Full wwPDB X-ray Structure Validation Report ⓘ

Dec 2, 2023 – 04:56 pm GMT

PDB ID	:	2JIE
Title	:	BETA-GLUCOSIDASE B FROM BACILLUS POLYMYXA COMPLEXED WITH 2-F-GLUCOSE
Authors	:	Isorna, P.; Polaina, J.; Sanz-Aparicio, J.
Deposited on	:	2007-02-28
Resolution	:	2.30 Å(reported)

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

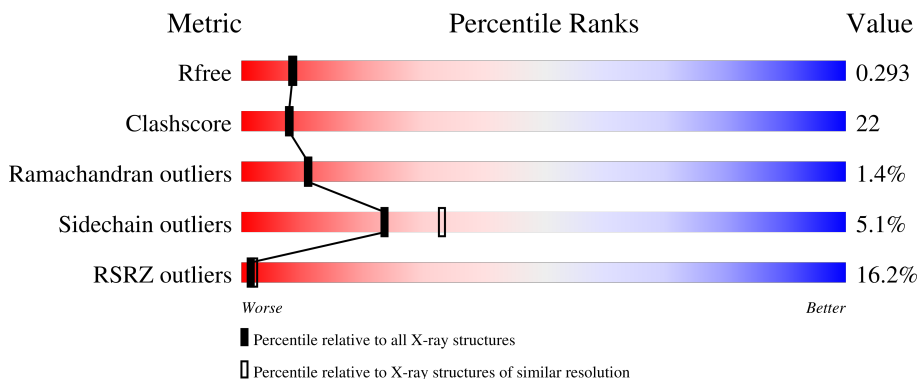|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1   Overall quality at a glance ⓘ

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

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	Percentile Ranks	Value
Rfree		0.293
Clashscore		22
Ramachandran outliers		1.4%
Sidechain outliers		5.1%
RSRZ outliers		16.2%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (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 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	454	16% 59% 35% • •

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 3759 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 BETA-GLUCOSIDASE B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	445	Total 3619	C 2324	N 610	O 665	S 20	0	0	0

- Molecule 2 is 2-deoxy-2-fluoro-alpha-D-glucopyranose (three-letter code: G2F) (formula: $C_6H_{11}FO_5$).
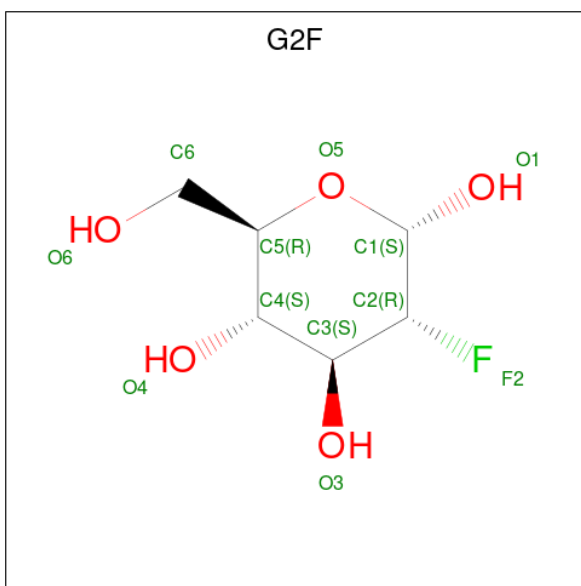
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 11	C 6	F 1	O 4	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	129	Total 129	O 129	0	0

