



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2014 – 01:14 AM GMT

PDB ID : 1GP2
Title : G PROTEIN HETEROTRIMER GI_ALPHA_1 BETA_1 GAMMA_2 WITH
GDP BOUND
Authors : Wall, M.A.; Sprang, S.R.
Deposited on : 1996-11-13
Resolution : 2.30 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

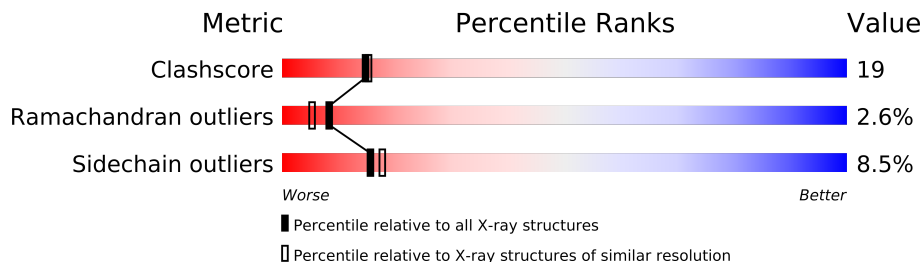
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.30 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))
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	353	
2	B	340	
3	G	71	

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 6197 atoms, of which 0 are hydrogen and 0 are deuterium.

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 G PROTEIN GI ALPHA 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	344	2759	1745	470	528	16	60	0	0

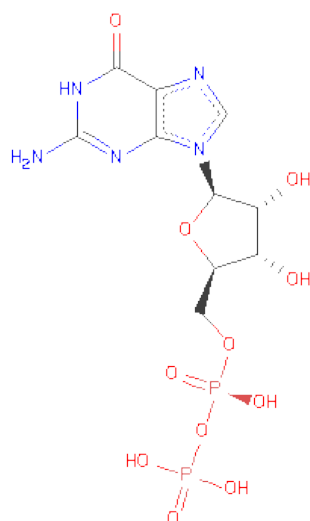
- Molecule 2 is a protein called G PROTEIN GI BETA 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	339	2607	1607	468	511	21	27	0	0

- Molecule 3 is a protein called G PROTEIN GI GAMMA 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	G	54	413	260	71	79	3	0	0	0

- Molecule 4 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



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

- Molecule 5 is water.

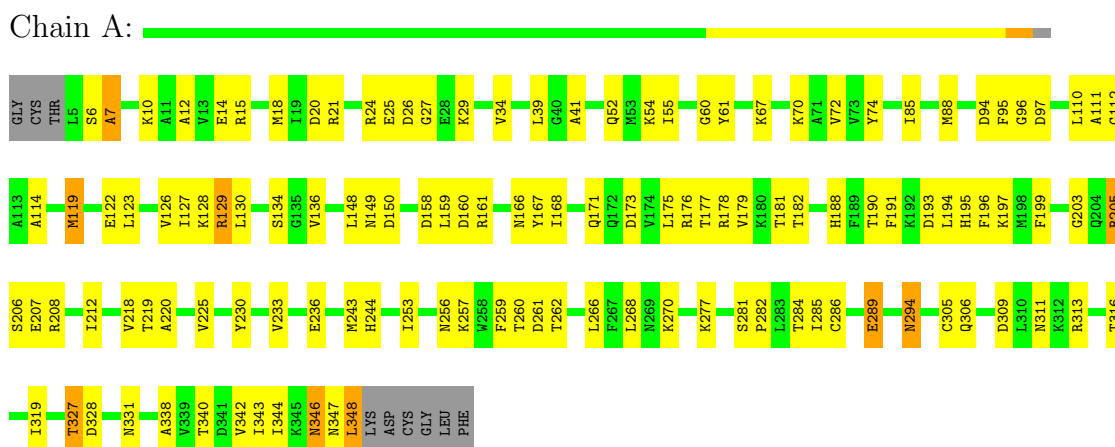
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	225	Total 225	O 225	0	0
5	B	142	Total 142	O 142	0	0
5	G	23	Total 23	O 23	0	0

