Full wwPDB X-ray Structure Validation Report (i)

Feb 14, 2017 – 10:34 am GMT

PDB ID	:	3P27
Title	:	Crystal structure of S. cerevisiae Hbs1 protein (GDP-bound form), a translational GTPase involved in RNA quality control pathways and interacting with Dom34/Pelota
Authors	:	van den Elzen, A.; Henri, J.; Lazar, N.; Gas, M.E.; Durand, D.; Lacroute, F.; Nicaise, M.; van Tilbeurgh, H.; Sraphin, B.; Graille, M.; Paris-Sud Yeast Structural Genomics (YSG)
Deposited on	:	2010-10-01
Resolution	:	2.95 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

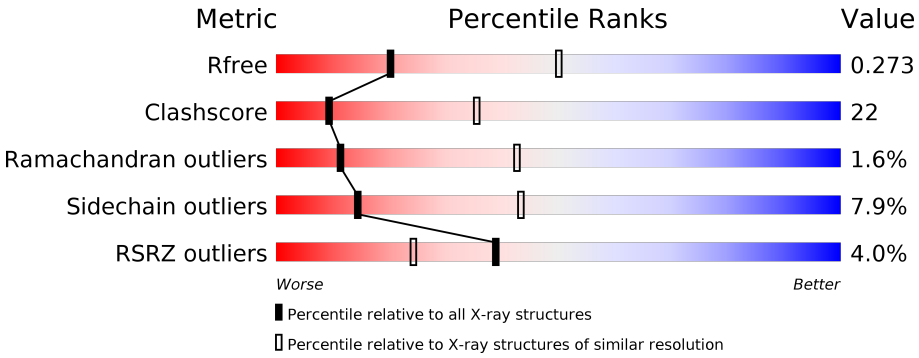
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

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 2.95 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}	100719	2395 (3.00-2.92)
Clashscore	112137	2773 (3.00-2.92)
Ramachandran outliers	110173	2680 (3.00-2.92)
Sidechain outliers	110143	2683 (3.00-2.92)
RSRZ outliers	101464	2421 (3.00-2.92)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	483	4% 54% 33% • 10%
1	B	483	4% 55% 33% • 8%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7043 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.

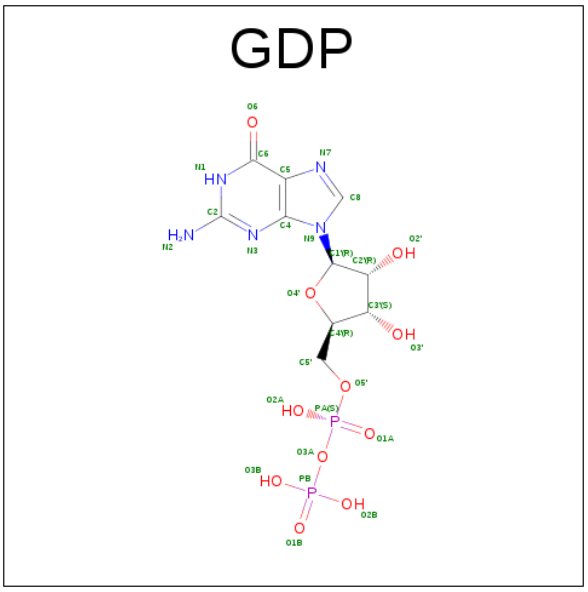
- Molecule 1 is a protein called Elongation factor 1 alpha-like protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	433	Total	C	N	O	S	Se	0	0	0
			3414	2178	583	639	5	9			
1	B	444	Total	C	N	O	S	Se	0	0	0
			3509	2232	605	658	5	9			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	612	HIS	-	EXPRESSION TAG	UNP P32769
A	613	HIS	-	EXPRESSION TAG	UNP P32769
A	614	HIS	-	EXPRESSION TAG	UNP P32769
A	615	HIS	-	EXPRESSION TAG	UNP P32769
A	616	HIS	-	EXPRESSION TAG	UNP P32769
A	617	HIS	-	EXPRESSION TAG	UNP P32769
B	612	HIS	-	EXPRESSION TAG	UNP P32769
B	613	HIS	-	EXPRESSION TAG	UNP P32769
B	614	HIS	-	EXPRESSION TAG	UNP P32769
B	615	HIS	-	EXPRESSION TAG	UNP P32769
B	616	HIS	-	EXPRESSION TAG	UNP P32769
B	617	HIS	-	EXPRESSION TAG	UNP P32769

- 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 28 10 5 11 2	0	0
2	B	1	Total C N O P 28 10 5 11 2	0	0

- Molecule 3 is water.

