



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:48 AM GMT

PDB ID : 2BTQ
Title : STRUCTURE OF BTUBAB HETERODIMER FROM PROSTHECOBACTER DEJONGEII
Authors : Schlieper, D.; Lowe, J.
Deposited on : 2005-06-06
Resolution : 3.20 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

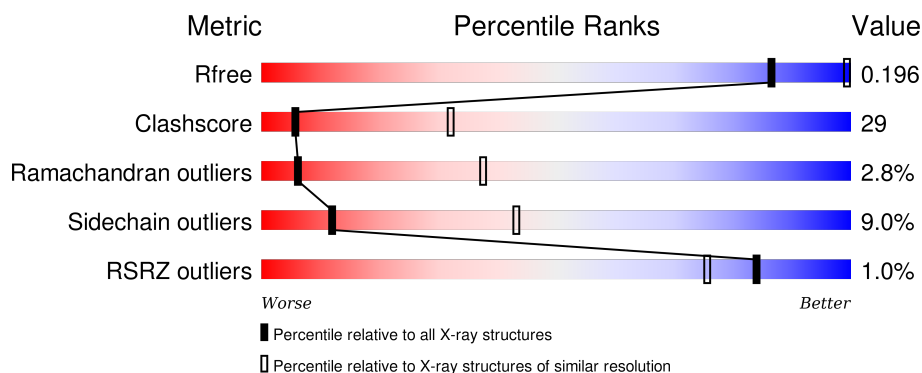
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 3.20 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}	91344	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	473	
2	B	426	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6402 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 TUBULIN BTUBA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	437	Total	C	N	O	S	0	0	1
			3323	2113	560	633	17			

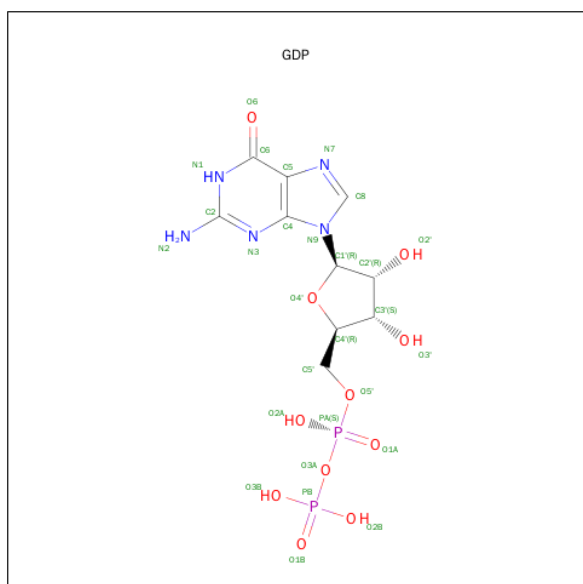
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	255	SER	THR	CONFLICT SEE REMARK 9	UNP Q8GCC5

- Molecule 2 is a protein called TUBULIN BTUBB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	391	Total	C	N	O	S	0	0	0
			3031	1923	526	571	11			

- Molecule 3 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).

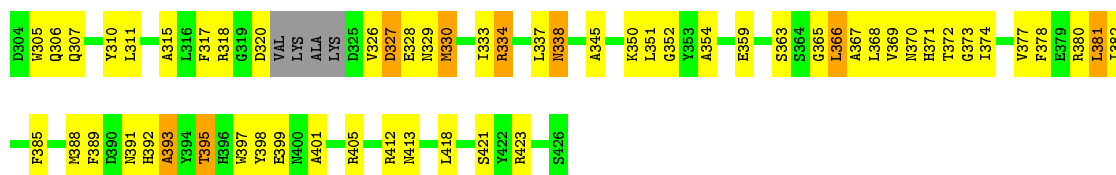


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	154.40 Å 154.40 Å 256.33 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	53.52 – 3.20 133.71 – 3.20	Depositor EDS
% Data completeness (in resolution range)	98.3 (53.52-3.20) 98.3 (133.71-3.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.22 (at 3.19 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.215 , 0.247 0.194 , 0.196	Depositor DCC
R_{free} test set	1539 reflections (5.40%)	DCC
Wilson B-factor (Å ²)	91.9	Xtriage
Anisotropy	0.302	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 68.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 30511 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6402	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.93% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, SO4

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	0.41	0/3390	0.67	0/4605
2	B	0.38	0/3090	0.64	1/4181 (0.0%)
All	All	0.40	0/6480	0.66	1/8786 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	175	LEU	CA-CB-CG	5.86	128.78	115.30

There are no chirality outliers.

There are no planarity outliers.

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	3323	0	3314	176	0
2	B	3031	0	2989	201	0
3	A	28	0	12	5	0
4	B	20	0	0	0	0
All	All	6402	0	6315	369	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 29.