3 Residue-property plots

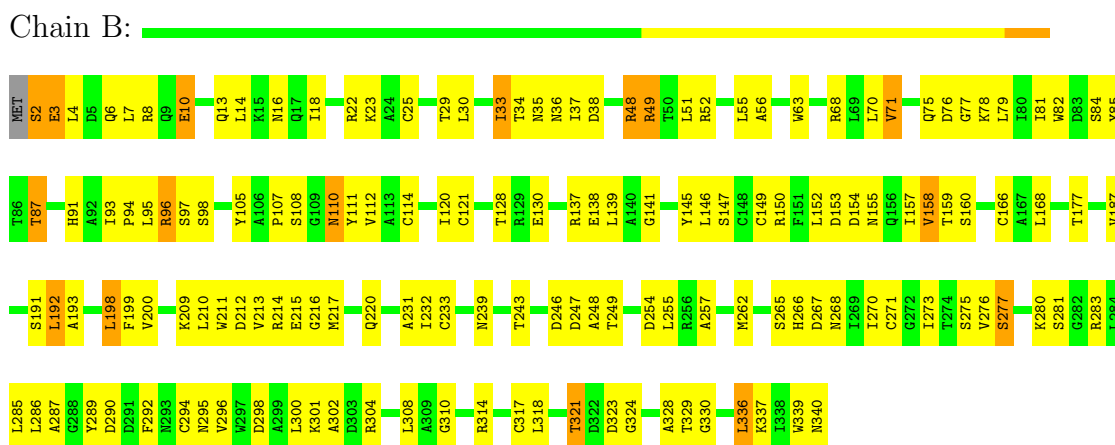
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

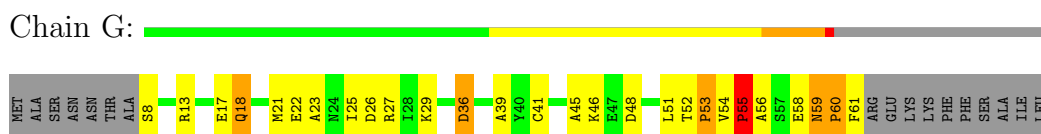
• Molecule 1: G PROTEIN GI ALPHA 1



• Molecule 2: G PROTEIN GI BETA 1



• Molecule 3: G PROTEIN GI GAMMA 2



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	84.29Å 84.29Å 132.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.30	Depositor
% Data completeness (in resolution range)	89.8 (15.00-2.30)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.226 , 0.307	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6197	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

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	0/2805	0.69	0/3775
2	B	0.49	1/2654 (0.0%)	0.78	0/3597
3	G	0.49	0/419	0.65	0/566
All	All	0.51	1/5878 (0.0%)	0.73	0/7938

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	130	GLU	CD-OE2	6.63	1.32	1.25

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2759	0	2739	83	0
2	B	2607	0	2510	127	0
3	G	413	0	423	20	0
4	A	28	0	12	1	0
5	A	225	0	0	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	142	0	0	5	0
5	G	23	0	0	2	0
All	All	6197	0	5684	218	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 19.

