



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:10 PM UTC

PDB ID : 2BO6 / pdb_00002bo6
Title : DISSECTION OF MANNOSYLGLYCERATE SYNTHASE: AN ARCHETYPAL MANNOSYLTRANSFERASE
Authors : Flint, J.; Taylor, E.; Yang, M.; Bolam, D.N.; Tailford, L.E.; Martinez-Fleites, C.; Dodson, E.J.; Davis, B.G.; Gilbert, H.J.; Davies, G.J.
Deposited on : 2005-04-08
Resolution : 2.45 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

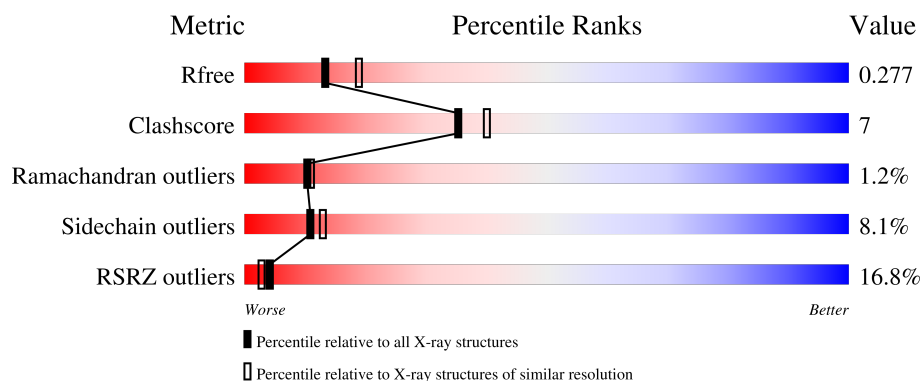
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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	397	15% 72% 21% ...
1	B	397	17% 76% 17% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	DGY	B	1382	-	X	-	-

2 Entry composition [i](#)

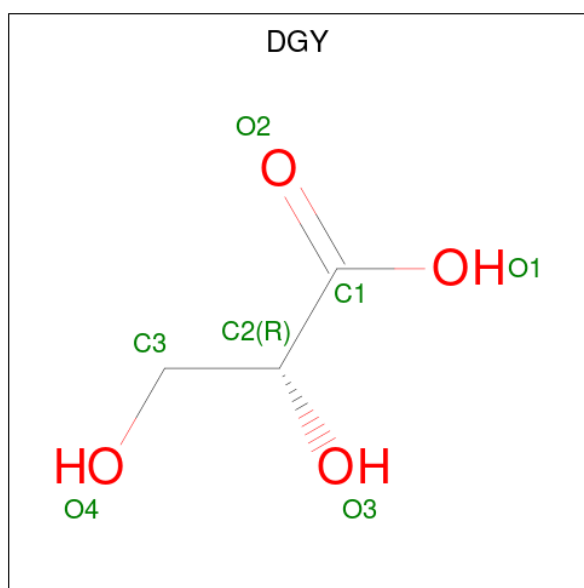
There are 4 unique types of molecules in this entry. The entry contains 6392 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 MANNOSYLGLYCERATE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	381	Total	C	N	O	S	0	0	1
			3138	2006	558	559	15			
1	B	381	Total	C	N	O	S	0	0	1
			3138	2006	558	559	15			

- Molecule 2 is (2R)-2,3-DIHYDROXYPROPANOIC ACID (CCD ID: DGY) (formula: $C_3H_6O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			7	3	4		
2	B	1	Total	C	O	0	0
			7	3	4		

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Mn 1	0	0
3	B	1	Total 1	Mn 1	0	0