3 Residue-property plots ⓘ

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

• Molecule 1: BETA-GLUCOSIDASE B
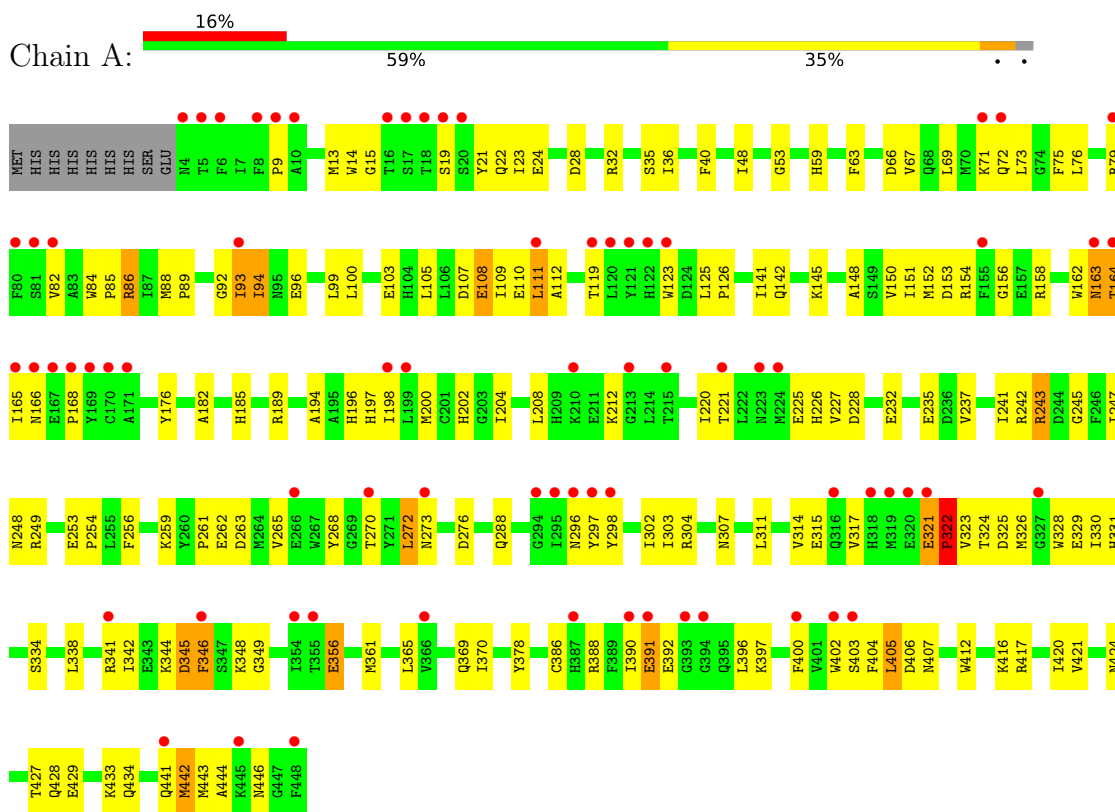
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	71.24Å 74.65Å 88.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.30 33.63 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.3 (25.00-2.30) 99.7 (33.63-2.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.31 (at 2.29Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.250 , 0.306 0.241 , 0.293	Depositor DCC
R_{free} test set	1484 reflections (6.88%)	wwPDB-VP
Wilson B-factor (Å^2)	38.9	Xtriage
Anisotropy	0.852	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 54.2	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.019 for k,h,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	3759	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.95% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: G2F

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	0.57	1/3730 (0.0%)	0.65	1/5057 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	356	GLU	CD-OE1	21.47	1.49	1.25

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	356	GLU	OE1-CD-OE2	6.26	130.81	123.30