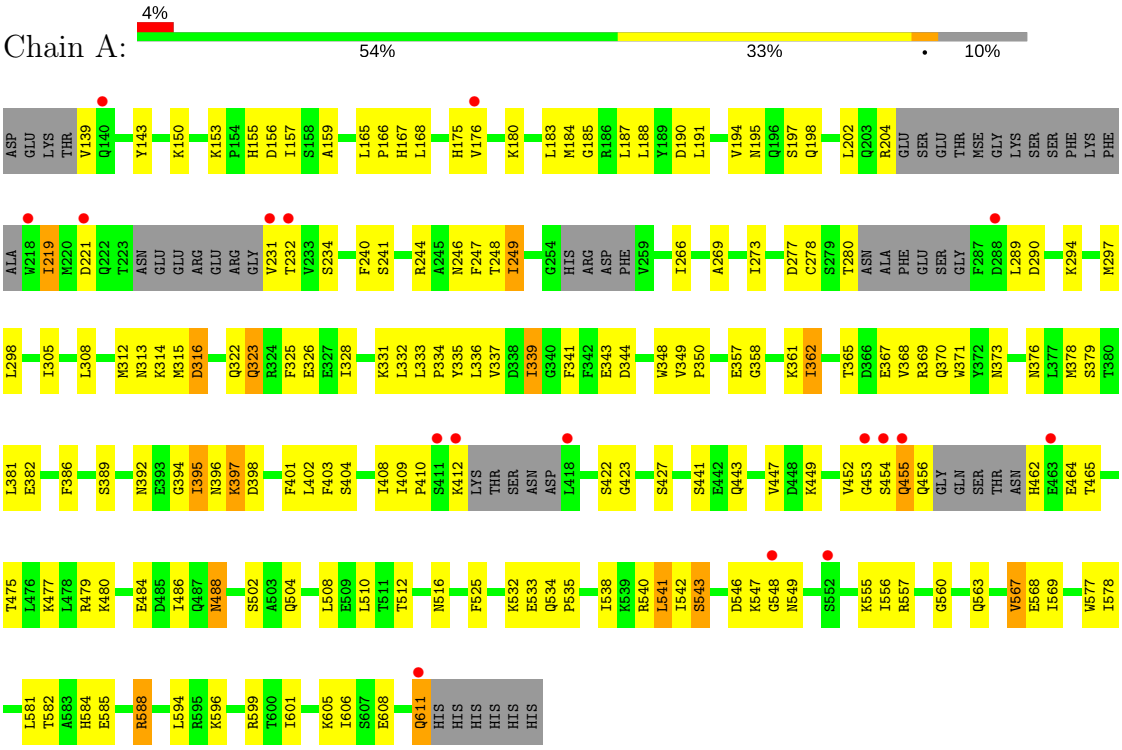
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	31	Total O 31 31	0	0
3	B	33	Total O 33 33	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

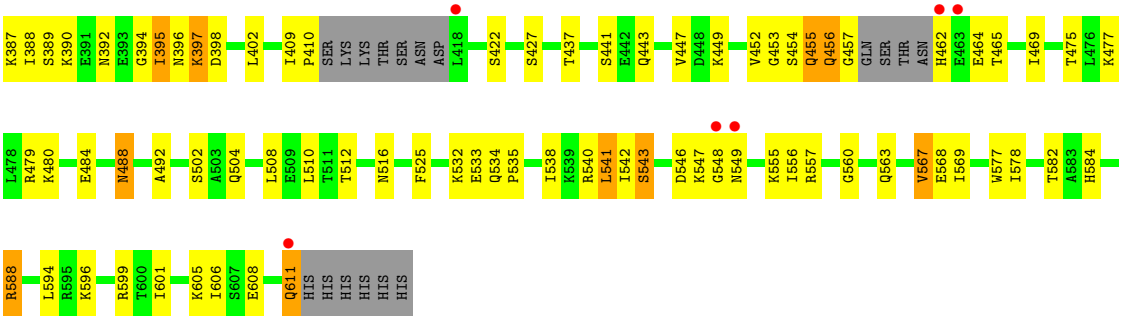
• Molecule 1: Elongation factor 1 alpha-like protein

Chain A:



• Molecule 1: Elongation factor 1 alpha-like protein

Chain B:


K387 I388 S389 K390 E391 N392 E393 G394 I395 N396 K397 D398 L402 I409 P410 SER LYS LYS THR SER ASN ASP L418 S422 S427 T437 S441 E442 Q443 V447 D448 K449 V452 G453 S454 Q455 Q456 G457 GLN SER THR ASN H462 E463 E464 T465 I469 T475 L476 K477
L478 R479 K480 E484 N488 A492 S502 A503 Q504 L508 E509 L510 T511 T512 N516 F525 K532 E533 Q534 P535 I538 K539 R540 L541 I542 S543 D546 K547 G548 N549 K555 I556 R557 G560 Q563 V567 E568 I569 W577 I578 T582 A583 H584
R588 L594 R595 K596 R599 T600 I601 K605 I606 S607 E608 Q611 HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α, β, γ	109.96Å 109.96Å 188.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 – 2.95 19.98 – 2.95	Depositor EDS
% Data completeness (in resolution range)	98.2 (19.98-2.95) 98.5 (19.98-2.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.35 (at 2.93Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.214 , 0.278 0.207 , 0.273	Depositor DCC
R_{free} test set	2304 reflections (5.08%)	DCC
Wilson B-factor (Å^2)	55.1	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 42.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7043	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.00 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.0560e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: 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	0.52	0/3467	0.67	0/4667
1	B	0.53	0/3566	0.67	0/4802
All	All	0.52	0/7033	0.67	0/9469

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3414	0	3457	155	0
1	B	3509	0	3535	168	0
2	A	28	0	12	5	0
2	B	28	0	12	3	0
3	A	31	0	0	3	0
3	B	33	0	0	0	0
All	All	7043	0	7016	306	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 22.