All (369) 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)
2:B:245:LYS:H	2:B:245:LYS:HE2	1.07	1.12
1:A:296:ILE:HG12	1:A:370:MET:HE1	1.33	1.05
2:B:245:LYS:HE2	2:B:245:LYS:N	1.83	0.92
2:B:31:THR:HG22	2:B:35:THR:H	1.32	0.92
2:B:338:ASN:H	2:B:338:ASN:HD22	1.13	0.90
1:A:299:LEU:HD11	1:A:370:MET:HG3	1.56	0.87
1:A:376:ASN:ND2	1:A:378:GLU:H	1.72	0.86
2:B:132:GLN:NE2	2:B:250:LEU:H	1.75	0.84
2:B:16:ILE:HD12	2:B:229:ILE:HG21	1.59	0.83
2:B:150:SER:HB3	2:B:192:ARG:HG3	1.62	0.81
2:B:67:VAL:HA	2:B:92:VAL:HG13	1.63	0.80
2:B:113:VAL:O	2:B:117:ILE:HG12	1.81	0.79
2:B:16:ILE:HB	2:B:137:THR:HG21	1.65	0.78
2:B:67:VAL:HG23	2:B:117:ILE:HD12	1.66	0.77
1:A:208:ASN:HD21	3:A:1443:GDP:HN22	1.33	0.77
1:A:216:HIS:O	1:A:220:ASN:HA	1.85	0.75
2:B:23:LEU:HD13	2:B:23:LEU:H	1.52	0.73
1:A:117:LEU:HB3	1:A:118:PRO:HD3	1.70	0.73
2:B:88:GLU:HA	2:B:91:ILE:HG23	1.71	0.73
1:A:296:ILE:HG12	1:A:370:MET:CE	2.17	0.72
1:A:296:ILE:HA	1:A:370:MET:HE2	1.70	0.72
1:A:435:ALA:H	2:B:391:ASN:HD22	1.38	0.72
2:B:31:THR:HG22	2:B:35:THR:N	2.03	0.72
1:A:13:GLN:HG3	1:A:77:VAL:HG21	1.72	0.72
1:A:319:THR:HG22	1:A:320:ALA:N	2.05	0.71
2:B:208:LEU:HD21	2:B:300:THR:HG23	1.73	0.70
1:A:387:CYS:HB3	1:A:417:ARG:NH1	2.07	0.70
2:B:300:THR:O	2:B:300:THR:HG22	1.89	0.70
1:A:296:ILE:HD12	1:A:336:ALA:HB3	1.72	0.70
2:B:95:ILE:HD12	2:B:95:ILE:N	2.06	0.70
1:A:185:GLU:OE2	1:A:186:PRO:HD3	1.92	0.70
1:A:45:PRO:HG2	1:A:49:TRP:CD1	2.27	0.69
1:A:328:GLU:HG2	1:A:329:ASP:N	2.05	0.69
1:A:257:ARG:O	1:A:261:THR:HG23	1.92	0.69
1:A:261:THR:HA	2:B:397:TRP:CE2	2.27	0.69
1:A:264:VAL:HB	2:B:397:TRP:HZ2	1.58	0.69
1:A:383:LEU:HD13	1:A:423:LEU:HD13	1.75	0.69
1:A:390:PHE:CD2	1:A:417:ARG:HD3	2.29	0.68
2:B:286:PHE:H	2:B:287:PRO:CD	2.06	0.68
1:A:273:MET:CE	1:A:376:ASN:HB3	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:329:ASN:O	2:B:333:ILE:HD13	1.94	0.68
1:A:212:PHE:HA	1:A:229:LEU:HD21	1.75	0.67
1:A:244:MET:CE	1:A:256:LEU:HB2	2.24	0.67
1:A:251:THR:HG22	1:A:253:GLU:H	1.60	0.67
1:A:274:CYS:HA	1:A:372:LEU:O	1.95	0.67
2:B:20:PHE:O	2:B:23:LEU:HD22	1.95	0.67
1:A:23:TRP:CZ2	1:A:68:ALA:HB2	2.30	0.66
2:B:338:ASN:HD22	2:B:338:ASN:N	1.84	0.66
2:B:25:LEU:HD23	2:B:52:PHE:HE2	1.60	0.66
2:B:132:GLN:HE22	2:B:250:LEU:H	1.45	0.65
2:B:102:TRP:CE3	2:B:188:LEU:HD13	2.32	0.65
2:B:395:THR:HG21	2:B:405:ARG:HE	1.62	0.65
2:B:56:ARG:NH1	2:B:59:LYS:HD2	2.11	0.65
2:B:91:ILE:O	2:B:91:ILE:HG13	1.97	0.65
2:B:228:ILE:HD12	2:B:228:ILE:H	1.60	0.65
1:A:292:ILE:HD11	1:A:329:ASP:OD1	1.98	0.64
1:A:271:PHE:CE1	1:A:423:LEU:HD11	2.33	0.63
1:A:208:ASN:HD22	1:A:211:LEU:HD12	1.64	0.63
2:B:101:ASN:HB3	2:B:104:ARG:HB2	1.81	0.63
2:B:66:LEU:HB2	2:B:91:ILE:HB	1.80	0.62
1:A:160:LYS:HD3	1:A:164:GLY:HA2	1.79	0.62
2:B:116:GLN:O	2:B:120:VAL:HG23	1.99	0.62
1:A:261:THR:HA	2:B:397:TRP:CZ2	2.34	0.62
2:B:208:LEU:CD2	2:B:300:THR:HG23	2.29	0.62
2:B:246:LEU:HD12	2:B:351:LEU:C	2.20	0.62
2:B:269:SER:O	2:B:366:LEU:HD22	2.00	0.61
1:A:104:ASN:HB3	1:A:107:VAL:HG23	1.81	0.61
1:A:222:GLU:HG2	1:A:223:SER:H	1.64	0.61
2:B:377:VAL:O	2:B:381:LEU:HD22	1.99	0.61
1:A:45:PRO:HG2	1:A:49:TRP:CG	2.34	0.61
1:A:197:ARG:HH22	1:A:422:GLU:CB	2.13	0.61
1:A:106:ALA:O	1:A:110:LEU:HD12	2.00	0.60
2:B:418:LEU:O	2:B:421:SER:HB3	2.01	0.60
1:A:95:ILE:N	1:A:95:ILE:HD12	2.17	0.60