All (218) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:128:LYS:HG3	1:A:159:LEU:HD23	1.38	1.06
1:A:181:THR:O	1:A:203:GLY:HA3	1.70	0.90
1:A:55:ILE:HA	1:A:60:GLY:HA2	1.59	0.82
1:A:149:ASN:OD1	1:A:178:ARG:HD3	1.80	0.81
1:A:311:ASN:HB2	1:A:319:ILE:HD11	1.62	0.81
2:B:48:ARG:HD3	2:B:340:ASN:HB2	1.65	0.79
1:A:112:GLY:HA2	5:A:405:HOH:O	1.84	0.77
1:A:282:PRO:HA	1:A:294:ASN:HD21	1.49	0.76
2:B:271:CYS:HB2	2:B:290:ASP:HB2	1.67	0.75
1:A:129:ARG:HG2	1:A:129:ARG:HH11	1.50	0.75
2:B:79:LEU:HG	2:B:95:LEU:HD21	1.68	0.73
2:B:289:TYR:CE1	2:B:295:ASN:HB2	2.24	0.73
2:B:198:LEU:HA	2:B:213:VAL:HG23	1.71	0.72
2:B:51:LEU:HD23	2:B:87:THR:HG22	1.70	0.72
2:B:48:ARG:HG2	3:G:61:PHE:HB3	1.73	0.71
1:A:7:ALA:HB3	5:A:359:HOH:O	1.91	0.70
1:A:230:TYR:O	1:A:286:CYS:HB2	1.91	0.70
1:A:282:PRO:HA	1:A:294:ASN:ND2	2.07	0.70
2:B:262:MET:SD	2:B:302:ALA:HB2	2.32	0.70
2:B:121:CYS:HB3	2:B:139:LEU:HB2	1.75	0.69
2:B:79:LEU:HD11	2:B:114:CYS:SG	2.32	0.68
2:B:212:ASP:HB3	2:B:215:GLU:HB2	1.75	0.67
2:B:6:GLN:O	2:B:10:GLU:HB2	1.94	0.67
1:A:52:GLN:NE2	1:A:175:LEU:HD21	2.10	0.67
2:B:96:ARG:H	2:B:96:ARG:HD3	1.61	0.66
2:B:48:ARG:HD3	2:B:340:ASN:CB	2.27	0.64
3:G:54:VAL:HG13	3:G:55:PRO:HD2	1.78	0.64
2:B:286:LEU:HD22	2:B:296:VAL:HG22	1.80	0.64
2:B:8:ARG:HG3	2:B:8:ARG:HH11	1.63	0.63
2:B:286:LEU:CD2	2:B:296:VAL:HG13	2.28	0.63
2:B:152:LEU:HD23	2:B:192:LEU:HD21	1.80	0.63
1:A:85:ILE:HA	1:A:88:MET:HE2	1.80	0.63
1:A:342:VAL:O	1:A:346:ASN:HB2	1.98	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:239:ASN:HA	2:B:255:LEU:HD12	1.80	0.62
2:B:166:CYS:SG	2:B:187:VAL:HG11	2.41	0.61
2:B:249:THR:HG22	2:B:265:SER:HB3	1.82	0.61
2:B:71:VAL:HG13	2:B:81:ILE:HG12	1.83	0.60
3:G:22:GLU:HB2	5:G:78:HOH:O	2.01	0.60
1:A:188:HIS:CD2	1:A:197:LYS:HG2	2.37	0.60
2:B:51:LEU:HD13	2:B:82:TRP:CG	2.37	0.59
1:A:266:LEU:HD21	1:A:268:LEU:HD21	1.84	0.59
1:A:61:TYR:HB2	1:A:171:GLN:HG2	1.85	0.59
2:B:340:ASN:HD22	3:G:61:PHE:HB2	1.68	0.58
3:G:52:THR:O	3:G:54:VAL:N	2.37	0.58
1:A:188:HIS:HD2	1:A:197:LYS:HG2	1.68	0.58
2:B:71:VAL:HG11	2:B:112:VAL:HG21	1.86	0.58
1:A:70:LYS:HE3	1:A:167:TYR:HD2	1.70	0.57
2:B:29:THR:O	2:B:33:ILE:HG23	2.05	0.57
2:B:96:ARG:HH21	2:B:97:SER:CB	2.18	0.56
1:A:67:LYS:HE2	5:A:388:HOH:O	2.05	0.56
1:A:277:LYS:HE2	5:A:476:HOH:O	2.04	0.56
3:G:36:ASP:O	3:G:39:ALA:HB3	2.05	0.56
2:B:283:ARG:HB3	3:G:51:LEU:HD11	1.86	0.56
2:B:200:VAL:HA	2:B:209:LYS:O	2.05	0.56
1:A:39:LEU:HD13	1:A:253:ILE:HG12	1.87	0.55
