



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:48 PM UTC

PDB ID : 1MKI / pdb_00001mki
Title : Crystal Structure of Bacillus Subtilis Probable Glutaminase, APC1040
Authors : Kim, Y.; Dementieva, I.; Vinokour, E.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on : 2002-08-29
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

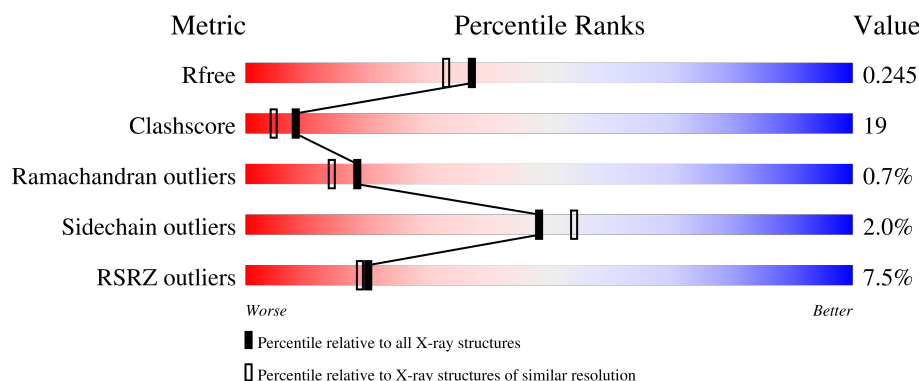
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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 $\leq 5\%$. 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	330	
1	B	330	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5193 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 Probable Glutaminase ybgJ.

Mol	Chain	Residues	Atoms								ZeroOcc	AltConf	Trace
1	A	312	Total	C	N	O	P	S	Se				
			2422	1545	403	456	1	5	12	0	0	0	
1	B	312	Total	C	N	O	P	S	Se				
			2422	1545	403	456	1	5	12	0	0	0	

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	cloning artifact	UNP O31465
A	-1	ASN	-	cloning artifact	UNP O31465
A	0	ALA	-	cloning artifact	UNP O31465
A	1	MSE	MET	modified residue	UNP O31465
A	60	MSE	MET	modified residue	UNP O31465
A	72	MSE	MET	modified residue	UNP O31465
A	74	SEP	SER	modified residue	UNP O31465
A	86	MSE	MET	modified residue	UNP O31465
A	124	MSE	MET	modified residue	UNP O31465
A	152	MSE	MET	modified residue	UNP O31465
A	207	MSE	MET	modified residue	UNP O31465
A	247	MSE	MET	modified residue	UNP O31465
A	252	MSE	MET	modified residue	UNP O31465
A	276	MSE	MET	modified residue	UNP O31465
A	313	MSE	MET	modified residue	UNP O31465
A	318	MSE	MET	modified residue	UNP O31465
B	-2	SER	-	cloning artifact	UNP O31465
B	-1	ASN	-	cloning artifact	UNP O31465
B	0	ALA	-	cloning artifact	UNP O31465
B	1	MSE	MET	modified residue	UNP O31465
B	60	MSE	MET	modified residue	UNP O31465
B	72	MSE	MET	modified residue	UNP O31465
B	74	SEP	SER	modified residue	UNP O31465
B	86	MSE	MET	modified residue	UNP O31465
B	124	MSE	MET	modified residue	UNP O31465

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	152	MSE	MET	modified residue	UNP O31465
B	207	MSE	MET	modified residue	UNP O31465
B	247	MSE	MET	modified residue	UNP O31465
B	252	MSE	MET	modified residue	UNP O31465
B	276	MSE	MET	modified residue	UNP O31465
B	313	MSE	MET	modified residue	UNP O31465
B	318	MSE	MET	modified residue	UNP O31465

- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is FORMIC ACID (CCD ID: FMT) (formula: CH_2O_2).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			3	1	2		