All (306) 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:175:HIS:CE1	1:A:176:VAL:HG12	2.04	0.93
1:A:611:GLN:HE21	1:B:611:GLN:HE21	1.13	0.92
1:B:175:HIS:CE1	1:B:176:VAL:HG12	2.05	0.91
1:A:167:HIS:HE1	1:A:248:THR:OG1	1.56	0.88
1:B:167:HIS:HE1	1:B:248:THR:OG1	1.59	0.86
1:B:187:LEU:HD11	1:B:378:MSE:CE	2.06	0.85
1:A:297:MSE:HE1	1:A:308:LEU:HD13	1.59	0.84
1:A:512:THR:HG22	1:A:563:GLN:H	1.41	0.83
1:A:187:LEU:HD11	1:A:378:MSE:CE	2.09	0.83
1:A:187:LEU:HD11	1:A:378:MSE:HE3	1.61	0.82
1:B:452:VAL:HG22	1:B:453:GLY:H	1.42	0.82
1:B:187:LEU:HD11	1:B:378:MSE:HE3	1.61	0.81
1:B:512:THR:HG22	1:B:563:GLN:H	1.46	0.80
1:B:240:PHE:HE1	1:B:249:ILE:HD11	1.46	0.80
1:A:240:PHE:HE1	1:A:249:ILE:HD11	1.46	0.80
1:A:297:MSE:CE	1:A:308:LEU:HD13	2.12	0.79
1:B:512:THR:CG2	1:B:563:GLN:H	1.94	0.79
1:A:452:VAL:HG22	1:A:453:GLY:H	1.46	0.78
1:A:488:ASN:H	1:A:488:ASN:HD22	1.30	0.77
1:A:512:THR:CG2	1:A:563:GLN:H	1.97	0.77
1:A:358:GLY:O	1:A:376:ASN:HB2	1.85	0.76
1:B:297:MSE:CE	1:B:308:LEU:HD13	2.15	0.76
1:B:488:ASN:HD22	1:B:488:ASN:H	1.33	0.76
1:B:367:GLU:O	1:B:370:GLN:HG2	1.86	0.76
1:A:231:VAL:HG13	1:A:232:THR:H	1.52	0.75
1:B:297:MSE:HE1	1:B:308:LEU:HD13	1.68	0.75
1:B:525:PHE:HZ	1:B:569:ILE:HD12	1.51	0.74
1:B:231:VAL:HG13	1:B:232:THR:H	1.53	0.74
1:A:525:PHE:HZ	1:A:569:ILE:HD12	1.54	0.73
1:A:297:MSE:HE1	1:A:308:LEU:CD1	2.19	0.72
1:B:240:PHE:CE1	1:B:249:ILE:HD11	2.24	0.72
1:A:449:LYS:HE2	1:A:464:GLU:OE2	1.90	0.72
1:A:240:PHE:CE1	1:A:249:ILE:HD11	2.24	0.71
1:B:452:VAL:HG22	1:B:453:GLY:N	2.04	0.71
1:B:333:LEU:O	1:B:337:VAL:HG23	1.91	0.70
1:B:358:GLY:O	1:B:376:ASN:HB2	1.90	0.69
1:B:278:CYS:SG	1:B:312:MSE:HE3	2.33	0.69
1:A:452:VAL:HG22	1:A:453:GLY:N	2.08	0.69
1:B:449:LYS:HE2	1:B:464:GLU:OE2	1.92	0.69
1:A:611:GLN:HE21	1:B:611:GLN:NE2	1.88	0.69
1:B:588:ARG:HH11	1:B:588:ARG:HG3	1.56	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:LEU:O	1:A:337:VAL:HG23	1.93	0.68
1:A:367:GLU:O	1:A:370:GLN:HG2	1.93	0.68
1:B:195:ASN:HD22	1:B:197:SER:H	1.41	0.68
1:B:258:PHE:HB3	1:B:261:ASN:HD22	1.58	0.68
1:B:331:LYS:O	1:B:334:PRO:HD2	1.93	0.67
1:A:608:GLU:HG3	1:B:608:GLU:HG3	1.75	0.67
1:A:611:GLN:NE2	1:B:611:GLN:HE21	1.91	0.67
1:A:549:ASN:HB3	1:B:605:LYS:NZ	2.09	0.67
1:A:331:LYS:O	1:A:334:PRO:HD2	1.94	0.65
1:B:297:MSE:HE1	1:B:308:LEU:HD22	1.76	0.65
1:B:508:LEU:HD22	1:B:569:ILE:HG13	1.78	0.65
1:A:605:LYS:NZ	1:B:549:ASN:HB3	2.11	0.65
1:A:512:THR:HG21	1:A:560:GLY:O	1.96	0.65
1:B:512:THR:HG21	1:B:560:GLY:O	1.96	0.64
1:B:297:MSE:HE1	1:B:308:LEU:CD1	2.28	0.64
1:B:397:LYS:HD3	1:B:397:LYS:N	2.13	0.63
1:A:195:ASN:HD22	1:A:197:SER:H	1.45	0.63
1:A:362:ILE:HG23	3:A:6:HOH:O	1.99	0.63
1:A:508:LEU:HD22	1:A:569:ILE:HG13	1.81	0.62
1:A:542:ILE:O	1:A:543:SER:HB3	1.99	0.61
1:A:588:ARG:HG3	1:A:588:ARG:HH11	1.64	0.61
1:B:534:GLN:NE2	1:B:535:PRO:HD2	2.16	0.61
1:B:313:ASN:OD1	1:B:314:LYS:N	2.33	0.61
1:B:180:LYS:HB2	2:B:663:GDP:O2B	2.01	0.61
1:B:218:TRP:C	1:B:218:TRP:CD1	2.74	0.61
1:A:326:GLU:HG3	3:A:18:HOH:O	1.99	0.61
1:B:308:LEU:HD11	1:B:341:PHE:CE1	2.36	0.60
1:B:322:GLN:HB2	1:B:371:TRP:CD2	2.36	0.60
1:A:534:GLN:NE2	1:A:535:PRO:HD2	2.16	0.60
1:B:240:PHE:HE1	1:B:249:ILE:CD1	2.15	0.60
1:A:175:HIS:CD2	1:A:290:ASP:OD2	2.54	0.60
1:A:397:LYS:N	1:A:397:LYS:HD3	2.17	0.60
1:A:240:PHE:HE1	1:A:249:ILE:CD1	2.13	0.60
1:B:525:PHE:CZ	1:B:569:ILE:HD12	2.35	0.60
1:A:278:CYS:SG	1:A:312:MSE:HE3	2.42	0.60
1:B:175:HIS:CD2	1:B:290:ASP:OD2	2.55	0.60