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	3619	0	3411	152	0
2	A	11	0	9	0	0
3	A	129	0	0	5	0
All	All	3759	0	3420	152	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 (152) 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:110:GLU:OE2	1:A:158:ARG:HD2	1.69	0.93
1:A:148:ALA:O	1:A:152:MET:HG3	1.70	0.91
1:A:390:ILE:HD11	1:A:396:LEU:HB3	1.60	0.83
1:A:82:VAL:HG11	1:A:151:ILE:HD11	1.60	0.82
1:A:93:ILE:HD12	1:A:94:ILE:H	1.45	0.79
1:A:325:ASP:O	1:A:416:LYS:HE3	1.82	0.79
1:A:303:ILE:HG23	1:A:314:VAL:HG13	1.64	0.79
1:A:321:GLU:O	1:A:323:VAL:HG13	1.86	0.76
1:A:72:GLN:HE22	1:A:73:LEU:HD13	1.52	0.74
1:A:356:GLU:HG3	1:A:402:TRP:HB2	1.70	0.71
1:A:67:VAL:HG21	1:A:108:GLU:HB3	1.72	0.71
1:A:245:GLY:HA2	1:A:249:ARG:HB2	1.73	0.71
1:A:342:ILE:O	1:A:345:ASP:O	2.08	0.70
1:A:93:ILE:HD12	1:A:94:ILE:N	2.08	0.68
1:A:296:ASN:CG	1:A:356:GLU:HB3	2.15	0.67
1:A:36:ILE:HD13	1:A:125:LEU:HB3	1.77	0.66
1:A:235:GLU:OE2	3:A:2070:HOH:O	2.13	0.66
1:A:48:ILE:HD12	1:A:412:TRP:HA	1.77	0.66
1:A:296:ASN:OD1	1:A:356:GLU:HB3	1.96	0.66
1:A:249:ARG:HH22	1:A:263:ASP:CG	1.98	0.65
1:A:321:GLU:HB3	1:A:322:PRO:HD2	1.78	0.65
1:A:22:GLN:O	1:A:407:ASN:HB2	1.97	0.65
1:A:304:ARG:HG3	1:A:315:GLU:HB3	1.77	0.65
1:A:427:THR:OG1	1:A:429:GLU:HG2	1.96	0.65
1:A:189:ARG:HH11	1:A:189:ARG:HG3	1.62	0.64
1:A:71:LYS:HD3	1:A:112:ALA:O	1.96	0.64
1:A:256:PHE:CD1	1:A:346:PHE:HB3	2.31	0.64
1:A:338:LEU:O	1:A:342:ILE:HG12	1.97	0.64
1:A:75:PHE:HA	1:A:443:MET:HE1	1.79	0.63
1:A:156:GLY:HA2	1:A:162:TRP:HZ2	1.63	0.63
1:A:390:ILE:O	1:A:391:GLU:HB3	1.99	0.62
1:A:93:ILE:HD12	1:A:93:ILE:H	1.64	0.61
1:A:348:LYS:O	1:A:349:GLY:N	2.33	0.61
1:A:194:ALA:O	1:A:198:ILE:HG22	2.01	0.61
1:A:298:TYR:HE2	1:A:356:GLU:OE2	1.83	0.60
1:A:225:GLU:H	1:A:248:ASN:HD21	1.48	0.59
1:A:249:ARG:O	1:A:253:GLU:HB2	2.03	0.59
1:A:79:ARG:NH2	1:A:163:ASN:OD1	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:ARG:NH2	1:A:263:ASP:OD1	2.36	0.58
1:A:330:ILE:HD12	1:A:378:TYR:CD2	2.38	0.58
1:A:243:ARG:CZ	1:A:247:ILE:HD11	2.34	0.57
1:A:253:GLU:HB3	1:A:254:PRO:HD3	1.85	0.57
1:A:93:ILE:CD1	1:A:94:ILE:N	2.66	0.57
1:A:370:ILE:O	1:A:434:GLN:HG2	2.05	0.56
1:A:321:GLU:HA	1:A:321:GLU:OE1	2.05	0.56
1:A:330:ILE:HD12	1:A:378:TYR:HD2	1.70	0.56