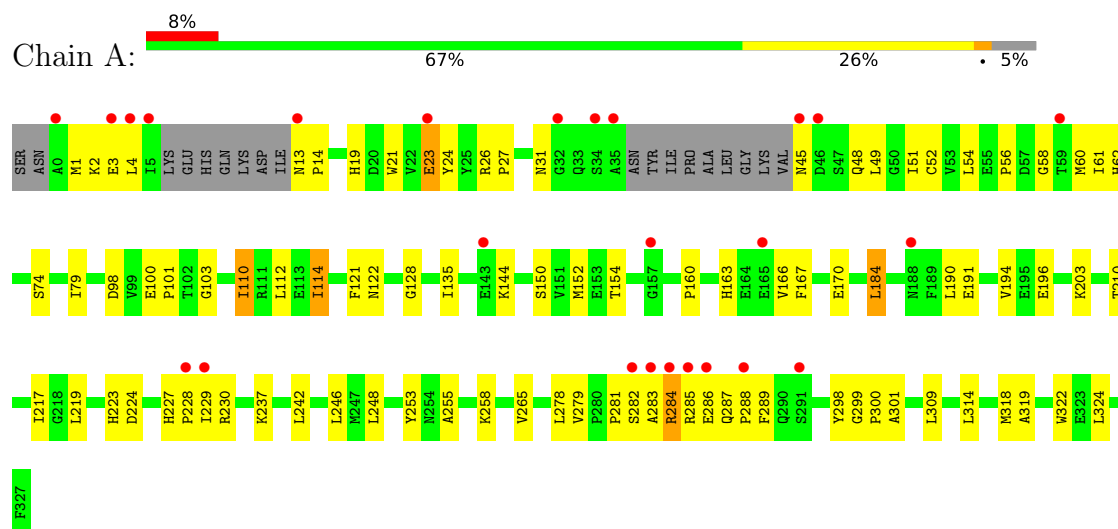
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	154	Total	O	0	0
			154	154		
4	B	176	Total	O	0	0
			176	176		

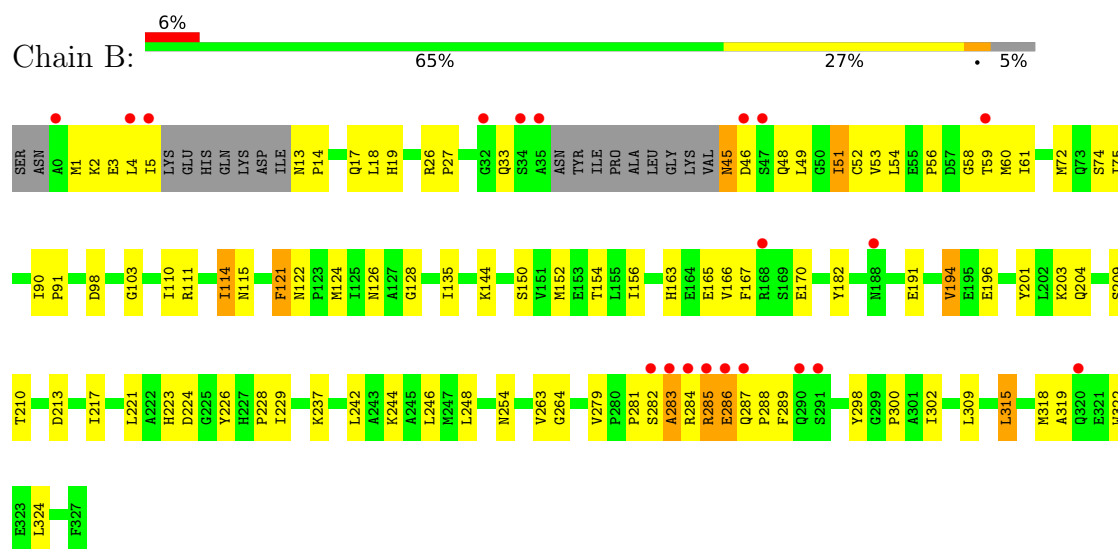
3 Residue-property plots [i](#)