1:B:316:ASP:N	1:B:316:ASP:OD1	2.31	0.60
1:A:167:HIS:CE1	1:A:248:THR:OG1	2.48	0.59
1:A:269:ALA:O	1:A:588:ARG:NH2	2.33	0.59
1:A:488:ASN:N	1:A:488:ASN:HD22	1.99	0.59
1:B:308:LEU:HD11	1:B:341:PHE:CZ	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:GLN:HB2	1:A:371:TRP:CD2	2.38	0.59
1:A:456:GLN:HG2	1:A:475:THR:OG1	2.03	0.58
1:B:185:GLY:HA2	1:B:219:ILE:HD11	1.85	0.58
1:B:297:MSE:HE1	1:B:308:LEU:CD2	2.33	0.58
1:B:452:VAL:CG2	1:B:453:GLY:H	2.16	0.58
1:A:308:LEU:HD11	1:A:341:PHE:CE1	2.39	0.58
1:B:258:PHE:HB3	1:B:261:ASN:ND2	2.19	0.58
1:B:456:GLN:HG2	1:B:475:THR:OG1	2.03	0.58
1:A:297:MSE:HE1	1:A:308:LEU:HD22	1.86	0.58
1:B:512:THR:HG22	1:B:563:GLN:N	2.16	0.58
1:B:183:LEU:O	1:B:183:LEU:HD12	2.04	0.58
1:B:542:ILE:O	1:B:543:SER:HB3	2.05	0.57
1:A:512:THR:HG22	1:A:563:GLN:N	2.14	0.57
1:A:549:ASN:HB3	1:B:605:LYS:HZ2	1.69	0.57
1:A:441:SER:OG	1:A:443:GLN:HG2	2.05	0.57
1:A:540:ARG:HB2	1:A:568:GLU:HB3	1.87	0.56
1:B:167:HIS:CE1	1:B:248:THR:OG1	2.50	0.56
1:B:512:THR:HG22	1:B:563:GLN:O	2.05	0.56
1:A:184:MSE:HA	1:A:184:MSE:HE2	1.86	0.56
1:A:316:ASP:OD2	2:A:663:GDP:N2	2.38	0.56
1:B:289:LEU:HG	1:B:294:LYS:HE3	1.87	0.56
1:B:455:GLN:O	1:B:457:GLY:N	2.39	0.56
1:A:297:MSE:CE	1:A:308:LEU:CD1	2.83	0.56
1:B:184:MSE:HE2	1:B:184:MSE:HA	1.87	0.56
1:A:289:LEU:HG	1:A:294:LYS:HE3	1.88	0.56
1:B:357:GLU:HA	1:B:362:ILE:HG13	1.87	0.56
1:A:175:HIS:CG	1:A:176:VAL:H	2.24	0.56
1:B:441:SER:OG	1:B:443:GLN:HG2	2.06	0.56
1:A:277:ASP:CG	1:A:314:LYS:HD2	2.25	0.55
1:B:277:ASP:CG	1:B:314:LYS:HD2	2.27	0.55
1:A:313:ASN:OD1	1:A:314:LYS:N	2.39	0.55
1:B:175:HIS:CG	1:B:176:VAL:H	2.24	0.55
1:B:488:ASN:N	1:B:488:ASN:HD22	2.01	0.55
1:A:357:GLU:HA	1:A:362:ILE:HG13	1.87	0.55
1:A:525:PHE:CZ	1:A:569:ILE:HD12	2.39	0.55
1:B:488:ASN:O	1:B:532:LYS:HE3	2.07	0.55
1:A:369:ARG:HH11	1:A:373:ASN:HA	1.72	0.54
1:A:277:ASP:OD2	1:A:314:LYS:HD2	2.08	0.54
1:B:269:ALA:O	1:B:588:ARG:NH2	2.41	0.54
1:B:277:ASP:OD2	1:B:314:LYS:HD2	2.08	0.53
1:A:297:MSE:HE1	1:A:308:LEU:CD2	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:479:ARG:O	1:A:480:LYS:HB2	2.08	0.53
1:B:230:GLY:O	1:B:231:VAL:C	2.47	0.53
1:A:183:LEU:O	1:A:183:LEU:HD12	2.09	0.53
1:B:365:THR:HB	1:B:368:VAL:HG23	1.90	0.53
1:B:258:PHE:HD1	1:B:261:ASN:HD21	1.56	0.53
1:B:333:LEU:HD11	1:B:343:GLU:HG3	1.90	0.53
1:A:488:ASN:O	1:A:532:LYS:HE3	2.08	0.53
1:B:218:TRP:C	1:B:218:TRP:HD1	2.12	0.53
1:A:308:LEU:HD11	1:A:341:PHE:CZ	2.44	0.53
1:B:582:THR:HG22	1:B:606:ILE:HG22	1.91	0.53
1:B:256:ARG:HD3	1:B:256:ARG:O	2.10	0.52
1:B:540:ARG:HB2	1:B:568:GLU:HB3	1.89	0.52
1:A:175:HIS:CG	1:A:176:VAL:N	2.77	0.52
1:A:333:LEU:HB3	1:A:334:PRO:HD3	1.92	0.52
1:A:190:ASP:OD2	1:A:361:LYS:HB2	2.10	0.52
1:A:185:GLY:HA2	1:A:219:ILE:HD11	1.92	0.51
1:A:315:MSE:HE1	1:A:325:PHE:HB2	1.91	0.51
1:A:452:VAL:CG2	1:A:453:GLY:H	2.20	0.51
1:B:175:HIS:CG	1:B:176:VAL:N	2.78	0.51
1:B:244:ARG:HD3	1:B:382:GLU:OE2	2.09	0.51
1:A:382:GLU:O	1:A:386:PHE:HD2	1.93	0.51
1:A:180:LYS:HB2	2:A:663:GDP:O2B	2.11	0.51
1:B:452:VAL:CG2	1:B:453:GLY:N	2.74	0.51
1:B:297:MSE:CE	1:B:308:LEU:CD1	2.86	0.51
1:B:333:LEU:HB3	1:B:334:PRO:HD3	1.92	0.51
1:A:605:LYS:HZ1	1:B:549:ASN:HB3	1.76	0.51
1:A:195:ASN:HB3	1:A:198:GLN:H	1.75	0.50
1:B:588:ARG:HH11	1:B:588:ARG:CG	2.23	0.50
1:A:195:ASN:N	1:A:198:GLN:OE1	2.43	0.50
1:A:202:LEU:HD11	1:A:219:ILE:HG13	1.92	0.50
1:A:362:ILE:O	1:A:362:ILE:HG13	2.11	0.50
1:A:512:THR:HG22	1:A:563:GLN:O	2.10	0.50