1:A:152:MET:HB2	1:A:212:LYS:HE3	1.88	0.56
1:A:390:ILE:HG22	1:A:391:GLU:N	2.21	0.56
1:A:326:MET:HG3	1:A:416:LYS:HD2	1.88	0.56
1:A:391:GLU:O	1:A:391:GLU:HG3	2.06	0.55
1:A:119:THR:HA	1:A:163:ASN:HB3	1.88	0.55
1:A:262:GLU:H	1:A:262:GLU:CD	2.09	0.55
1:A:69:LEU:O	1:A:69:LEU:HD23	2.06	0.55
1:A:141:ILE:CD1	1:A:200:MET:HE3	2.37	0.54
1:A:331:HIS:HD2	1:A:334:SER:OG	1.90	0.54
1:A:302:ILE:HB	1:A:317:VAL:HB	1.90	0.54
1:A:390:ILE:HG22	1:A:391:GLU:H	1.73	0.54
1:A:442:MET:O	1:A:442:MET:HE2	2.07	0.54
1:A:390:ILE:C	1:A:392:GLU:H	2.11	0.54
1:A:237:VAL:O	1:A:241:ILE:HG12	2.08	0.54
1:A:325:ASP:HB2	1:A:361:MET:HA	1.90	0.53
1:A:344:LYS:O	1:A:348:LYS:HD3	2.08	0.53
1:A:441:GLN:O	1:A:444:ALA:HB3	2.09	0.53
1:A:424:ASN:O	1:A:428:GLN:N	2.40	0.53
1:A:93:ILE:HD12	1:A:93:ILE:N	2.24	0.52
1:A:265:VAL:HG13	1:A:272:LEU:HD23	1.91	0.52
1:A:164:THR:OG1	1:A:202:HIS:HD2	1.93	0.52
1:A:268:TYR:CE1	1:A:311:LEU:HD11	2.46	0.51
1:A:123:TRP:N	1:A:123:TRP:CD1	2.79	0.51
1:A:242:ARG:HD3	3:A:2072:HOH:O	2.10	0.50
1:A:36:ILE:HG23	1:A:125:LEU:O	2.10	0.50
1:A:321:GLU:CB	1:A:322:PRO:HD2	2.41	0.50
1:A:14:TRP:HB2	1:A:443:MET:HE2	1.93	0.50
1:A:89:PRO:HD2	1:A:93:ILE:CD1	2.42	0.49
1:A:208:LEU:O	1:A:212:LYS:HG3	2.12	0.49
1:A:323:VAL:HG12	1:A:329:GLU:HA	1.94	0.49
1:A:388:ARG:O	1:A:392:GLU:HB2	2.12	0.49
1:A:273:ASN:HB3	1:A:276:ASP:OD1	2.13	0.49
1:A:402:TRP:O	1:A:403:SER:HB3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:ASP:OD1	1:A:417:ARG:HB3	2.13	0.49
1:A:99:LEU:HD22	1:A:154:ARG:HG2	1.95	0.48
1:A:420:ILE:O	1:A:433:LYS:HG3	2.12	0.48
1:A:84:TRP:HB3	1:A:85:PRO:HD3	1.95	0.48
1:A:202:HIS:HE1	1:A:288:GLN:O	1.97	0.47
1:A:103:GLU:HG3	1:A:158:ARG:HH22	1.80	0.47
1:A:67:VAL:HG21	1:A:108:GLU:CB	2.44	0.47
1:A:324:THR:CG2	1:A:330:ILE:HD11	2.44	0.47
1:A:326:MET:HE3	1:A:412:TRP:CD1	2.49	0.47
1:A:226:HIS:HE1	1:A:228:ASP:OD1	1.98	0.47
1:A:165:ILE:HG21	1:A:198:ILE:HD11	1.95	0.47
1:A:69:LEU:HD23	1:A:72:GLN:NE2	2.29	0.47
1:A:72:GLN:NE2	1:A:73:LEU:HD13	2.26	0.47
1:A:86:ARG:NH1	1:A:86:ARG:HG3	2.30	0.47
1:A:21:TYR:CZ	1:A:53:GLY:HA3	2.50	0.46
1:A:297:TYR:OH	1:A:334:SER:HB2	2.15	0.46
1:A:165:ILE:HD12	1:A:165:ILE:N	2.29	0.46
1:A:168:PRO:HA	1:A:198:ILE:HD13	1.96	0.46
1:A:323:VAL:HA	1:A:328:TRP:O	2.16	0.46
1:A:141:ILE:HD13	1:A:200:MET:HE3	1.97	0.46