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

• Molecule 1: Probable Glutaminase ybgJ



• Molecule 1: Probable Glutaminase ybgJ



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	71.33Å 181.48Å 51.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.69 – 2.00 40.69 – 2.00	Depositor EDS
% Data completeness (in resolution range)	95.2 (40.69-2.00) 95.2 (40.69-2.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.65 (at 2.00Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.212 , 0.245 0.213 , 0.245	Depositor DCC
R_{free} test set	4545 reflections (9.73%)	wwPDB-VP
Wilson B-factor (Å ²)	23.0	Xtriage
Anisotropy	0.869	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 40.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5193	wwPDB-VP
Average B, all atoms (Å ²)	31.0	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 34.14 % 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 7.1478e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: EDO, SEP, FMT

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	0.38	0/2453	0.88	9/3300 (0.3%)
1	B	0.37	0/2453	0.87	7/3300 (0.2%)
All	All	0.37	0/4906	0.88	16/6600 (0.2%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	121	PHE	N-CA-C	6.40	118.25	111.28
1	A	299	GLY	CA-C-N	5.88	127.19	119.84
1	A	299	GLY	C-N-CA	5.88	127.19	119.84
1	A	194	VAL	N-CA-C	5.73	115.92	110.42
1	A	103	GLY	N-CA-C	-5.71	107.77	115.36
1	B	210	THR	N-CA-C	-5.58	101.66	109.69
1	A	253	TYR	CB-CA-C	-5.51	110.24	116.63
1	A	210	THR	N-CA-C	-5.43	101.87	109.69
1	A	255	ALA	N-CA-C	-5.41	105.49	113.61
1	B	103	GLY	N-CA-C	-5.28	107.96	115.30
1	B	194	VAL	N-CA-C	5.28	115.42	110.30
1	A	114	ILE	N-CA-C	5.25	116.03	110.72
1	B	286	GLU	N-CA-C	-5.22	99.67	110.80
1	B	121	PHE	N-CA-C	5.20	116.94	111.28
1	B	264	GLY	N-CA-C	5.14	123.00	115.08
1	B	114	ILE	N-CA-C	5.04	115.26	110.42

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	2422	0	2395	89	0
1	B	2422	0	2395	98	0
2	A	12	0	18	0	0
2	B	4	0	6	0	0
3	A	3	0	1	0	0
4	A	154	0	0	3	0
4	B	176	0	0	1	0
All	All	5193	0	4815	187	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 19.