2:B:69:LEU:HD22	2:B:70:GLU:N	2.17	0.60
2:B:318:ARG:HA	2:B:354:ALA:O	2.01	0.60
2:B:378:PHE:O	2:B:382:ILE:HG12	2.02	0.59
1:A:175:PRO:HG2	1:A:185:GLU:OE1	2.02	0.59
1:A:376:ASN:HD22	1:A:378:GLU:H	1.45	0.59
2:B:366:LEU:HD13	2:B:367:ALA:N	2.17	0.59
1:A:124:LEU:HD13	1:A:159:LEU:HD13	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:ARG:HG3	1:A:198:ARG:HH21	1.68	0.58
2:B:125:VAL:O	2:B:128:THR:HB	2.03	0.58
2:B:395:THR:HG21	2:B:405:ARG:NE	2.17	0.58
2:B:371:HIS:CD2	2:B:373:GLY:H	2.21	0.58
2:B:9:VAL:HB	2:B:67:VAL:HG13	1.84	0.58
2:B:16:ILE:HD12	2:B:229:ILE:CG2	2.33	0.58
2:B:389:PHE:O	2:B:405:ARG:NH1	2.37	0.58
1:A:305:VAL:HG11	1:A:311:PRO:HG3	1.84	0.58
2:B:216:LEU:O	2:B:218:ARG:N	2.36	0.58
2:B:106:TYR:C	2:B:107:ASN:HD22	2.06	0.58
2:B:19:SER:O	2:B:22:ARG:HB3	2.04	0.58
1:A:244:MET:HE1	1:A:256:LEU:HB2	1.86	0.58
1:A:197:ARG:NH1	1:A:198:ARG:HH11	2.01	0.58
2:B:366:LEU:HD13	2:B:366:LEU:C	2.25	0.57
1:A:273:MET:HE1	1:A:376:ASN:HB3	1.86	0.57
2:B:3:GLU:O	2:B:131:LEU:HD12	2.04	0.57
2:B:7:ILE:HG12	2:B:65:VAL:CG2	2.34	0.57
2:B:203:LEU:HD13	2:B:229:ILE:HG23	1.87	0.57
1:A:184:THR:C	1:A:186:PRO:HD2	2.25	0.57
2:B:25:LEU:HD23	2:B:52:PHE:CE2	2.39	0.57
2:B:146:SER:HB2	2:B:189:THR:OG1	2.05	0.57
1:A:309:CYS:HB2	1:A:378:GLU:HB3	1.86	0.56
2:B:12:CYS:O	2:B:16:ILE:HG12	2.05	0.56
2:B:9:VAL:CG2	2:B:145:GLY:HA2	2.35	0.56
2:B:68:ASP:OD1	2:B:94:LYS:HD2	2.04	0.56
2:B:412:ARG:NH2	2:B:413:ASN:HD22	2.02	0.56
1:A:417:ARG:NH1	1:A:421:GLN:NE2	2.54	0.56
1:A:185:GLU:N	1:A:186:PRO:HD2	2.20	0.56
1:A:73:LEU:HA	1:A:97:ARG:HB2	1.88	0.56
1:A:273:MET:HE2	1:A:379:ILE:HB	1.88	0.56
2:B:303:ILE:HD13	2:B:303:ILE:N	2.21	0.56
1:A:185:GLU:HG3	1:A:186:PRO:HD3	1.88	0.56
2:B:131:LEU:O	2:B:163:LYS:HE3	2.06	0.55
2:B:250:LEU:O	2:B:254:VAL:HG23	2.07	0.55
2:B:21:TRP:HA	2:B:24:ALA:CB	2.37	0.55
2:B:246:LEU:HD12	2:B:352:GLY:N	2.21	0.55
2:B:68:ASP:OD1	2:B:94:LYS:HB2	2.07	0.55
1:A:208:ASN:HD21	3:A:1443:GDP:N2	2.02	0.55
2:B:202:LEU:HD12	2:B:374:ILE:HD11	1.88	0.55
1:A:143:ILE:CG1	1:A:192:ALA:HB3	2.37	0.55
2:B:217:ASN:HD22	2:B:218:ARG:H	1.55	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:THR:CG2	1:A:320:ALA:N	2.69	0.55
2:B:9:VAL:HG22	2:B:145:GLY:HA2	1.89	0.54
1:A:75:PRO:HD3	1:A:97:ARG:O	2.07	0.54
1:A:372:LEU:HD12	1:A:373:LEU:N	2.22	0.54
1:A:394:TRP:O	1:A:397:LYS:HD2	2.08	0.54
1:A:197:ARG:HH22	1:A:422:GLU:HB2	1.71	0.54
2:B:253:PHE:HE1	2:B:368:LEU:HD12	1.73	0.54
2:B:208:LEU:HB3	2:B:225:LEU:HG	1.89	0.54
2:B:351:LEU:HD12	2:B:351:LEU:N	2.23	0.54
2:B:2:ARG:O	2:B:50:VAL:HG13	2.08	0.54
1:A:391:ASP:O	1:A:395:GLN:HB2	2.08	0.54
1:A:429:VAL:HG21	1:A:440:GLN:HG3	1.88	0.54
2:B:167:THR:CG2	2:B:169:SER:OG	2.56	0.54
2:B:311:LEU:HB2	2:B:370:ASN:O	2.08	0.54
2:B:101:ASN:HB3	2:B:104:ARG:CB	2.37	0.53
2:B:350:LYS:C	2:B:351:LEU:HD12	2.29	0.53
1:A:281:PRO:C	1:A:283:ASP:H	2.12	0.53
1:A:95:ILE:HD11	1:A:123:ARG:HG3	1.90	0.53
2:B:167:THR:HG21	2:B:169:SER:OG	2.09	0.53
2:B:84:GLN:O	2:B:85:LEU:HG	2.09	0.53
2:B:289:LEU:HD22	2:B:317:PHE:CD2	2.43	0.53
2:B:88:GLU:HA	2:B:91:ILE:CG2	2.36	0.53
2:B:246:LEU:HD23	2:B:247:ASN:N	2.24	0.53
2:B:67:VAL:CG2	2:B:117:ILE:HD12	2.39	0.53
1:A:207:ASP:HB3	1:A:307:ALA:HA	1.91	0.53
1:A:13:GLN:O	1:A:17:GLN:HG3	2.09	0.52