1:B:219:ILE:O	1:B:223:THR:HG23	2.12	0.50
1:B:369:ARG:HH11	1:B:373:ASN:HA	1.75	0.50
1:A:488:ASN:ND2	1:A:488:ASN:H	2.05	0.50
1:A:333:LEU:HD11	1:A:343:GLU:HG3	1.93	0.50
1:A:502:SER:HB3	1:A:577:TRP:HB3	1.92	0.50
1:B:195:ASN:HB3	1:B:198:GLN:H	1.77	0.50
1:B:315:MSE:HE1	1:B:325:PHE:HB2	1.93	0.50
1:A:585:GLU:CD	1:B:540:ARG:HH22	2.14	0.50
1:B:258:PHE:HD1	1:B:261:ASN:ND2	2.09	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:453:GLY:O	1:B:456:GLN:HB2	2.12	0.49
1:B:362:ILE:O	1:B:362:ILE:HG13	2.12	0.49
1:A:312:MSE:HE1	1:A:328:ILE:HB	1.94	0.49
1:B:588:ARG:HG3	1:B:588:ARG:NH1	2.24	0.49
1:B:262:ALA:O	1:B:266:ILE:HG13	2.13	0.49
1:A:333:LEU:HD12	1:A:333:LEU:O	2.13	0.48
1:B:402:LEU:HB2	1:B:427:SER:HB3	1.95	0.48
1:A:156:ASP:HB3	1:A:159:ALA:HB3	1.95	0.48
1:B:538:ILE:HG21	1:B:541:LEU:HD13	1.93	0.48
1:A:608:GLU:HA	1:B:608:GLU:HG3	1.95	0.48
1:A:582:THR:HG22	1:A:606:ILE:HG22	1.95	0.48
1:A:336:LEU:O	1:A:339:ILE:HG22	2.13	0.48
1:B:312:MSE:HE1	1:B:328:ILE:HB	1.95	0.48
1:B:392:ASN:N	1:B:392:ASN:HD22	2.09	0.48
1:B:252:ALA:H	1:B:256:ARG:HH21	1.62	0.48
1:B:502:SER:HB3	1:B:577:TRP:HB3	1.93	0.48
1:A:538:ILE:HG21	1:A:541:LEU:HD13	1.96	0.48
1:A:143:TYR:C	1:A:143:TYR:CD2	2.86	0.48
1:B:227:ARG:HD3	1:B:457:GLY:HA3	1.95	0.48
1:A:605:LYS:HZ3	1:B:549:ASN:HB3	1.77	0.48
1:B:541:LEU:HD12	1:B:567:VAL:HG22	1.95	0.48
1:A:453:GLY:O	1:A:456:GLN:HB2	2.14	0.47
1:B:449:LYS:HB2	1:B:477:LYS:HB3	1.95	0.47
1:A:452:VAL:CG2	1:A:453:GLY:N	2.77	0.47
1:B:479:ARG:O	1:B:480:LYS:HB2	2.14	0.47
1:A:188:LEU:O	1:A:191:LEU:HB2	2.14	0.47
1:A:588:ARG:NH1	1:A:588:ARG:HG3	2.30	0.47
1:A:167:HIS:HA	1:A:246:ASN:O	2.15	0.47
1:A:608:GLU:HG3	1:B:608:GLU:CG	2.43	0.47
1:B:488:ASN:ND2	1:B:488:ASN:H	2.07	0.47
1:B:332:LEU:HD23	1:B:348:TRP:CZ3	2.50	0.47
1:A:549:ASN:HB3	1:B:605:LYS:HZ1	1.78	0.47
1:A:332:LEU:HD23	1:A:348:TRP:CZ3	2.50	0.47
1:B:184:MSE:HB3	1:B:219:ILE:HD13	1.97	0.47
1:A:599:ARG:O	1:A:601:ILE:HG23	2.15	0.46
1:B:588:ARG:NH1	1:B:588:ARG:CG	2.76	0.46
1:A:409:ILE:HA	1:A:410:PRO:HD3	1.73	0.46
1:A:244:ARG:HD3	1:A:382:GLU:OE2	2.15	0.46
1:A:516:ASN:HD21	1:A:599:ARG:HH21	1.62	0.46
1:A:392:ASN:N	1:A:392:ASN:HD22	2.14	0.46
1:A:488:ASN:ND2	1:A:488:ASN:N	2.61	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:THR:OG1	2:B:663:GDP:H8	1.99	0.46
1:A:365:THR:HB	1:A:368:VAL:HG23	1.97	0.46
1:A:449:LYS:HB2	1:A:477:LYS:HB3	1.98	0.46
1:B:156:ASP:HB3	1:B:159:ALA:HB3	1.97	0.46
1:A:323:GLN:NE2	3:A:47:HOH:O	2.49	0.45
1:A:349:VAL:HA	1:A:350:PRO:HD3	1.86	0.45
1:A:541:LEU:HD12	1:A:567:VAL:HG22	1.99	0.45
1:A:195:ASN:HB2	1:A:198:GLN:OE1	2.16	0.45
1:A:168:LEU:O	1:A:247:PHE:HA	2.17	0.45
1:B:190:ASP:OD2	1:B:361:LYS:HB2	2.16	0.45
1:A:298:LEU:HD13	1:A:339:ILE:HG12	1.98	0.45
1:A:510:LEU:HD11	1:A:594:LEU:HD22	1.98	0.45
1:A:396:ASN:HB3	1:A:398:ASP:H	1.81	0.45
1:A:408:ILE:HD11	1:A:486:ILE:HG22	1.98	0.45
1:B:382:GLU:O	1:B:386:PHE:HD2	2.00	0.45
1:A:608:GLU:CG	1:B:608:GLU:HG3	2.46	0.45
1:B:298:LEU:HA	1:B:339:ILE:HD11	1.98	0.45
1:B:396:ASN:HB3	1:B:398:ASP:H	1.81	0.45
1:B:336:LEU:O	1:B:339:ILE:HG22	2.16	0.45
1:A:153:LYS:O	1:A:155:HIS:HD2	2.00	0.44
1:A:402:LEU:HB2	1:A:427:SER:HB3	2.00	0.44
1:A:608:GLU:HG3	1:B:608:GLU:HA	2.00	0.44
1:B:143:TYR:CD2	1:B:143:TYR:C	2.90	0.44
1:B:510:LEU:HD11	1:B:594:LEU:HD22	1.98	0.44
1:A:150:LYS:HB2	1:A:150:LYS:HE3	1.79	0.44
1:A:294:LYS:HG2	1:A:335:TYR:CE1	2.53	0.44
1:B:168:LEU:O	1:B:247:PHE:HA	2.16	0.44
1:A:266:ILE:HG23	1:A:305:ILE:HD12	2.00	0.43