All (187) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:284:ARG:HG3	1:B:289:PHE:O	1.71	0.89
1:B:284:ARG:O	1:B:285:ARG:HB2	1.74	0.88
1:B:284:ARG:NH2	1:B:288:PRO:HG2	1.91	0.84
1:B:122:ASN:HD22	1:B:124:MSE:H	1.24	0.84
1:A:284:ARG:CZ	1:A:324:LEU:HD21	2.09	0.83
1:B:284:ARG:CZ	1:B:289:PHE:HD1	1.92	0.82
1:A:284:ARG:CZ	1:A:289:PHE:HD1	1.94	0.80
1:A:284:ARG:HD2	1:A:324:LEU:HD22	1.64	0.79
1:B:284:ARG:CZ	1:B:324:LEU:HD21	2.13	0.77
1:A:284:ARG:NE	1:A:289:PHE:HB2	1.99	0.77
1:A:284:ARG:NH2	1:A:289:PHE:HD1	1.83	0.76
1:B:284:ARG:NH1	1:B:289:PHE:HD1	1.84	0.75
1:A:284:ARG:HH21	1:A:288:PRO:HG2	1.53	0.74
1:A:279:VAL:CG1	1:A:284:ARG:HG2	2.19	0.72
1:B:285:ARG:HD3	1:B:287:GLN:O	1.89	0.72
1:B:1:MSE:HE1	1:B:19:HIS:HB2	1.71	0.72
1:A:284:ARG:CZ	1:A:289:PHE:CD1	2.76	0.69
1:B:284:ARG:NH1	1:B:324:LEU:HD21	2.07	0.69
1:B:17:GLN:HE22	1:B:322:TRP:HE1	1.36	0.69
1:B:279:VAL:HG11	1:B:284:ARG:HD2	1.75	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:VAL:HG11	1:A:284:ARG:HG2	1.76	0.68
1:B:284:ARG:HD2	1:B:324:LEU:HD22	1.75	0.68
1:B:284:ARG:CZ	1:B:324:LEU:CD2	2.72	0.67
1:A:166:VAL:O	1:A:170:GLU:HG2	1.94	0.67
1:A:265:VAL:HG13	1:A:278:LEU:O	1.95	0.67
1:A:13:ASN:HB2	1:A:14:PRO:HD3	1.76	0.67
1:A:284:ARG:CZ	1:A:324:LEU:CD2	2.73	0.67
1:B:284:ARG:NE	1:B:289:PHE:HB2	2.10	0.66
1:A:56:PRO:HG3	1:A:223:HIS:NE2	2.10	0.65
1:B:45:ASN:HD22	1:B:46:ASP:H	1.44	0.65
1:B:135:ILE:HG22	1:B:191:GLU:HG3	1.77	0.64
1:A:224:ASP:HB3	1:A:237:LYS:HG3	1.80	0.64
1:A:3:GLU:HG3	1:A:60:MSE:HE2	1.80	0.63
1:A:112:LEU:HD13	1:A:184:LEU:HD13	1.80	0.63
1:A:135:ILE:HG22	1:A:191:GLU:HG3	1.80	0.62
1:A:152:MSE:HG2	1:A:160:PRO:HG3	1.81	0.62
1:B:51:ILE:HD11	1:B:53:VAL:HG23	1.82	0.61
1:B:282:SER:C	1:B:284:ARG:H	2.09	0.61
1:B:45:ASN:HD22	1:B:46:ASP:N	1.98	0.61
1:A:45:ASN:HD22	1:A:48:GLN:HG3	1.65	0.61
1:B:286:GLU:O	1:B:287:GLN:HG3	2.00	0.61
1:A:26:ARG:HB3	1:A:27:PRO:HD3	1.81	0.61
1:A:1:MSE:HE1	1:A:19:HIS:HB2	1.81	0.61
1:A:152:MSE:HG2	1:A:160:PRO:CG	2.31	0.60
1:B:110:ILE:O	1:B:114:ILE:HD13	2.02	0.60
1:B:284:ARG:NH1	1:B:324:LEU:CD2	2.65	0.59
1:B:284:ARG:NH1	1:B:289:PHE:CD1	2.70	0.59
1:B:3:GLU:C	1:B:4:LEU:HD12	2.28	0.59
1:B:111:ARG:HH11	1:B:115:ASN:HD21	1.50	0.58
1:A:284:ARG:CD	1:A:324:LEU:HD22	2.32	0.58
1:B:152:MSE:HE1	1:B:217:ILE:HD11	1.83	0.58
1:A:135:ILE:HG22	1:A:191:GLU:CG	2.32	0.58
1:B:18:LEU:HD13	1:B:51:ILE:HD12	1.86	0.58
1:B:284:ARG:HH22	1:B:288:PRO:HG2	1.64	0.58
1:A:79:ILE:HG13	1:A:152:MSE:HE1	1.85	0.57
1:A:284:ARG:HG3	1:A:289:PHE:O	2.04	0.57
1:B:263:VAL:HG11	1:B:315:LEU:HD13	1.86	0.57
1:B:224:ASP:HB3	1:B:237:LYS:HG3	1.86	0.57
1:A:60:MSE:HE3	1:A:62:HIS:HD2	1.69	0.56
1:A:31:ASN:HB2	1:A:309:LEU:HD21	1.86	0.56
1:B:45:ASN:ND2	1:B:46:ASP:N	2.53	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:TYR:O	1:B:228:PRO:HD3	2.05	0.56