2:B:392:HIS:HA	2:B:405:ARG:HH11	1.73	0.52
1:A:143:ILE:HG12	1:A:192:ALA:HB3	1.92	0.52
2:B:48:MET:C	2:B:50:VAL:H	2.12	0.52
1:A:397:LYS:NZ	1:A:410:GLU:OE2	2.42	0.52
2:B:259:PRO:O	2:B:260:PHE:HB2	2.09	0.52
2:B:208:LEU:HD21	2:B:300:THR:CG2	2.37	0.52
1:A:204:LEU:HD13	1:A:206:PHE:CE1	2.45	0.52
1:A:350:ILE:N	1:A:351:PRO:HD3	2.23	0.52
1:A:290:LEU:HD22	1:A:294:GLU:OE1	2.10	0.51
2:B:132:GLN:NE2	2:B:250:LEU:N	2.52	0.51
2:B:371:HIS:O	2:B:374:ILE:HG22	2.10	0.51
2:B:228:ILE:CD1	2:B:228:ILE:H	2.23	0.51
1:A:427:TYR:O	1:A:430:ALA:HB3	2.10	0.51
2:B:418:LEU:HD13	2:B:418:LEU:C	2.31	0.51
1:A:415:VAL:O	1:A:418:ALA:HB3	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:ASN:ND2	3:A:1443:GDP:HN22	2.06	0.51
2:B:330:MET:HE1	2:B:334:ARG:HB2	1.93	0.51
1:A:182:VAL:HG12	1:A:184:THR:H	1.76	0.50
2:B:286:PHE:N	2:B:287:PRO:CD	2.73	0.50
1:A:425:GLN:O	1:A:429:VAL:HG23	2.11	0.50
2:B:31:THR:CG2	2:B:35:THR:H	2.16	0.50
1:A:275:ALA:HB3	1:A:372:LEU:HB3	1.93	0.50
1:A:319:THR:HG23	1:A:372:LEU:HD11	1.93	0.50
1:A:104:ASN:HB3	1:A:107:VAL:CG2	2.42	0.50
1:A:72:ASP:HB3	1:A:78:ILE:HD13	1.94	0.50
1:A:208:ASN:ND2	1:A:211:LEU:HD12	2.24	0.50
2:B:382:ILE:O	2:B:385:PHE:HB3	2.12	0.50
2:B:181:VAL:HG21	2:B:398:TYR:HE1	1.77	0.50
2:B:365:GLY:O	2:B:366:LEU:HB2	2.12	0.50
2:B:267:THR:HG22	2:B:268:ALA:N	2.27	0.50
2:B:8:HIS:HD1	2:B:137:THR:HB	1.77	0.50
2:B:187:ILE:CD1	2:B:381:LEU:HB3	2.42	0.50
2:B:301:ALA:O	2:B:303:ILE:HD13	2.11	0.50
2:B:240:LEU:HD21	2:B:253:PHE:CE2	2.47	0.50
1:A:43:VAL:HG22	1:A:44:ALA:N	2.27	0.50
2:B:320:ASP:H	2:B:363:SER:HB3	1.77	0.49
1:A:244:MET:HE3	1:A:256:LEU:HB2	1.93	0.49
2:B:37:LYS:O	2:B:37:LYS:HG3	2.12	0.49
2:B:326:VAL:C	2:B:328:GLU:H	2.15	0.49
2:B:391:ASN:O	2:B:392:HIS:HB2	2.12	0.49
2:B:175:LEU:HD21	2:B:206:GLU:HA	1.93	0.49
2:B:102:TRP:HB2	2:B:185:ASN:OD1	2.12	0.49
2:B:303:ILE:HD11	2:B:305:TRP:CE2	2.47	0.49
2:B:21:TRP:HA	2:B:24:ALA:HB3	1.94	0.49
1:A:227:ASP:O	1:A:231:LEU:HD13	2.12	0.49
1:A:350:ILE:O	1:A:350:ILE:HG22	2.11	0.49
2:B:369:VAL:HG12	2:B:371:HIS:HB2	1.94	0.49
2:B:243:PRO:O	2:B:244:GLY:O	2.30	0.49
2:B:26:ARG:HG2	2:B:359:GLU:OE2	2.12	0.49
2:B:227:ASN:O	2:B:228:ILE:C	2.50	0.49
1:A:376:ASN:HD22	1:A:378:GLU:N	2.10	0.49
1:A:197:ARG:HH22	1:A:422:GLU:HB3	1.77	0.48
2:B:294:PHE:CE1	2:B:315:ALA:HB2	2.48	0.48
1:A:22:PHE:O	1:A:26:VAL:HG23	2.12	0.48
1:A:74:GLU:OE2	1:A:76:SER:HB2	2.13	0.48
2:B:310:TYR:CZ	2:B:337:LEU:HD22	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:PRO:O	2:B:393:ALA:O	2.32	0.48
2:B:286:PHE:H	2:B:287:PRO:HD2	1.77	0.48
1:A:435:ALA:N	2:B:391:ASN:HD22	2.06	0.48
2:B:330:MET:HG2	2:B:351:LEU:HD13	1.96	0.48
2:B:318:ARG:O	2:B:363:SER:HA	2.14	0.48
2:B:338:ASN:ND2	2:B:338:ASN:N	2.56	0.48
1:A:115:GLU:O	1:A:118:PRO:HD2	2.13	0.48
1:A:197:ARG:HH11	1:A:198:ARG:HH11	1.62	0.48
2:B:2:ARG:NH1	2:B:3:GLU:HG3	2.29	0.48
1:A:349:TRP:C	1:A:351:PRO:HD3	2.33	0.48
1:A:400:ALA:HB1	1:A:404:LEU:CD2	2.44	0.48
2:B:134:PHE:CZ	2:B:160:TYR:CD2	3.02	0.48
1:A:324:ARG:HA	1:A:359:VAL:O	2.13	0.48
2:B:228:ILE:N	2:B:228:ILE:HD12	2.27	0.47
2:B:303:ILE:H	2:B:303:ILE:HD13	1.79	0.47
1:A:78:ILE:HG22	1:A:82:LYS:HE2	1.95	0.47
1:A:328:GLU:CG	1:A:329:ASP:N	2.76	0.47
1:A:75:PRO:O	1:A:79:ASP:HB2	2.14	0.47
2:B:16:ILE:HB	2:B:137:THR:CG2	2.42	0.47