3:G:51:LEU:O	3:G:53:PRO:HD3	2.06	0.55
2:B:37:ILE:HG22	2:B:38:ASP:N	2.22	0.55
2:B:271:CYS:CB	2:B:290:ASP:HB2	2.36	0.54
2:B:168:LEU:O	2:B:177:THR:N	2.40	0.54
1:A:18:MET:HA	1:A:21:ARG:NH1	2.22	0.54
2:B:75:GLN:HG2	2:B:98:SER:O	2.07	0.54
2:B:275:SER:HB3	5:B:395:HOH:O	2.07	0.54
2:B:51:LEU:HB3	2:B:82:TRP:CE3	2.43	0.53
1:A:72:VAL:HG11	1:A:179:VAL:HG12	1.91	0.53
1:A:12:ALA:O	1:A:15:ARG:HG2	2.07	0.53
2:B:271:CYS:SG	2:B:290:ASP:HB2	2.49	0.53
1:A:338:ALA:O	1:A:342:VAL:HG23	2.09	0.53
2:B:233:CYS:HB2	2:B:276:VAL:HG23	1.91	0.53
2:B:209:LYS:HD2	2:B:211:TRP:CZ2	2.44	0.53
2:B:270:ILE:HG22	2:B:270:ILE:O	2.09	0.53
2:B:150:ARG:C	2:B:157:ILE:HG13	2.29	0.53
1:A:313:ARG:HB3	1:A:316:THR:HB	1.91	0.53
1:A:256:ASN:HB3	1:A:259:PHE:HD2	1.74	0.53
2:B:3:GLU:HA	2:B:6:GLN:OE1	2.09	0.53
1:A:168:ILE:O	1:A:168:ILE:HG13	2.09	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:328:ASP:HB3	1:A:331:ASN:HB3	1.92	0.52
2:B:14:LEU:O	2:B:18:ILE:HG13	2.08	0.52
2:B:271:CYS:HB2	2:B:290:ASP:CB	2.39	0.52
1:A:67:LYS:HE3	1:A:168:ILE:HG22	1.91	0.52
1:A:305:CYS:O	1:A:309:ASP:HB2	2.09	0.52
1:A:344:ILE:HG23	1:A:348:LEU:HD12	1.91	0.52
2:B:153:ASP:O	2:B:155:ASN:N	2.43	0.52
2:B:108:SER:OG	2:B:110:ASN:HB2	2.10	0.52
2:B:191:SER:O	2:B:199:PHE:HB2	2.10	0.52
2:B:49:ARG:HD2	2:B:84:SER:O	2.09	0.52
2:B:49:ARG:HG2	2:B:87:THR:HG23	1.91	0.52
2:B:51:LEU:HB3	2:B:82:TRP:CZ3	2.45	0.52
1:A:243:MET:HG2	1:A:286:CYS:SG	2.50	0.51
1:A:244:HIS:HE1	1:A:286:CYS:O	1.92	0.51
2:B:110:ASN:HB3	2:B:111:TYR:CD1	2.46	0.51
2:B:18:ILE:HG12	3:G:23:ALA:HA	1.93	0.51
2:B:7:LEU:HD22	3:G:13:ARG:HG2	1.93	0.50
2:B:48:ARG:HG2	3:G:61:PHE:CB	2.39	0.50
2:B:77:GLY:C	2:B:78:LYS:HD2	2.31	0.50
2:B:51:LEU:CD2	2:B:87:THR:HG22	2.40	0.50
1:A:256:ASN:HB3	1:A:259:PHE:CD2	2.46	0.50
1:A:306:GLN:HA	1:A:306:GLN:NE2	2.26	0.50
1:A:191:PHE:HE2	1:A:340:THR:HG1	1.59	0.50
2:B:34:THR:O	2:B:36:ASN:N	2.45	0.50
2:B:267:ASP:O	2:B:268:ASN:HB2	2.11	0.50
2:B:96:ARG:HH21	2:B:97:SER:HB3	1.76	0.49
1:A:129:ARG:NH1	1:A:129:ARG:HG2	2.24	0.49
2:B:317:CYS:SG	2:B:330:GLY:HA3	2.53	0.49
2:B:13:GLN:HA	2:B:16:ASN:HD22	1.77	0.49
1:A:128:LYS:HG3	1:A:159:LEU:CD2	2.27	0.49
2:B:318:LEU:HD23	2:B:329:THR:HG22	1.94	0.49
2:B:120:ILE:HG21	2:B:138:GLU:HB3	1.95	0.49
2:B:281:SER:HB3	3:G:48:ASP:HB2	1.94	0.48
1:A:188:HIS:HB3	1:A:195:HIS:CE1	2.47	0.48
2:B:308:LEU:HB3	2:B:339:TRP:CZ3	2.48	0.48
3:G:46:LYS:O	3:G:46:LYS:HD3	2.14	0.48