1:A:176:TYR:HA	1:A:185:HIS:HB2	1.96	0.46
1:A:220:ILE:HG22	3:A:2080:HOH:O	2.14	0.46
1:A:89:PRO:HD2	1:A:93:ILE:HD13	1.97	0.46
1:A:105:LEU:O	1:A:109:ILE:HG12	2.16	0.46
1:A:302:ILE:C	1:A:303:ILE:HD12	2.37	0.45
1:A:196:HIS:O	1:A:200:MET:HG3	2.16	0.45
1:A:59:HIS:O	1:A:63:PHE:HB3	2.17	0.44
1:A:202:HIS:CD2	1:A:220:ILE:HB	2.52	0.44
1:A:253:GLU:CB	1:A:254:PRO:HD3	2.47	0.44
1:A:243:ARG:CZ	1:A:247:ILE:CD1	2.95	0.44
1:A:99:LEU:HD11	1:A:150:VAL:CG1	2.47	0.44
1:A:369:GLN:HB2	1:A:434:GLN:NE2	2.33	0.44
1:A:84:TRP:N	1:A:85:PRO:CD	2.81	0.44
1:A:96:GLU:O	1:A:100:LEU:HG	2.18	0.44
1:A:326:MET:HG3	1:A:416:LYS:CD	2.47	0.44
1:A:79:ARG:HH12	1:A:166:ASN:ND2	2.16	0.44
1:A:168:PRO:HD2	3:A:2066:HOH:O	2.17	0.44
1:A:153:ASP:OD2	1:A:212:LYS:HD3	2.18	0.43
1:A:404:PHE:O	1:A:421:VAL:HB	2.19	0.43
1:A:189:ARG:HG3	1:A:189:ARG:NH1	2.30	0.43
1:A:197:HIS:HA	1:A:200:MET:HE2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:ARG:HB2	1:A:86:ARG:HG3	1.99	0.43
1:A:165:ILE:CG2	1:A:198:ILE:HD11	2.48	0.43
1:A:200:MET:O	1:A:204:ILE:HG12	2.19	0.43
1:A:220:ILE:HG12	1:A:221:THR:N	2.34	0.43
1:A:348:LYS:O	1:A:349:GLY:HA3	2.18	0.43
1:A:197:HIS:HD2	1:A:200:MET:CE	2.32	0.43
1:A:446:ASN:O	1:A:446:ASN:OD1	2.36	0.42
1:A:73:LEU:HD23	1:A:404:PHE:HE1	1.83	0.42
1:A:261:PRO:O	1:A:265:VAL:HG23	2.19	0.42
1:A:40:PHE:CB	1:A:182:ALA:HB2	2.49	0.42
1:A:324:THR:HG23	1:A:330:ILE:HD11	2.00	0.42
1:A:15:GLY:O	1:A:400:PHE:HA	2.20	0.42
1:A:23:ILE:HG13	1:A:24:GLU:N	2.35	0.42
1:A:145:LYS:HG3	1:A:208:LEU:HD11	2.01	0.42
1:A:13:MET:HG3	1:A:397:LYS:O	2.20	0.42
1:A:378:TYR:CD1	1:A:378:TYR:C	2.93	0.42
1:A:386:CYS:HB3	1:A:396:LEU:CD2	2.50	0.42
1:A:73:LEU:HD12	1:A:73:LEU:HA	1.85	0.41
1:A:125:LEU:HA	1:A:126:PRO:HD3	1.93	0.41
1:A:163:ASN:HD22	1:A:163:ASN:HA	1.57	0.41
1:A:321:GLU:O	1:A:322:PRO:C	2.58	0.41
1:A:59:HIS:HD2	1:A:66:ASP:OD2	2.02	0.41
1:A:256:PHE:CE1	1:A:346:PHE:HB3	2.54	0.41
1:A:28:ASP:OD1	1:A:28:ASP:N	2.46	0.41
1:A:19:SER:HB3	1:A:22:GLN:OE1	2.21	0.41
1:A:341:ARG:NE	3:A:2101:HOH:O	2.54	0.41
1:A:403:SER:OG	1:A:405:LEU:O	2.34	0.41
1:A:35:SER:CB	1:A:85:PRO:HG2	2.50	0.41
1:A:76:LEU:O	1:A:76:LEU:HD12	2.21	0.41
1:A:88:MET:HA	1:A:93:ILE:HD11	2.02	0.41
1:A:107:ASP:O	1:A:111:LEU:HB2	2.21	0.41
1:A:227:VAL:HG13	1:A:303:ILE:HD13	2.03	0.41