1:B:218:TRP:O	1:B:218:TRP:HD1	2.01	0.43
1:B:312:MSE:HE1	1:B:328:ILE:CG2	2.48	0.43
1:B:317:ASN:OD1	2:B:663:GDP:N2	2.52	0.43
1:A:156:ASP:O	1:A:159:ALA:HB3	2.18	0.43
1:B:376:ASN:OD1	1:B:379:SER:HB2	2.18	0.43
1:B:556:ILE:O	1:B:556:ILE:HG23	2.19	0.43
1:A:394:GLY:O	1:A:395:ILE:C	2.57	0.43
1:B:333:LEU:N	1:B:334:PRO:CD	2.82	0.43
1:A:455:GLN:OE1	1:A:462:HIS:HB3	2.19	0.43
1:A:176:VAL:O	2:A:663:GDP:O1B	2.37	0.43
1:B:255:HIS:CB	1:B:258:PHE:HB2	2.49	0.43
1:B:258:PHE:CD1	1:B:261:ASN:ND2	2.86	0.43
1:A:369:ARG:HA	1:A:369:ARG:HD3	1.65	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:488:ASN:ND2	1:B:488:ASN:N	2.62	0.42
1:A:581:LEU:HA	1:A:581:LEU:HD12	1.75	0.42
1:B:167:HIS:HA	1:B:246:ASN:O	2.19	0.42
1:B:596:LYS:HB2	1:B:596:LYS:HE3	1.81	0.42
1:A:401:PHE:CZ	1:A:403:PHE:HB2	2.54	0.42
1:B:195:ASN:HB2	1:B:198:GLN:OE1	2.19	0.42
1:A:298:LEU:HA	1:A:339:ILE:HD11	2.01	0.42
1:B:455:GLN:OE1	1:B:462:HIS:HB3	2.19	0.42
1:B:156:ASP:O	1:B:159:ALA:HB3	2.19	0.42
1:B:231:VAL:HG13	1:B:232:THR:N	2.29	0.42
1:B:596:LYS:HG2	1:B:601:ILE:HD13	2.02	0.42
1:A:273:ILE:HD11	1:A:381:LEU:HD21	2.01	0.42
1:A:314:LYS:NZ	2:A:663:GDP:O4'	2.52	0.42
1:B:188:LEU:HD12	1:B:219:ILE:HG12	2.01	0.42
1:B:298:LEU:HA	1:B:339:ILE:CD1	2.50	0.42
1:B:516:ASN:HD21	1:B:599:ARG:HH21	1.67	0.42
1:A:298:LEU:HA	1:A:339:ILE:CD1	2.50	0.42
1:A:504:GLN:HG2	1:A:577:TRP:HH2	1.85	0.41
1:B:455:GLN:C	1:B:457:GLY:H	2.23	0.41
1:B:402:LEU:HD23	1:B:402:LEU:HA	1.85	0.41
1:A:231:VAL:HG13	1:A:232:THR:N	2.28	0.41
1:A:556:ILE:O	1:A:556:ILE:HG23	2.20	0.41
1:B:188:LEU:CD1	1:B:219:ILE:HG12	2.50	0.41
1:A:452:VAL:HG11	1:A:465:THR:HG23	2.02	0.41
1:A:187:LEU:HA	1:A:187:LEU:HD12	1.67	0.41
1:A:588:ARG:CG	1:A:588:ARG:NH1	2.82	0.41
1:B:195:ASN:N	1:B:198:GLN:OE1	2.45	0.41
1:A:557:ARG:NH1	1:B:396:ASN:HD22	2.18	0.41
1:A:404:SER:O	1:A:423:GLY:HA3	2.20	0.41
1:B:357:GLU:OE1	1:B:368:VAL:HG21	2.21	0.41
1:B:392:ASN:ND2	1:B:392:ASN:N	2.69	0.41
1:B:452:VAL:HG11	1:B:465:THR:HG23	2.03	0.41
1:B:394:GLY:O	1:B:395:ILE:C	2.59	0.41
1:B:555:LYS:HB3	1:B:557:ARG:HH21	1.86	0.41
1:A:596:LYS:HE3	1:A:596:LYS:HB2	1.87	0.41
1:B:150:LYS:HA	1:B:151:PRO:HD3	1.88	0.41
1:B:258:PHE:CD2	1:B:260:PRO:HD2	2.56	0.41
1:B:217:ALA:HA	1:B:219:ILE:HG22	2.02	0.41
1:A:175:HIS:O	1:A:180:LYS:HE2	2.21	0.41
1:B:218:TRP:O	1:B:218:TRP:CD1	2.73	0.40
1:B:266:ILE:HG23	1:B:305:ILE:HD12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:388:ILE:O	1:B:390:LYS:N	2.54	0.40
1:B:409:ILE:HA	1:B:410:PRO:HD3	1.73	0.40
1:B:504:GLN:HG2	1:B:577:TRP:HH2	1.86	0.40
1:A:165:LEU:HA	1:A:166:PRO:HD3	1.91	0.40
1:A:188:LEU:HB3	1:A:194:VAL:HG23	2.02	0.40
1:A:538:ILE:HG21	1:A:541:LEU:CD1	2.51	0.40
1:B:333:LEU:O	1:B:333:LEU:HD12	2.21	0.40
1:B:437:THR:O	1:B:492:ALA:HA	2.21	0.40
1:B:599:ARG:O	1:B:601:ILE:HG23	2.21	0.40
1:A:314:LYS:HE2	2:A:663:GDP:O4'	2.21	0.40
1:A:157:ILE:HA	1:A:157:ILE:HD13	1.85	0.40
1:A:369:ARG:NH1	1:A:373:ASN:HA	2.36	0.40
1:A:555:LYS:HB3	1:A:557:ARG:HH21	1.87	0.40
1:B:175:HIS:O	1:B:180:LYS:HE2	2.21	0.40
1:B:187:LEU:HA	1:B:187:LEU:HD12	1.66	0.40
1:B:525:PHE:CE2	1:B:594:LEU:HG	2.56	0.40
1:A:585:GLU:OE1	1:B:540:ARG:NH2	2.54	0.40
1:A:312:MSE:HE1	1:A:328:ILE:CG2	2.50	0.40
1:B:384:ALA:O	1:B:387:LYS:HB2	2.21	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	419/483 (87%)	383 (91%)	30 (7%)	6 (1%)	13	46
1	B	434/483 (90%)	395 (91%)	31 (7%)	8 (2%)	10	39
All	All	853/966 (88%)	778 (91%)	61 (7%)	14 (2%)	11	42

