116	SER	8.8
1	C	114	GLY	8.6
1	C	115	GLY	7.5
1	D	339	GLU	6.3
1	C	153	SER	6.0
1	D	380	PRO	5.8
1	B	374	ILE	5.7
1	B	155	SER	5.7
1	D	155	SER	5.6
1	C	118	ARG	5.2
1	C	152	ASP	5.0
1	D	375	CYS	5.0
1	D	337	GLN	4.9
1	C	117	GLU	4.9
1	D	40	VAL	4.8
1	D	116	SER	4.6
1	A	339	GLU	4.5
1	B	156	THR	4.4
1	D	385	ASN	4.4
1	A	39	ILE	4.4
1	B	387	LEU	4.3

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Mol	Chain	Res	Type	RSRZ
1	C	156	THR	4.3
1	D	341	LEU	4.1
1	A	374	ILE	4.1
1	D	376	GLY	4.0
1	D	340	GLU	4.0
1	A	115	GLY	3.9
1	B	375	CYS	3.9
1	A	44	HIS	3.9
1	D	378	ASP	3.8
1	A	158	ARG	3.8
1	D	39	ILE	3.8
1	D	338	GLY	3.7
1	B	386	ASP	3.7
1	D	384	PRO	3.7
1	B	378	ASP	3.5
1	A	373	GLU	3.5
1	C	150	THR	3.4
1	B	392	LEU	3.4
1	D	374	ILE	3.3
1	B	116	SER	3.2
1	A	428	LEU	3.2
1	A	381	PHE	3.2
1	B	389	THR	3.2
1	B	377	GLY	3.1
1	A	388	GLN	3.0
1	D	44	HIS	3.0
1	D	377	GLY	3.0
1	B	376	GLY	3.0
1	C	157	LEU	2.9
1	D	118	ARG	2.9
1	A	387	LEU	2.9
1	C	110	PHE	2.8
1	B	371	MET	2.8
1	D	432	TYR	2.8
1	A	377	GLY	2.8
1	C	42	ASP	2.8
1	B	396	GLU	2.7
1	D	158	ARG	2.7
1	A	159	ASP	2.6
1	A	38	LEU	2.6
1	C	40	VAL	2.6
1	A	389	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	115	GLY	2.6
1	D	379	LYS	2.6
1	D	154	GLN	2.6
1	D	153	SER	2.6
1	D	386	ASP	2.6
1	C	378	ASP	2.5
1	D	42	ASP	2.5
1	D	149	GLY	2.5
1	D	41	LYS	2.4
1	A	378	ASP	2.4
1	B	107	LEU	2.3
1	D	157	LEU	2.3
1	D	388	GLN	2.3
1	D	425	ILE	2.3
1	C	119	GLU	2.3
1	B	365	ASP	2.2
1	B	370	LYS	2.2
1	D	431	GLN	2.2
1	A	380	PRO	2.2
1	C	155	SER	2.2
1	A	116	SER	2.2
1	B	380	PRO	2.2
1	B	363	ALA	2.2
1	D	48	LEU	2.2
1	B	393	GLN	2.1
1	B	428	LEU	2.1
1	D	382	LEU	2.1
1	A	41	LYS	2.1
1	B	154	GLN	2.1
1	B	96	SER	2.1
1	A	340	GLU	2.1
1	B	40	VAL	2.0
1	B	431	GLN	2.0
1	B	385	ASN	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 monosaccharides in this entry.