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	441/454 (97%)	412 (93%)	23 (5%)	6 (1%)	11	11

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	322	PRO
1	A	94	ILE
1	A	346	PHE
1	A	92	GLY
1	A	164	THR
1	A	9	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	376/385 (98%)	357 (95%)	19 (5%)	24	33

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	ARG
1	A	93	ILE
1	A	108	GLU
1	A	111	LEU
1	A	142	GLN
1	A	163	ASN
1	A	232	GLU
1	A	243	ARG
1	A	259	LYS
1	A	270	THR
1	A	272	LEU

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Mol	Chain	Res	Type
1	A	307	ASN
1	A	321	GLU
1	A	322	PRO
1	A	345	ASP
1	A	365	LEU
1	A	391	GLU
1	A	405	LEU
1	A	442	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
1	A	59	HIS
1	A	72	GLN
1	A	95	ASN
1	A	127	GLN
1	A	166	ASN
1	A	197	HIS
1	A	202	HIS
1	A	207	ASN
1	A	209	HIS
1	A	226	HIS
1	A	248	ASN
1	A	257	ASN
1	A	287	GLN
1	A	288	GLN
1	A	307	ASN
1	A	313	GLN
1	A	331	HIS
1	A	369	GLN
1	A	434	GLN
1	A	441	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 monosaccharides 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	$\#|Z| > 2$
2	G2F	A	1449	1	11,11,12	1.70	3 (27%)	10,15,17	0.98	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
2	G2F	A	1449	1	-	0/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1449	G2F	C1-C2	3.39	1.57	1.52
2	A	1449	G2F	F2-C2	2.58	1.47	1.40
2	A	1449	G2F	C2-C3	2.43	1.54	1.51

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	348:LYS	C	349:GLY	N	3.30

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	445/454 (98%)	0.79	72 (16%)	1	2	27, 46, 60, 77	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	319	MET	7.8
1	A	4	ASN	6.6
1	A	403	SER	5.6
1	A	366	VAL	5.5
1	A	123	TRP	4.6
1	A	165	ILE	4.6
1	A	119	THR	4.5
1	A	321	GLU	4.5
1	A	122	HIS	4.1
1	A	17	SER	4.0
1	A	93	ILE	4.0
1	A	166	ASN	4.0
1	A	297	TYR	3.9
1	A	391	GLU	3.7
1	A	448	PHE	3.7
1	A	111	LEU	3.6
1	A	18	THR	3.6
1	A	402	TRP	3.6
1	A	19	SER	3.4
1	A	390	ILE	3.4
1	A	213	GLY	3.4
1	A	168	PRO	3.3
1	A	355	THR	3.3
1	A	121	TYR	3.2
1	A	320	GLU	3.2
1	A	270	THR	3.2
1	A	10	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	387	HIS	3.1
1	A	273	ASN	3.0
1	A	171	ALA	3.0
1	A	82	VAL	3.0
1	A	296	ASN	3.0
1	A	81	SER	2.9
1	A	170	CYS	2.9
1	A	16	THR	2.9
1	A	80	PHE	2.8
1	A	215	THR	2.8
1	A	72	GLN	2.8
1	A	394	GLY	2.8
1	A	223	ASN	2.8
1	A	167	GLU	2.8
1	A	198	ILE	2.7
1	A	8	PHE	2.7
1	A	164	THR	2.7
1	A	298	TYR	2.6
1	A	9	PRO	2.6
1	A	295	ILE	2.6
1	A	79	ARG	2.5
1	A	5	THR	2.5
1	A	71	LYS	2.5
1	A	20	SER	2.4
1	A	120	LEU	2.4
1	A	354	ILE	2.4
1	A	199	LEU	2.4
1	A	210	LYS	2.4
1	A	393	GLY	2.3
1	A	221	THR	2.3
1	A	266	GLU	2.3
1	A	341	ARG	2.3
1	A	155	PHE	2.2
1	A	400	PHE	2.2
1	A	169	TYR	2.2
1	A	318	HIS	2.2
1	A	6	PHE	2.2
1	A	346	PHE	2.2
1	A	294	GLY	2.1
1	A	441	GLN	2.1
1	A	445	LYS	2.1
1	A	316	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	163	ASN	2.0
1	A	224	MET	2.0
1	A	327	GLY	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	G2F	A	1449	11/12	0.92	0.33	27,31,35,39	0

6.5 Other polymers ⓘ

There are no such residues in this entry.

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PROTEIN DATA BANK