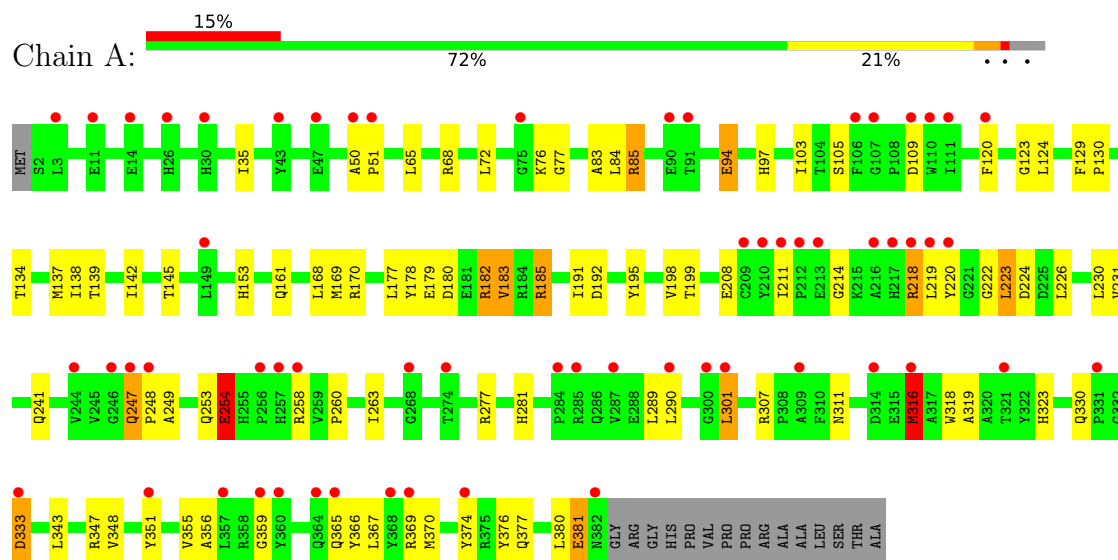
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	47	Total 47	O 47	0	0
4	B	53	Total 53	O 53	0	0

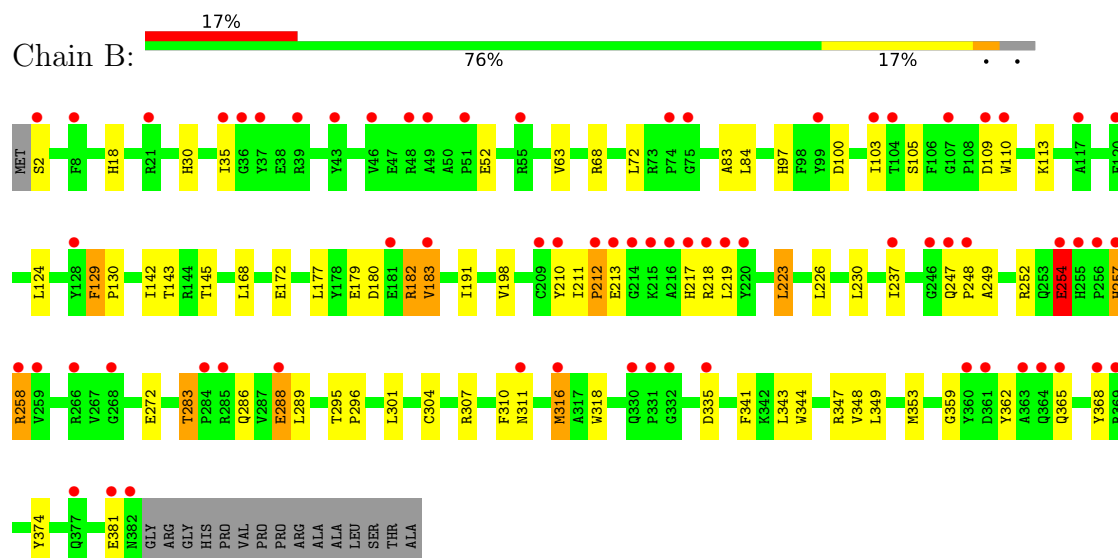
3 Residue-property plots

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: MANNOSYLGLYCERATE SYNTHASE



• Molecule 1: MANNOSYLGLYCERATE SYNTHASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	150.23Å 150.23Å 154.28Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	36.99 – 2.45 36.99 – 2.45	Depositor EDS
% Data completeness (in resolution range)	98.6 (36.99-2.45) 98.5 (36.99-2.45)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.253 , 0.277 0.255 , 0.277	Depositor DCC
R_{free} test set	3694 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	58.6	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 35.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.017 for -h,-k,l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	6392	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% 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, 0.333 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: DGY, MN

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	1.05	10/3229 (0.3%)	0.99	2/4394 (0.0%)
1	B	0.97	6/3229 (0.2%)	0.97	1/4394 (0.0%)
All	All	1.01	16/6458 (0.2%)	0.98	3/8788 (0.0%)

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	333	ASP	CG-OD2	11.82	1.47	1.25
1	A	316	MET	SD-CE	11.16	2.07	1.79
1	A	254	GLU	CD-OE1	8.84	1.42	1.25
1	A	359	GLY	C-O	7.37	1.33	1.23
1	B	359	GLY	C-O	6.42	1.32	1.23
1	B	254	GLU	CG-CD	6.30	1.67	1.52
1	B	288	GLU	CD-OE2	6.01	1.36	1.25
1	A	381	GLU	C-N	-5.84	1.25	1.33
1	A	218	ARG	NE-CZ	5.69	1.39	1.33
1	A	370	MET	SD-CE	-5.67	1.65	1.79
1	B	368	TYR	CA-CB	5.59	1.62	1.53
1	B	381	GLU	C-N	-5.58	1.25	1.33
1	A	185	ARG	NE-CZ	5.48	1.39	1.33
1	A	231	VAL	CA-CB	5.32	1.61	1.54
1	B	311	ASN	CB-CG	5.28	1.65	1.52
1	A	356	ALA	C-O	5.10	1.30	1.24