2:B:102:TRP:CD2	2:B:188:LEU:HD13	2.49	0.47
1:A:212:PHE:CE1	1:A:224:PRO:HD2	2.49	0.47
1:A:319:THR:HG22	1:A:320:ALA:H	1.76	0.47
2:B:176:ILE:HG23	2:B:176:ILE:O	2.14	0.47
1:A:291:GLY:O	1:A:292:ILE:C	2.51	0.47
1:A:388:HIS:O	1:A:391:ASP:N	2.48	0.47
1:A:310:SER:O	1:A:378:GLU:HG3	2.15	0.47
2:B:217:ASN:HD22	2:B:218:ARG:N	2.13	0.47
2:B:23:LEU:HD13	2:B:23:LEU:N	2.25	0.46
1:A:390:PHE:CD2	1:A:417:ARG:CD	2.97	0.46
2:B:412:ARG:NH2	2:B:413:ASN:ND2	2.63	0.46
1:A:13:GLN:HG3	1:A:77:VAL:CG2	2.43	0.46
2:B:378:PHE:CE1	2:B:418:LEU:HD11	2.50	0.46
1:A:299:LEU:CD1	1:A:370:MET:HG3	2.36	0.46
1:A:4:ASN:HB2	1:A:253:GLU:OE2	2.15	0.46
1:A:344:LEU:HA	1:A:345:PRO:HD3	1.67	0.46
1:A:16:ASN:OD1	1:A:70:MET:HB3	2.16	0.46
1:A:273:MET:HE3	1:A:376:ASN:HB3	1.98	0.46
2:B:16:ILE:CB	2:B:137:THR:HG21	2.39	0.46
2:B:229:ILE:O	2:B:233:VAL:HG23	2.16	0.46
2:B:378:PHE:CE1	2:B:418:LEU:CD1	2.98	0.46
2:B:294:PHE:HE1	2:B:315:ALA:HB2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:69:LEU:HD12	2:B:91:ILE:HD11	1.97	0.46
2:B:187:ILE:HG22	2:B:188:LEU:N	2.31	0.46
2:B:5:LEU:HB3	2:B:134:PHE:HD1	1.81	0.46
2:B:399:GLU:C	2:B:401:ALA:H	2.19	0.45
1:A:3:VAL:HG22	1:A:253:GLU:OE2	2.17	0.45
2:B:114:ILE:HG23	2:B:115:ASP:N	2.32	0.45
2:B:216:LEU:HD13	2:B:218:ARG:HH22	1.81	0.45
2:B:5:LEU:HB3	2:B:134:PHE:CD1	2.52	0.45
1:A:198:ARG:HG3	1:A:198:ARG:NH2	2.32	0.45
1:A:30:HIS:CE1	1:A:245:ARG:HB3	2.52	0.45
1:A:66:PRO:HG2	1:A:88:LEU:CD1	2.47	0.45
1:A:222:GLU:HG2	1:A:223:SER:N	2.31	0.45
2:B:249:ASP:OD1	2:B:251:SER:HB2	2.17	0.45
2:B:368:LEU:HD23	2:B:368:LEU:HA	1.80	0.45
1:A:424:VAL:O	1:A:428:GLN:HG3	2.17	0.45
1:A:217:ARG:NH1	1:A:218:LYS:HE2	2.32	0.45
2:B:303:ILE:HD11	2:B:305:TRP:NE1	2.32	0.44
2:B:5:LEU:CD1	2:B:121:ILE:HG23	2.47	0.44
2:B:69:LEU:HD12	2:B:91:ILE:CD1	2.47	0.44
2:B:371:HIS:HD2	2:B:372:THR:N	2.16	0.44
2:B:53:HIS:O	2:B:60:TYR:HA	2.17	0.44
1:A:291:GLY:O	1:A:294:GLU:N	2.48	0.44
1:A:116:VAL:O	1:A:117:LEU:C	2.55	0.44
1:A:319:THR:CG2	1:A:320:ALA:H	2.30	0.44
2:B:56:ARG:HH11	2:B:59:LYS:HD2	1.80	0.44
1:A:205:ILE:O	1:A:205:ILE:HG22	2.18	0.44
1:A:185:GLU:N	1:A:186:PRO:CD	2.80	0.44
1:A:55:LYS:HG2	1:A:64:TYR:CE2	2.53	0.44
2:B:317:PHE:CD1	2:B:317:PHE:N	2.85	0.44
2:B:303:ILE:HG22	2:B:374:ILE:HA	2.00	0.44
1:A:95:ILE:CD1	1:A:95:ILE:N	2.80	0.44
1:A:281:PRO:O	1:A:283:ASP:N	2.51	0.44
2:B:133:GLY:HA3	2:B:164:ARG:O	2.18	0.44
2:B:261:PRO:O	2:B:264:HIS:HD2	2.01	0.44
2:B:176:ILE:HD13	2:B:225:LEU:HD22	2.00	0.43
1:A:148:GLY:O	1:A:152:GLY:HA3	2.18	0.43
1:A:124:LEU:CD1	1:A:159:LEU:HD13	2.47	0.43
1:A:185:GLU:CG	1:A:186:PRO:HD3	2.48	0.43
1:A:23:TRP:CE2	1:A:68:ALA:HB2	2.53	0.43
2:B:289:LEU:HD22	2:B:317:PHE:HD2	1.83	0.43
2:B:388:MET:CA	2:B:393:ALA:HB2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:ALA:HB1	1:A:399:PHE:CD1	2.53	0.43
2:B:303:ILE:HD11	2:B:305:TRP:CZ2	2.54	0.43
2:B:412:ARG:HH21	2:B:413:ASN:HD22	1.65	0.43
1:A:262:ASN:HD21	2:B:179:SER:HA	1.83	0.43
2:B:95:ILE:HD13	2:B:113:VAL:HG11	2.00	0.43
2:B:209:PHE:HA	2:B:225:LEU:HD11	2.01	0.43
1:A:11:ILE:HD12	1:A:152:GLY:HA2	2.00	0.43
1:A:306:PHE:CD1	1:A:306:PHE:N	2.86	0.43
2:B:175:LEU:O	2:B:176:ILE:HB	2.19	0.43
1:A:264:VAL:HB	2:B:397:TRP:CZ2	2.46	0.43
1:A:167:PRO:HA	1:A:201:ASP:OD2	2.19	0.43
1:A:195:THR:O	1:A:196:LEU:C	2.57	0.43