1:B:166:VAL:O	1:B:170:GLU:HG3	2.06	0.55
1:B:5:ILE:HD13	1:B:60:MSE:HE2	1.88	0.55
1:B:152:MSE:HE1	1:B:217:ILE:CD1	2.37	0.55
1:A:1:MSE:O	1:A:61:ILE:HA	2.06	0.55
1:B:56:PRO:HG3	1:B:223:HIS:NE2	2.22	0.55
1:B:284:ARG:CZ	1:B:289:PHE:CD1	2.82	0.55
1:B:163:HIS:CE1	1:B:165:GLU:HB3	2.41	0.54
1:B:5:ILE:HD13	1:B:60:MSE:CE	2.36	0.54
1:A:152:MSE:CG	1:A:160:PRO:HG3	2.37	0.54
1:A:287:GLN:HB3	1:A:288:PRO:HD3	1.88	0.54
1:B:221:LEU:O	1:B:244:LYS:HD2	2.08	0.54
1:A:60:MSE:HE3	1:A:62:HIS:CD2	2.43	0.53
1:A:279:VAL:HG11	1:A:284:ARG:HD2	1.90	0.53
1:A:167:PHE:CZ	1:A:203:LYS:HE3	2.43	0.53
1:B:279:VAL:CG1	1:B:284:ARG:HG2	2.39	0.53
1:B:98:ASP:HB3	1:B:121:PHE:O	2.07	0.53
1:B:279:VAL:HG11	1:B:284:ARG:CD	2.38	0.53
1:A:184:LEU:HB3	1:A:190:LEU:HG	1.89	0.53
1:B:26:ARG:HB3	1:B:27:PRO:HD3	1.89	0.53
1:A:110:ILE:CG2	1:A:114:ILE:HD12	2.39	0.52
1:B:229:ILE:N	1:B:229:ILE:HD12	2.23	0.52
1:A:285:ARG:HH11	1:A:322:TRP:HA	1.74	0.52
1:B:45:ASN:HD22	1:B:45:ASN:N	2.07	0.52
1:B:45:ASN:HB2	1:B:48:GLN:NE2	2.25	0.52
1:B:51:ILE:CD1	1:B:53:VAL:HG23	2.39	0.52
1:B:318:MSE:HE3	1:B:322:TRP:HZ3	1.73	0.52
1:B:5:ILE:HD11	1:B:54:LEU:HD11	1.92	0.52
1:A:150:SER:O	1:A:154:THR:HG23	2.09	0.51
1:A:227:HIS:HD2	1:A:229:ILE:H	1.56	0.51
1:A:45:ASN:ND2	1:A:48:GLN:HG3	2.25	0.51
1:A:284:ARG:NH2	1:A:288:PRO:HG2	2.25	0.50
1:A:284:ARG:NH1	1:A:324:LEU:HD21	2.26	0.50
1:B:122:ASN:O	1:B:128:GLY:HA3	2.11	0.50
1:A:284:ARG:CB	1:A:289:PHE:O	2.60	0.49
1:B:13:ASN:CG	1:B:14:PRO:HD3	2.36	0.49
1:B:51:ILE:HD13	1:B:52:CYS:N	2.27	0.49
1:B:284:ARG:CD	1:B:324:LEU:HD22	2.42	0.49
1:B:33:GLN:O	1:B:302:ILE:HG12	2.11	0.49
1:B:51:ILE:HD11	1:B:53:VAL:CG2	2.41	0.49
1:B:135:ILE:HG22	1:B:191:GLU:CG	2.41	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:HIS:HE1	1:B:165:GLU:HB3	1.76	0.49
1:B:298:TYR:CZ	1:B:300:PRO:HG3	2.48	0.49
1:B:114:ILE:N	1:B:114:ILE:HD12	2.28	0.49
1:A:2:LYS:HA	1:A:60:MSE:O	2.14	0.48
1:B:45:ASN:O	1:B:48:GLN:HG3	2.14	0.48
1:A:24:TYR:HB3	4:A:1432:HOH:O	2.13	0.47
1:B:2:LYS:HE3	1:B:59:THR:HG21	1.95	0.47
1:A:79:ILE:HD11	1:A:217:ILE:HD13	1.95	0.47
1:B:319:ALA:HA	1:B:324:LEU:HG	1.95	0.47
1:B:122:ASN:HD22	1:B:124:MSE:N	2.03	0.47
1:B:163:HIS:CE1	1:B:166:VAL:HG23	2.50	0.47
1:B:279:VAL:HG11	1:B:284:ARG:HG2	1.97	0.47
1:A:258:LYS:HE3	4:B:1472:HOH:O	2.14	0.47
1:A:279:VAL:HG11	1:A:284:ARG:CG	2.44	0.47
1:A:287:GLN:HB3	1:A:288:PRO:CD	2.44	0.47
1:B:1:MSE:O	1:B:61:ILE:HA	2.14	0.47
1:B:284:ARG:O	1:B:285:ARG:CB	2.52	0.46
1:A:248:LEU:C	1:A:248:LEU:HD13	2.40	0.46
1:B:45:ASN:HB2	1:B:48:GLN:HE21	1.79	0.46
1:B:111:ARG:HH11	1:B:115:ASN:ND2	2.14	0.46
1:A:282:SER:C	1:A:284:ARG:H	2.23	0.46
1:B:45:ASN:HA	1:B:48:GLN:HG3	1.97	0.46
1:A:23:GLU:HA	1:A:23:GLU:OE1	2.16	0.45
1:A:45:ASN:HD22	1:A:48:GLN:CG	2.27	0.45
1:B:284:ARG:CG	1:B:289:PHE:O	2.54	0.45