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	307	ARG	N-CA-C	6.23	113.73	108.13
1	B	191	ILE	N-CA-C	5.75	116.49	110.62
1	A	241	GLN	N-CA-C	5.67	118.23	111.71

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	3138	0	3037	55	1
1	B	3138	0	3037	39	1
2	A	7	0	5	0	0
2	B	7	0	5	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	47	0	0	1	0
4	B	53	0	0	1	0
All	All	6392	0	6084	92	1

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 7.

All (92) 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:316:MET:CE	1:A:316:MET:SD	2.07	1.43
1:A:85:ARG:NH1	1:A:85:ARG:HG2	1.55	1.05
1:A:85:ARG:HH11	1:A:85:ARG:CG	1.70	1.03
1:B:316:MET:HA	1:B:316:MET:HE2	1.47	0.96
1:A:85:ARG:HG2	1:A:85:ARG:HH11	0.79	0.96
1:A:94:GLU:HA	1:A:94:GLU:OE1	1.68	0.93
1:A:94:GLU:OE1	1:A:94:GLU:CA	2.35	0.74
1:A:316:MET:HA	1:A:316:MET:HE2	1.70	0.73
1:B:143:THR:HA	1:B:237:ILE:HD11	1.71	0.73
1:A:145:THR:HG23	1:A:374:TYR:CE1	2.27	0.70
1:B:283:THR:HG21	1:B:335:ASP:OD2	1.91	0.70
1:A:319:ALA:HB2	1:A:374:TYR:CE2	2.27	0.69
1:B:316:MET:HA	1:B:316:MET:CE	2.25	0.63
1:A:316:MET:CE	1:A:316:MET:HA	2.29	0.63
1:A:316:MET:HE1	1:A:377:GLN:OE1	1.99	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:TRP:CE2	1:B:211:ILE:HD13	2.34	0.62
1:A:76:LYS:NZ	1:A:192:ASP:OD2	2.34	0.60
1:B:180:ASP:HB3	1:B:183:VAL:HG13	1.83	0.60
1:A:222:GLY:O	1:A:224:ASP:N	2.36	0.59
1:B:142:ILE:HD11	1:B:230:LEU:CD1	2.33	0.58
1:B:362:TYR:O	1:B:365:GLN:NE2	2.37	0.58
1:B:223:LEU:HD21	1:B:348:VAL:HG11	1.84	0.58
1:A:85:ARG:HD3	1:A:178:TYR:OH	2.04	0.57
1:A:208:GLU:HB2	1:A:253:GLN:HB3	1.88	0.56
1:A:177:LEU:CD2	1:A:198:VAL:CG2	2.84	0.56
1:B:18:HIS:NE2	4:B:2002:HOH:O	2.33	0.56
1:A:311:ASN:HD21	1:B:272:GLU:HB3	1.72	0.55
1:B:129:PHE:CE1	1:B:211:ILE:HD12	2.42	0.55
1:A:77:GLY:HA2	1:A:191:ILE:HD13	1.89	0.54
1:B:142:ILE:CD1	1:B:230:LEU:CD1	2.86	0.54
1:A:223:LEU:HD21	1:A:348:VAL:HG11	1.91	0.53
1:B:35:ILE:HD12	1:B:83:ALA:HB2	1.91	0.52
1:B:318:TRP:HB2	1:B:347:ARG:HD3	1.90	0.52
1:A:247:GLN:N	1:A:248:PRO:CD	2.73	0.51
1:A:123:GLY:HA2	1:A:170:ARG:HG3	1.92	0.51
1:B:362:TYR:CG	1:B:365:GLN:NE2	2.79	0.51
1:A:129:PHE:CE1	1:A:211:ILE:HD12	2.47	0.50
1:A:222:GLY:C	1:A:224:ASP:N	2.71	0.49
1:B:180:ASP:OD1	1:B:182:ARG:HD3	2.11	0.49
1:B:177:LEU:HD23	1:B:198:VAL:CG2	2.42	0.49
1:A:177:LEU:HD23	1:A:198:VAL:CG2	2.42	0.49