1:A:197:ARG:HH11	1:A:198:ARG:HE	1.67	0.43
2:B:87:ASP:C	2:B:89:SER:H	2.22	0.43
1:A:337:LEU:HD13	1:A:354:PHE:HE2	1.83	0.42
1:A:276:PHE:CG	1:A:277:ALA:N	2.87	0.42
2:B:132:GLN:HE21	2:B:250:LEU:H	1.59	0.42
2:B:260:PHE:CD1	2:B:260:PHE:C	2.93	0.42
2:B:51:PHE:O	2:B:63:ARG:HB2	2.19	0.42
2:B:95:ILE:CD1	2:B:95:ILE:N	2.76	0.42
1:A:145:GLY:N	3:A:1443:GDP:H5"	2.34	0.42
2:B:184:TYR:OH	2:B:393:ALA:HB3	2.20	0.42
2:B:106:TYR:CD2	2:B:107:ASN:ND2	2.88	0.42
1:A:421:GLN:HA	1:A:421:GLN:NE2	2.35	0.42
1:A:349:TRP:CE3	1:A:434:GLY:HA3	2.55	0.42
1:A:7:ILE:HA	1:A:67:ARG:O	2.20	0.42
2:B:306:GLN:HE21	2:B:306:GLN:HB3	1.60	0.42
2:B:286:PHE:HB3	2:B:287:PRO:HD3	2.01	0.42
2:B:326:VAL:HG13	2:B:327:ASP:N	2.35	0.42
2:B:157:ARG:HH22	2:B:165:ILE:HG13	1.85	0.42
1:A:97:ARG:CZ	1:A:116:VAL:HG12	2.50	0.42
1:A:193:LEU:HD23	1:A:193:LEU:HA	1.87	0.42
2:B:395:THR:HG21	2:B:405:ARG:CD	2.50	0.42
1:A:129:ASP:C	1:A:131:CYS:H	2.23	0.42
1:A:330:LYS:HB3	1:A:331:PRO:HD3	2.01	0.42
1:A:319:THR:HB	1:A:354:PHE:CD1	2.55	0.42
2:B:269:SER:HB3	2:B:299:PHE:CG	2.54	0.42
2:B:48:MET:C	2:B:50:VAL:N	2.73	0.42
1:A:281:PRO:HA	1:A:282:PRO:HD3	1.83	0.41
2:B:318:ARG:HB3	2:B:354:ALA:HB3	2.03	0.41
2:B:3:GLU:OE1	2:B:128:THR:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:HIS:NE2	1:A:245:ARG:HB3	2.35	0.41
1:A:203:CYS:HB3	1:A:271:PHE:CD2	2.55	0.41
1:A:104:ASN:OD1	1:A:106:ALA:HB3	2.20	0.41
2:B:21:TRP:CZ3	2:B:62:PRO:HB3	2.55	0.41
1:A:65:VAL:HG23	1:A:65:VAL:O	2.20	0.41
2:B:295:ALA:O	2:B:296:GLN:C	2.59	0.41
1:A:372:LEU:HD12	1:A:373:LEU:H	1.84	0.41
1:A:269:LEU:HD22	1:A:427:TYR:CD2	2.55	0.41
1:A:417:ARG:HH12	1:A:421:GLN:NE2	2.19	0.41
2:B:257:LEU:O	2:B:259:PRO:HD3	2.20	0.41
1:A:202:ALA:HA	1:A:270:HIS:HB2	2.01	0.41
1:A:244:MET:HE3	1:A:256:LEU:CA	2.50	0.41
2:B:366:LEU:C	2:B:366:LEU:CD1	2.89	0.41
1:A:5:ASN:HD22	1:A:67:ARG:NE	2.19	0.41
2:B:172:PRO:O	2:B:380:ARG:NH1	2.53	0.41
1:A:417:ARG:NH1	1:A:421:GLN:HE21	2.19	0.41
1:A:383:LEU:CD1	1:A:423:LEU:HD13	2.46	0.41
1:A:256:LEU:O	1:A:260:LEU:HG	2.21	0.41
2:B:90:SER:HA	2:B:120:VAL:HG13	2.02	0.41
2:B:122:ASP:O	2:B:125:VAL:HG22	2.20	0.41
2:B:217:ASN:ND2	2:B:218:ARG:N	2.68	0.41
2:B:7:ILE:HG12	2:B:65:VAL:HG22	2.03	0.41
2:B:21:TRP:HA	2:B:24:ALA:HB2	2.03	0.41
2:B:5:LEU:HD12	2:B:134:PHE:HE1	1.85	0.41
1:A:60:SER:C	1:A:62:GLY:H	2.24	0.41
2:B:423:ARG:HD3	2:B:423:ARG:HA	1.93	0.41
1:A:292:ILE:O	1:A:296:ILE:HG13	2.21	0.41
1:A:14:ALA:HB2	3:A:1443:GDP:C5	2.55	0.41
1:A:177:PRO:C	1:A:179:VAL:H	2.25	0.41
1:A:95:ILE:CD1	1:A:95:ILE:H	2.34	0.40
1:A:217:ARG:HD2	1:A:218:LYS:HE3	2.02	0.40
1:A:393:LEU:HD22	1:A:398:ALA:HB3	2.03	0.40
1:A:329:ASP:OD2	1:A:329:ASP:N	2.54	0.40
2:B:267:THR:HG23	2:B:301:ALA:CB	2.50	0.40
2:B:167:THR:HG22	2:B:168:PHE:N	2.36	0.40
2:B:8:HIS:CG	2:B:17:ALA:HB2	2.57	0.40
2:B:2:ARG:HE	2:B:2:ARG:N	2.19	0.40
1:A:279:LEU:HD23	1:A:279:LEU:HA	1.95	0.40
1:A:95:ILE:HD12	1:A:95:ILE:H	1.86	0.40
1:A:12:GLY:O	1:A:16:ASN:ND2	2.40	0.40
1:A:36:THR:HB	1:A:38:GLN:HG3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:ALA:HA	1:A:41:PRO:HD3	1.99	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	433/473 (92%)	383 (88%)	43 (10%)	7 (2%)	12	54
2	B	381/426 (89%)	306 (80%)	59 (16%)	16 (4%)	3	26
All	All	814/899 (90%)	689 (85%)	102 (12%)	23 (3%)	6	37