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	231	VAL
1	A	546	ASP
1	B	546	ASP
1	A	455	GLN
1	B	389	SER
1	B	455	GLN
1	B	456	GLN
1	B	543	SER
1	A	395	ILE
1	A	543	SER
1	B	395	ILE
1	B	548	GLY
1	A	389	SER
1	A	548	GLY

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	383/417 (92%)	354 (92%)	29 (8%)	15	46
1	B	391/417 (94%)	359 (92%)	32 (8%)	13	41
All	All	774/834 (93%)	713 (92%)	61 (8%)	14	43

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	139	VAL
1	A	204	ARG
1	A	219	ILE
1	A	221	ASP
1	A	234	SER
1	A	241	SER
1	A	249	ILE
1	A	280	THR
1	A	316	ASP
1	A	323	GLN

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Mol	Chain	Res	Type
1	A	339	ILE
1	A	344	ASP
1	A	362	ILE
1	A	379	SER
1	A	397	LYS
1	A	412	LYS
1	A	422	SER
1	A	447	VAL
1	A	454	SER
1	A	484	GLU
1	A	488	ASN
1	A	533	GLU
1	A	541	LEU
1	A	547	LYS
1	A	567	VAL
1	A	578	ILE
1	A	584	HIS
1	A	588	ARG
1	A	611	GLN
1	B	139	VAL
1	B	204	ARG
1	B	218	TRP
1	B	221	ASP
1	B	234	SER
1	B	241	SER
1	B	249	ILE
1	B	250	VAL
1	B	256	ARG
1	B	274	LEU
1	B	280	THR
1	B	316	ASP
1	B	323	GLN
1	B	339	ILE
1	B	344	ASP
1	B	362	ILE
1	B	379	SER
1	B	397	LYS
1	B	422	SER
1	B	447	VAL
1	B	454	SER
1	B	469	ILE
1	B	484	GLU