2:B:152:LEU:CD2	2:B:192:LEU:HD21	2.44	0.48
2:B:294:CYS:HB3	2:B:308:LEU:HB2	1.95	0.48
3:G:17:GLU:HG3	5:G:89:HOH:O	2.13	0.48
2:B:266:HIS:CD2	2:B:304:ARG:HH11	2.32	0.48
2:B:149:CYS:HA	2:B:158:VAL:O	2.14	0.48
2:B:63:TRP:CZ3	2:B:70:LEU:HD23	2.49	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:246:ASP:C	2:B:248:ALA:H	2.18	0.48
1:A:166:ASN:HB2	5:A:441:HOH:O	2.13	0.47
1:A:130:LEU:O	1:A:136:VAL:HG21	2.13	0.47
2:B:68:ARG:NH1	2:B:85:TYR:HD2	2.11	0.47
2:B:275:SER:O	2:B:287:ALA:HA	2.14	0.47
1:A:61:TYR:H	1:A:171:GLN:NE2	2.12	0.47
1:A:122:GLU:O	1:A:126:VAL:HG23	2.14	0.47
1:A:270:LYS:HG2	4:A:355:GDP:C6	2.49	0.47
1:A:52:GLN:HE22	1:A:175:LEU:HD21	1.75	0.47
1:A:52:GLN:HA	1:A:52:GLN:OE1	2.14	0.47
1:A:179:VAL:HG22	5:A:532:HOH:O	2.14	0.47
2:B:107:PRO:HD2	5:B:397:HOH:O	2.14	0.46
1:A:34:VAL:HB	1:A:196:PHE:CD2	2.50	0.46
1:A:191:PHE:CE2	1:A:340:THR:HG21	2.50	0.46
1:A:27:GLY:HA2	2:B:55:LEU:HD11	1.96	0.46
2:B:191:SER:HB2	2:B:232:ILE:HG23	1.98	0.46
3:G:18:GLN:O	3:G:21:MET:HB2	2.15	0.46
1:A:55:ILE:HA	1:A:60:GLY:CA	2.39	0.46
2:B:79:LEU:HB2	2:B:93:ILE:HB	1.98	0.46
2:B:292:PHE:HA	2:B:314:ARG:HA	1.98	0.46
2:B:289:TYR:HE1	2:B:295:ASN:HB2	1.79	0.45
2:B:96:ARG:CD	2:B:96:ARG:H	2.22	0.45
1:A:20:ASP:O	1:A:24:ARG:HG3	2.16	0.45
2:B:193:ALA:HB2	2:B:198:LEU:HD12	1.97	0.45
1:A:127:ILE:HB	1:A:159:LEU:HD21	1.98	0.45
1:A:208:ARG:HG3	1:A:208:ARG:HH11	1.81	0.45
2:B:280:LYS:HB2	2:B:324:GLY:HA3	1.99	0.45
2:B:159:THR:O	2:B:166:CYS:HA	2.15	0.45
1:A:203:GLY:O	1:A:205:ARG:N	2.48	0.45
1:A:282:PRO:HB2	1:A:284:THR:HG22	1.99	0.44
2:B:30:LEU:HD23	2:B:262:MET:HB2	1.99	0.44
2:B:96:ARG:N	2:B:96:ARG:HD3	2.30	0.44
2:B:254:ASP:HB3	2:B:257:ALA:HB3	1.99	0.44
1:A:34:VAL:HG13	1:A:219:THR:HG21	2.00	0.44
2:B:56:ALA:H	2:B:76:ASP:HB3	1.81	0.44
1:A:181:THR:HG23	5:A:447:HOH:O	2.17	0.44
1:A:110:LEU:O	1:A:112:GLY:N	2.50	0.44
2:B:51:LEU:HB2	2:B:336:LEU:HB2	1.98	0.44
1:A:74:TYR:CE1	1:A:119:MET:HG2	2.52	0.44
1:A:54:LYS:HE3	1:A:60:GLY:O	2.18	0.44
2:B:81:ILE:HB	2:B:91:HIS:HB2	2.00	0.44
1:A:266:LEU:CD2	1:A:268:LEU:HD21	2.47	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:232:ILE:HG13	2:B:243:THR:HG22	1.99	0.44
1:A:281:SER:OG	1:A:285:ILE:HD12	2.18	0.44
2:B:137:ARG:HH11	2:B:137:ARG:HG2	1.83	0.43
1:A:206:SER:HB3	2:B:145:TYR:HE1	1.83	0.43
2:B:337:LYS:HB2	2:B:339:TRP:HE1	1.83	0.43
2:B:239:ASN:ND2	5:B:472:HOH:O	2.51	0.43
2:B:160:SER:HB2	2:B:187:VAL:HG12	2.00	0.43
2:B:276:VAL:HA	2:B:286:LEU:O	2.17	0.43