1:B:111:ARG:HG2	1:B:115:ASN:ND2	2.32	0.45
1:B:126:ASN:HD22	1:B:126:ASN:N	2.13	0.45
1:A:3:GLU:CG	1:A:60:MSE:HE2	2.45	0.45
1:B:13:ASN:N	1:B:14:PRO:CD	2.79	0.45
1:B:201:TYR:O	1:B:204:GLN:HG2	2.17	0.45
1:B:248:LEU:C	1:B:248:LEU:HD13	2.42	0.45
1:B:284:ARG:NH2	1:B:288:PRO:CG	2.73	0.45
1:A:144:LYS:HE2	1:A:196:GLU:OE2	2.16	0.45
1:A:319:ALA:HA	1:A:324:LEU:HG	2.00	0.44
1:B:122:ASN:ND2	1:B:124:MSE:H	2.03	0.44
1:A:1:MSE:HE2	1:A:62:HIS:O	2.18	0.44
1:A:227:HIS:CD2	1:A:230:ARG:H	2.36	0.44
1:A:122:ASN:O	1:A:128:GLY:HA3	2.17	0.44
1:A:167:PHE:CE2	1:A:203:LYS:HE3	2.53	0.44
1:A:284:ARG:HH21	1:A:288:PRO:CG	2.25	0.44
1:B:209:SER:HB2	1:B:213:ASP:HB2	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:ASP:O	1:A:122:ASN:HA	2.17	0.44
1:B:242:LEU:O	1:B:246:LEU:HD23	2.17	0.44
1:B:248:LEU:HD13	1:B:248:LEU:O	2.18	0.44
1:A:248:LEU:HD13	1:A:248:LEU:O	2.18	0.44
1:B:284:ARG:CD	1:B:289:PHE:HB2	2.47	0.44
1:A:13:ASN:HB2	1:A:14:PRO:CD	2.45	0.43
1:B:5:ILE:HG12	1:B:54:LEU:HD21	1.99	0.43
1:A:219:LEU:HG	1:A:228:PRO:HG3	2.00	0.43
1:A:242:LEU:O	1:A:246:LEU:HD23	2.17	0.43
1:B:72:MSE:HE2	1:B:75:ILE:HG22	2.00	0.43
1:A:4:LEU:HA	1:A:58:GLY:O	2.18	0.43
1:A:13:ASN:CB	1:A:14:PRO:HD3	2.47	0.42
1:A:110:ILE:HG22	1:A:114:ILE:HD12	2.01	0.42
1:B:4:LEU:HA	1:B:58:GLY:O	2.18	0.42
1:B:152:MSE:HE2	1:B:156:ILE:HG23	2.00	0.42
1:A:51:ILE:CD1	1:A:318:MSE:SE	3.16	0.42
1:B:163:HIS:ND1	1:B:166:VAL:HG23	2.34	0.42
1:A:284:ARG:CZ	1:A:289:PHE:HB2	2.49	0.42
1:A:287:GLN:CB	1:A:288:PRO:HD3	2.49	0.42
1:A:298:TYR:CZ	1:A:300:PRO:HG3	2.54	0.42
1:A:21:TRP:HA	4:A:1432:HOH:O	2.18	0.42
1:B:281:PRO:C	1:B:283:ALA:H	2.27	0.42
1:B:111:ARG:HB3	1:B:115:ASN:HD22	1.84	0.42
1:B:284:ARG:HE	1:B:284:ARG:HB3	1.58	0.42
1:A:51:ILE:HG12	1:A:52:CYS:N	2.34	0.42
1:B:254:ASN:OD1	1:B:254:ASN:N	2.53	0.42
1:B:150:SER:O	1:B:154:THR:HG23	2.20	0.41
1:A:284:ARG:CD	1:A:289:PHE:HB2	2.49	0.41
1:A:281:PRO:C	1:A:283:ALA:H	2.28	0.41
1:A:287:GLN:CB	1:A:288:PRO:CD	2.98	0.41
1:B:167:PHE:CE2	1:B:203:LYS:HE3	2.55	0.41
1:B:90:ILE:HB	1:B:91:PRO:HD3	2.02	0.41
1:A:54:LEU:HG	1:A:219:LEU:HD22	2.02	0.41
1:A:163:HIS:CD2	1:A:166:VAL:H	2.38	0.41
1:B:182:TYR:CD1	1:B:194:VAL:HG21	2.55	0.41
1:A:284:ARG:NE	1:A:324:LEU:HD22	2.36	0.41
1:A:284:ARG:CG	1:A:289:PHE:O	2.67	0.40
1:A:285:ARG:O	1:A:287:GLN:N	2.54	0.40
1:A:284:ARG:NH1	1:A:324:LEU:CD2	2.84	0.40
1:A:301:ALA:HB3	4:A:1412:HOH:O	2.20	0.40
1:B:144:LYS:HE2	1:B:196:GLU:OE2	2.20	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:VAL:HG11	1:A:284:ARG:CD	2.51	0.40
1:A:100:GLU:HA	1:A:101:PRO:HD3	1.98	0.40
1:A:318:MSE:HE3	1:A:322:TRP:HZ3	1.87	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	305/330 (92%)	290 (95%)	13 (4%)	2 (1%)	18	14
1	B	305/330 (92%)	287 (94%)	16 (5%)	2 (1%)	18	14
All	All	610/660 (92%)	577 (95%)	29 (5%)	4 (1%)	18	14