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	179	VAL
1	A	292	ILE
2	B	176	ILE
2	B	217	ASN
2	B	345	ALA
2	B	366	LEU
1	A	442	SER
2	B	57	ASP
2	B	239	SER
2	B	244	GLY
1	A	59	SER
1	A	178	GLN
1	A	220	ASN
1	A	282	PRO
2	B	88	GLU
2	B	327	ASP
2	B	393	ALA

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Mol	Chain	Res	Type
2	B	238	ALA
2	B	261	PRO
2	B	18	ASP
2	B	286	PHE
2	B	108	VAL
2	B	96	PRO

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	360/387 (93%)	332 (92%)	28 (8%)	16	53
2	B	319/341 (94%)	286 (90%)	33 (10%)	9	36
All	All	679/728 (93%)	618 (91%)	61 (9%)	12	43

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

Mol	Chain	Res	Type
1	A	56	LEU
1	A	98	THR
1	A	110	LEU
1	A	133	ASN
1	A	140	LEU
1	A	141	HIS
1	A	165	GLU
1	A	178	GLN
1	A	204	LEU
1	A	205	ILE
1	A	208	ASN
1	A	222	GLU
1	A	225	THR
1	A	227	ASP
1	A	253	GLU
1	A	256	LEU
1	A	270	HIS