2:B:34:THR:O	2:B:37:ILE:HG13	2.17	0.43
2:B:292:PHE:CD1	2:B:292:PHE:N	2.87	0.43
1:A:260:THR:HG22	1:A:261:ASP:OD1	2.19	0.43
1:A:212:ILE:HD12	1:A:212:ILE:HA	1.84	0.43
2:B:193:ALA:CB	2:B:198:LEU:HD12	2.48	0.43
1:A:188:HIS:HB3	1:A:195:HIS:HE1	1.84	0.43
2:B:277:SER:O	2:B:285:LEU:HD12	2.17	0.43
1:A:161:ARG:HD2	5:A:439:HOH:O	2.18	0.43
2:B:146:LEU:HD11	2:B:159:THR:HB	1.99	0.43
2:B:340:ASN:ND2	3:G:61:PHE:HB2	2.33	0.43
2:B:96:ARG:HH21	2:B:97:SER:HB2	1.83	0.43
1:A:225:VAL:HB	1:A:268:LEU:HD23	2.00	0.43
2:B:318:LEU:CD2	2:B:329:THR:HG22	2.49	0.43
5:A:465:HOH:O	2:B:55:LEU:HD13	2.18	0.43
2:B:210:LEU:HB3	2:B:220:GLN:H	1.83	0.43
2:B:147:SER:OG	2:B:187:VAL:O	2.24	0.42
1:A:95:PHE:HB3	1:A:97:ASP:O	2.19	0.42
2:B:25:CYS:HB3	3:G:29:LYS:HA	1.99	0.42
2:B:93:ILE:HA	2:B:94:PRO:HD3	1.81	0.42
1:A:39:LEU:HD13	1:A:253:ILE:CG1	2.49	0.42
3:G:46:LYS:C	3:G:46:LYS:HD3	2.39	0.42
1:A:123:LEU:O	1:A:127:ILE:HG13	2.17	0.42
1:A:220:ALA:HA	1:A:262:THR:HG23	2.01	0.42
1:A:179:VAL:HA	5:A:515:HOH:O	2.19	0.42
2:B:18:ILE:O	2:B:22:ARG:HG3	2.19	0.42
2:B:328:ALA:HA	2:B:337:LYS:O	2.19	0.42
2:B:150:ARG:O	2:B:157:ILE:HG13	2.20	0.42
2:B:301:LYS:O	2:B:302:ALA:HB3	2.20	0.42
2:B:8:ARG:HG3	2:B:8:ARG:NH1	2.32	0.42
2:B:231:ALA:HB2	2:B:275:SER:HA	2.02	0.42
1:A:289:GLU:CD	1:A:289:GLU:H	2.23	0.42
1:A:340:THR:O	1:A:343:ILE:HB	2.19	0.41
2:B:68:ARG:HG3	2:B:85:TYR:CD2	2.55	0.41
1:A:176:ARG:HD3	1:A:327:THR:HG21	2.01	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:25:GLU:O	1:A:29:LYS:HG3	2.21	0.41
2:B:339:TRP:CD1	2:B:339:TRP:N	2.88	0.41
2:B:2:SER:O	2:B:4:LEU:N	2.53	0.41
2:B:192:LEU:HA	2:B:192:LEU:HD12	1.80	0.41
1:A:148:LEU:HA	1:A:148:LEU:HD12	1.89	0.41
2:B:212:ASP:O	2:B:216:GLY:N	2.45	0.41
2:B:298:ASP:CG	2:B:301:LYS:HB2	2.41	0.41
2:B:192:LEU:HD23	5:B:360:HOH:O	2.20	0.41
2:B:214:ARG:NH2	5:B:480:HOH:O	2.54	0.41
2:B:96:ARG:HE	2:B:97:SER:HB3	1.86	0.40
2:B:321:THR:HB	2:B:323:ASP:OD1	2.21	0.40
2:B:300:LEU:HD21	3:G:41:CYS:SG	2.61	0.40
3:G:59:ASN:O	3:G:61:PHE:N	2.55	0.40
1:A:96:GLY:HA3	1:A:134:SER:OG	2.21	0.40
2:B:273:ILE:HG13	2:B:289:TYR:CE2	2.57	0.40
2:B:77:GLY:O	2:B:78:LYS:HD2	2.21	0.40
1:A:173:ASP:O	1:A:177:THR:HG23	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	342/353 (97%)	314 (92%)	21 (6%)	7 (2%)	11	8
2	B	337/340 (99%)	307 (91%)	23 (7%)	7 (2%)	11	8
3	G	52/71 (73%)	39 (75%)	8 (15%)	5 (10%)	1	0
All	All	731/764 (96%)	660 (90%)	52 (7%)	19 (3%)	8	5