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	285	ARG
1	A	286	GLU
1	B	283	ALA
1	A	110	ILE

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	255/259 (98%)	250 (98%)	5 (2%)	48	54
1	B	255/259 (98%)	250 (98%)	5 (2%)	48	54
All	All	510/518 (98%)	500 (98%)	10 (2%)	48	54

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	GLU
1	A	49	LEU
1	A	184	LEU
1	A	284	ARG
1	A	314	LEU
1	B	45	ASN
1	B	49	LEU
1	B	51	ILE
1	B	309	LEU
1	B	315	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	ASN
1	A	45	ASN
1	A	62	HIS
1	A	163	HIS
1	A	227	HIS
1	A	290	GLN
1	A	307	ASN
1	A	320	GLN
1	B	17	GLN
1	B	45	ASN
1	B	62	HIS
1	B	67	ASN
1	B	115	ASN
1	B	122	ASN
1	B	126	ASN
1	B	188	ASN
1	B	233	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	SEP	A	74	1	8,9,10	1.65	2 (25%)	7,12,14	1.35	0
1	SEP	B	74	1	8,9,10	1.74	2 (25%)	7,12,14	1.40	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
1	SEP	A	74	1	-	1/6/8/10	-
1	SEP	B	74	1	-	0/6/8/10	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	74	SEP	P-OG	-3.25	1.50	1.60
1	A	74	SEP	P-OG	-3.03	1.50	1.60
1	B	74	SEP	P-O1P	2.89	1.59	1.50
1	A	74	SEP	P-O1P	2.84	1.59	1.50