1:A:351:TYR:OH	1:A:367:LEU:HD11	2.12	0.48
1:A:195:TYR:O	1:A:199:THR:HG23	2.13	0.48
1:A:142:ILE:CD1	1:A:230:LEU:CD1	2.92	0.48
1:A:319:ALA:HB2	1:A:374:TYR:HE2	1.78	0.48
1:B:145:THR:HG23	1:B:374:TYR:CE1	2.49	0.48
1:A:218:ARG:NH1	1:A:219:LEU:O	2.47	0.47
1:B:2:SER:N	1:B:30:HIS:HB2	2.29	0.47
1:B:230:LEU:HD22	1:B:344:TRP:CE3	2.50	0.46
1:A:77:GLY:HA2	1:A:191:ILE:CD1	2.45	0.46
1:A:318:TRP:HB2	1:A:347:ARG:HD3	1.98	0.46
1:A:138:ILE:O	1:A:139:THR:C	2.57	0.46
1:A:290:LEU:HD21	1:A:301:LEU:HD12	1.98	0.46
1:B:247:GLN:N	1:B:248:PRO:CD	2.79	0.46
1:A:145:THR:HG23	1:A:374:TYR:CD1	2.50	0.46
1:A:137:MET:HA	1:A:137:MET:HE2	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:HIS:HB3	1:A:247:GLN:NE2	2.31	0.45
1:B:129:PHE:HE1	1:B:211:ILE:HD12	1.81	0.45
1:A:323:HIS:HB3	4:A:2042:HOH:O	2.15	0.45
1:A:351:TYR:O	1:A:355:VAL:HB	2.17	0.44
1:B:210:TYR:HB3	1:B:254:GLU:OE2	2.17	0.44
1:B:349:LEU:O	1:B:353:MET:HG2	2.18	0.44
1:A:311:ASN:HD21	1:B:272:GLU:CB	2.30	0.44
1:A:220:TYR:CD2	1:A:220:TYR:O	2.71	0.44
1:A:365:GLN:CD	1:A:366:TYR:N	2.76	0.44
1:B:304:CYS:HA	1:B:307:ARG:O	2.19	0.43
1:B:283:THR:HG22	1:B:286:GLN:H	1.84	0.43
1:B:295:THR:HB	1:B:296:PRO:HD3	2.00	0.43
1:B:142:ILE:HD13	1:B:230:LEU:HD12	2.00	0.43
1:B:113:LYS:NZ	1:B:210:TYR:O	2.43	0.43
1:B:211:ILE:O	1:B:212:PRO:C	2.62	0.42
1:A:97:HIS:CE1	1:A:168:LEU:HD12	2.55	0.42
1:A:180:ASP:OD1	1:A:182:ARG:HD3	2.20	0.42
1:B:210:TYR:N	1:B:254:GLU:OE2	2.52	0.42
1:A:129:PHE:HB3	1:A:130:PRO:HD2	2.02	0.42
1:A:277:ARG:CZ	1:A:281:HIS:HD2	2.33	0.42
1:A:50:ALA:N	1:A:51:PRO:CD	2.82	0.42
1:A:222:GLY:C	1:A:224:ASP:H	2.28	0.41
1:A:377:GLN:O	1:A:381:GLU:HG2	2.20	0.41
1:A:180:ASP:HB3	1:A:183:VAL:HG13	2.03	0.41
1:A:35:ILE:HD12	1:A:83:ALA:HB2	2.03	0.41
1:B:257:HIS:HD2	1:B:258:ARG:H	1.69	0.41
1:B:97:HIS:NE2	1:B:168:LEU:HD12	2.36	0.41
1:B:129:PHE:HB3	1:B:130:PRO:HD2	2.02	0.41
1:A:103:ILE:HG13	1:A:103:ILE:O	2.21	0.41
1:B:177:LEU:CD2	1:B:198:VAL:CG2	2.99	0.41
1:A:376:TYR:CZ	1:A:380:LEU:HD11	2.56	0.40
1:B:230:LEU:HD21	1:B:341:PHE:HA	2.03	0.40
1:A:260:PRO:HD2	1:A:263:ILE:HD12	2.04	0.40
1:A:330:GLN:OE1	1:A:333:ASP:OD2	2.38	0.40
1:B:129:PHE:CB	1:B:130:PRO:HD2	2.51	0.40
1:A:253:GLN:O	1:A:254:GLU:C	2.65	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:GLN:OE1	1:B:288:GLU:OE2[2_664]	2.17	0.03