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	35	ASN
3	G	55	PRO

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Mol	Chain	Res	Type
3	G	60	PRO
1	A	7	ALA
1	A	114	ALA
1	A	236	GLU
2	B	3	GLU
2	B	128	THR
2	B	154	ASP
3	G	45	ALA
3	G	56	ALA
1	A	41	ALA
1	A	119	MET
1	A	6	SER
2	B	247	ASP
1	A	111	ALA
2	B	310	GLY
3	G	53	PRO
2	B	141	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	296/303 (98%)	272 (92%)	24 (8%)	17	20
2	B	282/283 (100%)	263 (93%)	19 (7%)	23	29
3	G	44/58 (76%)	34 (77%)	10 (23%)	1	1
All	All	622/644 (97%)	569 (92%)	53 (8%)	15	18

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LYS
1	A	14	GLU
1	A	26	ASP
1	A	94	ASP
1	A	129	ARG
1	A	150	ASP

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Mol	Chain	Res	Type
1	A	158	ASP
1	A	160	ASP
1	A	182	THR
1	A	190	THR
1	A	193	ASP
1	A	194	LEU
1	A	199	PHE
1	A	205	ARG
1	A	207	GLU
1	A	218	VAL
1	A	233	VAL
1	A	257	LYS
1	A	289	GLU
1	A	294	ASN
1	A	327	THR
1	A	346	ASN
1	A	347	ASN
1	A	348	LEU
2	B	2	SER
2	B	10	GLU
2	B	23	LYS
2	B	33	ILE
2	B	48	ARG
2	B	49	ARG
2	B	52	ARG
2	B	71	VAL
2	B	87	THR
2	B	96	ARG
2	B	105	TYR
2	B	110	ASN
2	B	158	VAL
2	B	192	LEU
2	B	198	LEU
2	B	217	MET
2	B	277	SER
2	B	321	THR
2	B	336	LEU
3	G	8	SER
3	G	18	GLN
3	G	25	ILE
3	G	26	ASP
3	G	27	ARG

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Mol	Chain	Res	Type
3	G	36	ASP
3	G	55	PRO
3	G	58	GLU
3	G	59	ASN
3	G	60	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	HIS
1	A	188	HIS
1	A	195	HIS
1	A	306	GLN
1	A	331	ASN
2	B	110	ASN
2	B	175	GLN
2	B	266	HIS
2	B	340	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

1 ligand is 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	$\# Z > 2$
4	GDP	A	355	-	30,30,30	2.08	5 (16%)	44,47,47	5.73	14 (31%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GDP	A	355	-	-	0/16/32/32	0/1/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	355	GDP	O4'-C1'	7.19	1.52	1.41
4	A	355	GDP	PB-O3A	4.01	1.67	1.60
4	A	355	GDP	C6-N1	3.59	1.43	1.37
4	A	355	GDP	C8-N7	-2.94	1.28	1.34
4	A	355	GDP	PB-O3B	-2.05	1.47	1.54

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	355	GDP	C6-C5-N7	-32.13	129.81	134.14
4	A	355	GDP	O4'-C1'-N9	16.89	124.15	108.44
4	A	355	GDP	C6-N1-C2	3.84	126.23	119.51
4	A	355	GDP	C8-N9-C4	-3.68	104.09	106.90
4	A	355	GDP	C4'-O4'-C1'	-3.14	106.34	109.75
4	A	355	GDP	O2B-PB-O1B	2.85	119.77	110.44
4	A	355	GDP	N2-C2-N1	2.75	120.89	117.86
4	A	355	GDP	O3'-C3'-C4'	-2.48	103.76	111.08
4	A	355	GDP	C4-C5-N7	2.42	111.59	109.52
4	A	355	GDP	O3A-PB-O1B	-2.40	94.58	111.00
4	A	355	GDP	C2'-C1'-N9	-2.30	107.36	113.27
4	A	355	GDP	O2'-C2'-C3'	2.28	119.26	111.83
4	A	355	GDP	C1'-N9-C4	-2.06	123.08	126.64
4	A	355	GDP	N2-C2-N3	-2.04	117.54	120.30

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.