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	74	SEP	CA-CB-OG-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	$\# Z > 2$
2	EDO	A	1303	-	3,3,3	0.60	0	2,2,2	0.39	0
2	EDO	A	1305	-	3,3,3	0.71	0	2,2,2	0.39	0
2	EDO	B	1304	-	3,3,3	0.65	0	2,2,2	0.34	0
2	EDO	A	1302	-	3,3,3	0.63	0	2,2,2	0.38	0
3	FMT	A	1301	-	2,2,2	0.68	0	1,1,1	0.26	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	EDO	A	1303	-	-	1/1/1/1	-
2	EDO	A	1305	-	-	0/1/1/1	-
2	EDO	B	1304	-	-	1/1/1/1	-
2	EDO	A	1302	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1302	EDO	O1-C1-C2-O2
2	A	1303	EDO	O1-C1-C2-O2
2	B	1304	EDO	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

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, 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	299/330 (90%)	0.52	25 (8%) 17 15	17, 26, 53, 70	4 (1%)
1	B	299/330 (90%)	0.41	20 (6%) 24 22	16, 26, 58, 99	0
All	All	598/660 (90%)	0.47	45 (7%) 20 19	16, 26, 57, 99	4 (0%)

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	284	ARG	13.0
1	B	284	ARG	11.7
1	A	283	ALA	11.5
1	B	283	ALA	8.0
1	A	0	ALA	6.6
1	A	286	GLU	5.9
1	A	285	ARG	5.9
1	B	35	ALA	5.4
1	A	35	ALA	5.3
1	A	5	ILE	5.2
1	B	5	ILE	4.7
1	B	188	ASN	4.3
1	A	229	ILE	4.0
1	B	4	LEU	3.9
1	B	34	SER	3.5
1	A	23	GLU	3.5
1	A	34	SER	3.3
1	A	46	ASP	3.3
1	B	32	GLY	3.1
1	A	13	ASN	3.1
1	B	46	ASP	3.1
1	A	188	ASN	3.0
1	A	4	LEU	2.8
1	A	157	GLY	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	59	THR	2.7
1	B	282	SER	2.7
1	A	3	GLU	2.6
1	B	285	ARG	2.5
1	A	32	GLY	2.5
1	A	143	GLU	2.5
1	B	0	ALA	2.4
1	B	286	GLU	2.4
1	B	287	GLN	2.4
1	A	288	PRO	2.4
1	B	320	GLN	2.3
1	A	291	SER	2.3
1	A	45	ASN	2.3
1	B	291	SER	2.3
1	B	168	ARG	2.2
1	B	47	SER	2.2
1	A	228	PRO	2.2
1	A	59	THR	2.2
1	A	165	GLU	2.2
1	B	290	GLN	2.1
1	A	282	SER	2.1

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
1	SEP	A	74	10/11	0.87	0.10	17,21,25,39	0
1	SEP	B	74	10/11	0.91	0.09	19,21,27,39	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 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($\text{\AA}^2$)	Q<0.9
2	EDO	A	1302	4/4	0.54	0.23	48,48,49,49	0
2	EDO	A	1303	4/4	0.74	0.20	37,37,39,40	0
2	EDO	B	1304	4/4	0.76	0.18	37,37,38,40	0
3	FMT	A	1301	3/3	0.77	0.18	40,40,45,45	0
2	EDO	A	1305	4/4	0.79	0.16	40,43,43,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.