6.4 Ligands (i)

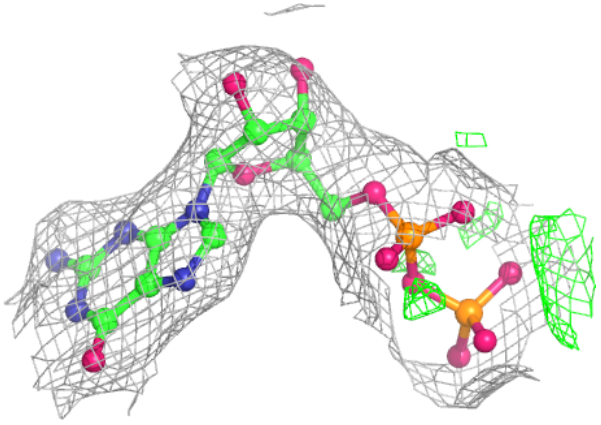
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

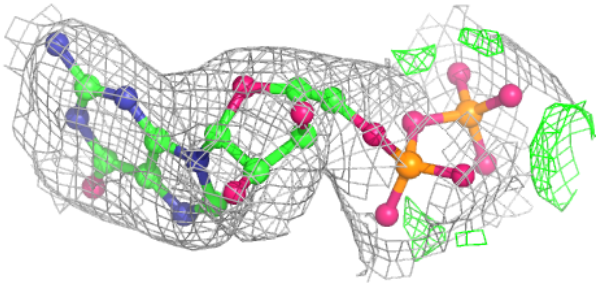
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	D	595	1/1	0.86	0.14	69,69,69,69	0
3	MG	C	595	1/1	0.89	0.19	57,57,57,57	0
3	MG	B	595	1/1	0.94	0.21	70,70,70,70	0
2	GDP	A	593	28/28	0.95	0.16	35,54,69,75	0
3	MG	A	595	1/1	0.96	0.29	68,68,68,68	0
2	GDP	B	593	28/28	0.96	0.14	32,46,70,76	0
2	GDP	D	593	28/28	0.97	0.13	35,49,61,69	0
2	GDP	C	593	28/28	0.98	0.15	38,47,56,65	0

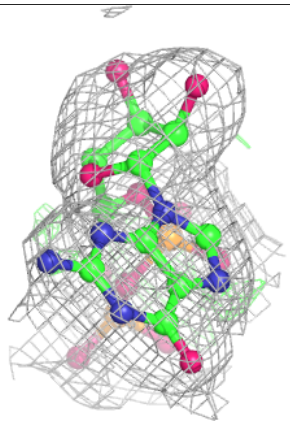
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GDP A 593:

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

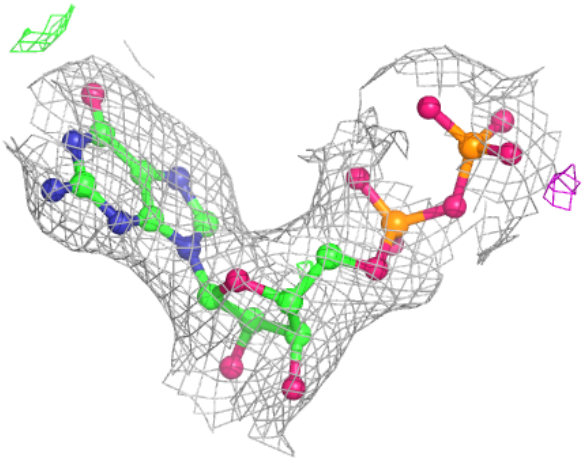


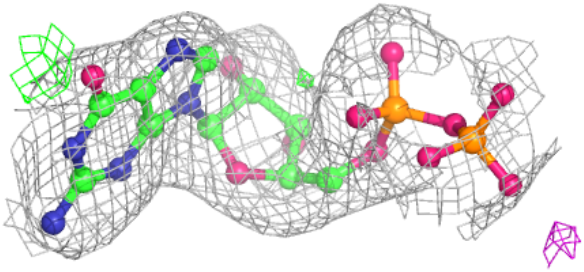


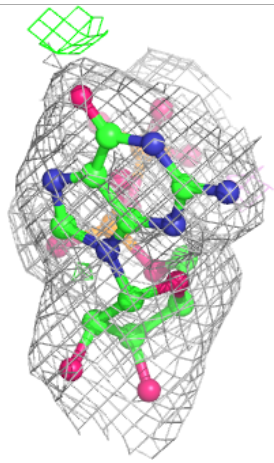


Electron density around GDP B 593:

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

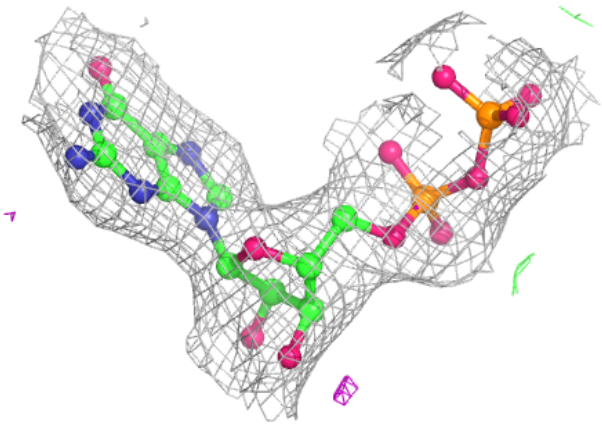


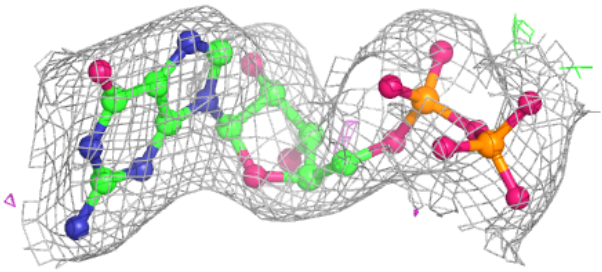


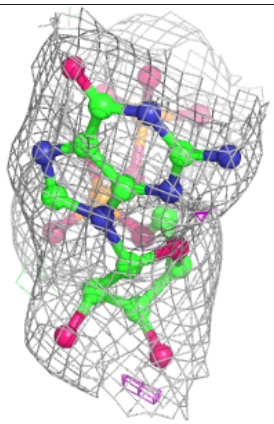


Electron density around GDP D 593:

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

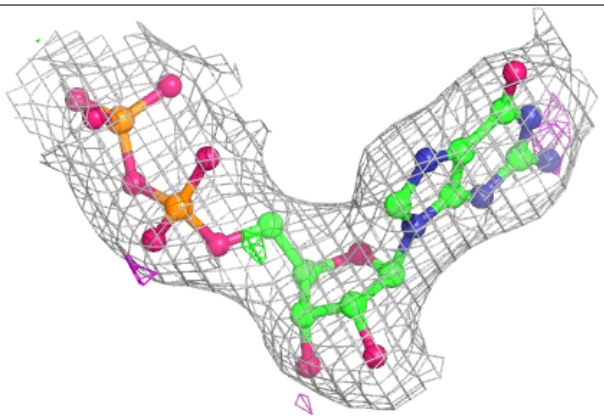


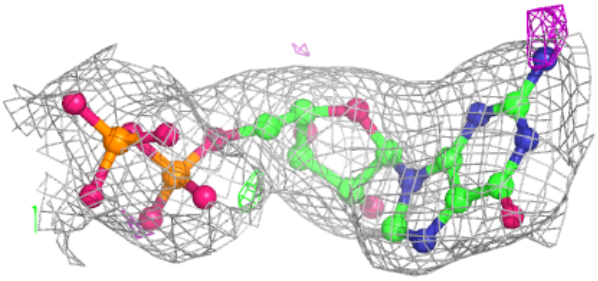


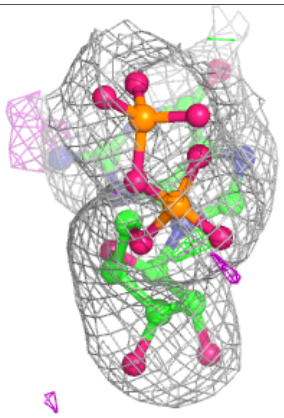


Electron density around GDP C 593:

$2mF_o$-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.