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Mol	Chain	Res	Type
1	B	488	ASN
1	B	533	GLU
1	B	541	LEU
1	B	547	LYS
1	B	567	VAL
1	B	578	ILE
1	B	584	HIS
1	B	588	ARG
1	B	611	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	155	HIS
1	A	167	HIS
1	A	175	HIS
1	A	195	ASN
1	A	222	GLN
1	A	239	HIS
1	A	261	ASN
1	A	323	GLN
1	A	347	ASN
1	A	383	ASN
1	A	392	ASN
1	A	451	GLN
1	A	487	GLN
1	A	488	ASN
1	A	516	ASN
1	A	534	GLN
1	B	155	HIS
1	B	167	HIS
1	B	175	HIS
1	B	195	ASN
1	B	222	GLN
1	B	239	HIS
1	B	261	ASN
1	B	323	GLN
1	B	347	ASN
1	B	383	ASN
1	B	392	ASN
1	B	451	GLN
1	B	487	GLN

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Mol	Chain	Res	Type
1	B	488	ASN
1	B	534	GLN
1	B	611	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 carbohydrates in this entry.

5.6 Ligand geometry

2 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	GDP	A	663	-	25,30,30	1.19	2 (8%)	26,47,47	2.00	6 (23%)
2	GDP	B	663	-	25,30,30	1.14	2 (8%)	26,47,47	1.95	6 (23%)

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	A	663	-	-	0/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GDP	B	663	-	-	0/12/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	663	GDP	C5-C4	3.04	1.47	1.40
2	A	663	GDP	C5-C4	3.11	1.47	1.40
2	B	663	GDP	C6-C5	3.84	1.48	1.41
2	A	663	GDP	C6-C5	3.99	1.48	1.41

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	663	GDP	C6-C5-C4	-4.13	116.74	120.84
2	B	663	GDP	C6-C5-C4	-3.62	117.24	120.84
2	B	663	GDP	C5-C6-N1	-3.43	118.59	123.48
2	A	663	GDP	C5-C6-N1	-3.21	118.91	123.48
2	A	663	GDP	N3-C2-N1	-3.16	122.85	127.46
2	A	663	GDP	C4-C5-N7	-3.00	106.51	109.41
2	B	663	GDP	N3-C2-N1	-2.99	123.09	127.46
2	B	663	GDP	C4-C5-N7	-2.90	106.61	109.41
2	B	663	GDP	C6-N1-C2	3.87	121.63	116.06
2	A	663	GDP	C6-N1-C2	3.93	121.71	116.06
2	B	663	GDP	C2-N3-C4	5.31	121.35	115.16
2	A	663	GDP	C2-N3-C4	5.39	121.45	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	663	GDP	5	0
2	B	663	GDP	3	0

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	424/483 (87%)	-0.24	17 (4%)	39	24	23, 47, 83, 132	0
1	B	435/483 (90%)	-0.19	17 (3%)	40	25	24, 47, 91, 122	0
All	All	859/966 (88%)	-0.21	34 (3%)	39	24	23, 47, 88, 132	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	218	TRP	4.8
1	A	218	TRP	4.7
1	A	455	GLN	4.3
1	A	231	VAL	4.2
1	B	418	LEU	3.9
1	B	288	ASP	3.5
1	B	255	HIS	3.3
1	B	548	GLY	3.2
1	B	462	HIS	3.2
1	A	611	GLN	3.0
1	A	232	THR	2.9
1	B	463	GLU	2.9
1	A	176	VAL	2.8
1	B	611	GLN	2.8
1	B	204	ARG	2.7
1	B	549	ASN	2.7
1	B	243	HIS	2.7
1	A	288	ASP	2.6
1	B	221	ASP	2.6
1	B	176	VAL	2.6
1	A	418	LEU	2.4
1	A	454	SER	2.4
1	A	221	ASP	2.4
1	B	177	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	463	GLU	2.3
1	A	548	GLY	2.3
1	A	411	SER	2.2
1	A	453	GLY	2.2
1	A	140	GLN	2.2
1	B	228	GLU	2.2
1	B	140	GLN	2.1
1	A	552	SER	2.1
1	A	412	LYS	2.1
1	B	287	PHE	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å^2)	Q<0.9
2	GDP	A	663	28/28	0.93	0.19	-0.34	57,77,84,90	0
2	GDP	B	663	28/28	0.97	0.17	-0.51	56,76,85,86	0

6.5 Other polymers (i)

There are no such residues in this entry.