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Mol	Chain	Res	Type
1	A	301	ASP
1	A	317	LEU
1	A	337	LEU
1	A	341	ARG
1	A	348	TYR
1	A	352	THR
1	A	361	GLN
1	A	373	LEU
1	A	396	ARG
1	A	417	ARG
1	A	423	LEU
2	B	2	ARG
2	B	5	LEU
2	B	9	VAL
2	B	23	LEU
2	B	26	ARG
2	B	32	GLU
2	B	47	ASN
2	B	69	LEU
2	B	91	ILE
2	B	92	VAL
2	B	111	GLU
2	B	138	HIS
2	B	157	ARG
2	B	166	PHE
2	B	175	LEU
2	B	181	VAL
2	B	217	ASN
2	B	218	ARG
2	B	245	LYS
2	B	246	LEU
2	B	249	ASP
2	B	253	PHE
2	B	255	THR
2	B	261	PRO
2	B	272	PRO
2	B	297	ASP
2	B	303	ILE
2	B	307	GLN
2	B	330	MET
2	B	334	ARG
2	B	338	ASN

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Mol	Chain	Res	Type
2	B	381	LEU
2	B	395	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	208	ASN
1	A	262	ASN
1	A	266	GLN
1	A	361	GLN
1	A	376	ASN
1	A	405	ASN
1	A	421	GLN
1	A	440	GLN
2	B	14	ASN
2	B	47	ASN
2	B	84	GLN
2	B	100	ASN
2	B	107	ASN
2	B	116	GLN
2	B	132	GLN
2	B	191	GLN
2	B	217	ASN
2	B	227	ASN
2	B	247	ASN
2	B	256	ASN
2	B	264	HIS
2	B	296	GLN
2	B	306	GLN
2	B	338	ASN
2	B	384	GLN
2	B	391	ASN
2	B	392	HIS
2	B	396	HIS
2	B	400	ASN
2	B	413	ASN

5.3.3 RNA ⓘ

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

5 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$
3	GDP	A	1443	-	23,30,30	1.76	7 (30%)	30,47,47	2.37	5 (16%)
4	SO4	B	1427	-	4,4,4	3.07	2 (50%)	6,6,6	0.92	0
4	SO4	B	1428	-	4,4,4	3.25	2 (50%)	6,6,6	0.98	0
4	SO4	B	1429	-	4,4,4	3.29	2 (50%)	6,6,6	0.96	0
4	SO4	B	1430	-	4,4,4	3.26	2 (50%)	6,6,6	0.97	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GDP	A	1443	-	-	0/12/32/32	0/3/3/3
4	SO4	B	1427	-	-	0/0/0/0	0/0/0/0
4	SO4	B	1428	-	-	0/0/0/0	0/0/0/0
4	SO4	B	1429	-	-	0/0/0/0	0/0/0/0
4	SO4	B	1430	-	-	0/0/0/0	0/0/0/0

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1430	SO4	O3-S	-4.64	1.30	1.47
4	B	1429	SO4	O3-S	-4.52	1.31	1.47
4	B	1428	SO4	O3-S	-4.38	1.31	1.47
4	B	1427	SO4	O3-S	-4.29	1.31	1.47
3	A	1443	GDP	C8-N7	-2.60	1.29	1.34
3	A	1443	GDP	PB-O2B	-2.42	1.46	1.54
3	A	1443	GDP	C6-C5	2.08	1.45	1.41
3	A	1443	GDP	O4'-C1'	2.21	1.44	1.41
3	A	1443	GDP	C4-N3	2.52	1.39	1.35
3	A	1443	GDP	C2-N1	2.61	1.40	1.35
4	B	1427	SO4	O1-S	4.32	1.61	1.47
4	B	1430	SO4	O1-S	4.49	1.62	1.47
4	B	1429	SO4	O1-S	4.67	1.63	1.47
4	B	1428	SO4	O1-S	4.70	1.63	1.47
3	A	1443	GDP	C6-N1	5.08	1.42	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1443	GDP	C5-C6-N1	-8.43	112.06	123.59
3	A	1443	GDP	N3-C2-N1	-3.08	122.76	127.44
3	A	1443	GDP	C1'-N9-C4	-2.08	123.80	126.94
3	A	1443	GDP	O2B-PB-O1B	2.60	118.96	110.58
3	A	1443	GDP	C6-N1-C2	6.93	125.55	115.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1443	GDP	5	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	437/473 (92%)	0.24	2 (0%) 91 87	38, 61, 101, 142	0
2	B	391/426 (91%)	0.27	6 (1%) 76 63	40, 74, 128, 177	0
All	All	828/899 (92%)	0.25	8 (0%) 84 75	38, 66, 123, 177	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	443	ALA	2.4
2	B	222	TYR	2.3
1	A	296	ILE	2.1
2	B	60	TYR	2.1
2	B	166	PHE	2.1
2	B	61	VAL	2.1
2	B	28	HIS	2.0
2	B	131	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	GDP	A	1443	28/28	0.91	0.36	1.65	70,105,112,115	0
4	SO4	B	1427	5/5	0.96	0.18	-0.55	74,76,81,84	0
4	SO4	B	1428	5/5	0.97	0.17	-1.00	96,96,97,98	0
4	SO4	B	1430	5/5	0.91	0.18	-	135,136,137,137	0
4	SO4	B	1429	5/5	0.89	0.18	-	149,150,152,153	0

6.5 Other polymers [i](#)

There are no such residues in this entry.