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	379/397 (96%)	357 (94%)	18 (5%)	4 (1%)	11	12
1	B	379/397 (96%)	360 (95%)	14 (4%)	5 (1%)	9	9
All	All	758/794 (96%)	717 (95%)	32 (4%)	9 (1%)	10	11

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	223	LEU
1	A	120	PHE
1	A	249	ALA
1	B	249	ALA
1	B	217	HIS
1	B	310	PHE
1	A	214	GLY
1	B	103	ILE
1	B	212	PRO

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	326/338 (96%)	301 (92%)	25 (8%)	12	15
1	B	326/338 (96%)	298 (91%)	28 (9%)	10	11
All	All	652/676 (96%)	599 (92%)	53 (8%)	11	13

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

Mol	Chain	Res	Type
1	A	65	LEU
1	A	68	ARG
1	A	72	LEU
1	A	84	LEU
1	A	85	ARG
1	A	94	GLU
1	A	105	SER
1	A	109	ASP
1	A	124	LEU
1	A	134	THR
1	A	161	GLN
1	A	169	MET
1	A	179	GLU
1	A	182	ARG
1	A	183	VAL
1	A	185	ARG
1	A	226	LEU
1	A	247	GLN
1	A	254	GLU
1	A	258	ARG
1	A	289	LEU
1	A	301	LEU
1	A	316	MET
1	A	343	LEU
1	A	369	ARG
1	B	52	GLU
1	B	63	VAL
1	B	68	ARG
1	B	72	LEU
1	B	84	LEU
1	B	100	ASP
1	B	105	SER
1	B	109	ASP
1	B	124	LEU
1	B	129	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	172	GLU
1	B	179	GLU
1	B	182	ARG
1	B	183	VAL
1	B	213	GLU
1	B	218	ARG
1	B	219	LEU
1	B	223	LEU
1	B	226	LEU
1	B	252	ARG
1	B	254	GLU
1	B	257	HIS
1	B	258	ARG
1	B	283	THR
1	B	289	LEU
1	B	301	LEU
1	B	316	MET
1	B	343	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	10	HIS
1	A	66	GLN
1	A	81	ASN
1	A	217	HIS
1	A	247	GLN
1	A	276	HIS
1	A	281	HIS
1	A	311	ASN
1	A	328	HIS
1	A	364	GLN
1	B	10	HIS
1	B	66	GLN
1	B	81	ASN
1	B	161	GLN
1	B	202	GLN
1	B	255	HIS
1	B	257	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	DGY	A	1382	-	6,6,6	0.96	0	6,7,7	2.56	2 (33%)
2	DGY	B	1382	-	6,6,6	1.01	1 (16%)	6,7,7	2.23	2 (33%)

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	DGY	A	1382	-	-	5/6/6/6	-
2	DGY	B	1382	-	-	5/6/6/6	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1382	DGY	O1-C1	-2.05	1.24	1.30

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1382	DGY	O1-C1-C2	4.50	122.26	112.74
2	B	1382	DGY	O1-C1-C2	4.28	121.79	112.74
2	A	1382	DGY	O2-C1-C2	-3.67	115.27	122.60
2	B	1382	DGY	O2-C1-C2	-2.25	118.10	122.60

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1382	DGY	O3-C2-C3-O4
2	B	1382	DGY	O3-C2-C3-O4
2	A	1382	DGY	O1-C1-C2-O3
2	A	1382	DGY	O2-C1-C2-O3
2	B	1382	DGY	O1-C1-C2-O3
2	A	1382	DGY	O1-C1-C2-C3
2	A	1382	DGY	O2-C1-C2-C3
2	B	1382	DGY	O1-C1-C2-C3
2	B	1382	DGY	O2-C1-C2-O3
2	B	1382	DGY	O2-C1-C2-C3

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	381/397 (95%)	1.22	60 (15%) 5 3	27, 29, 32, 36	0
1	B	381/397 (95%)	1.27	68 (17%) 4 3	27, 30, 32, 36	0
All	All	762/794 (95%)	1.24	128 (16%) 4 3	27, 29, 32, 36	0

All (128) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	247	GLN	8.1
1	B	257	HIS	7.3
1	B	368	TYR	7.2
1	A	382	ASN	6.3
1	A	220	TYR	6.0
1	B	258	ARG	5.7
1	B	109	ASP	5.6
1	A	257	HIS	5.5
1	A	110	TRP	5.2
1	A	247	GLN	5.2
1	A	219	LEU	5.1
1	B	284	PRO	5.0
1	A	374	TYR	5.0
1	A	333	ASP	4.7
1	B	246	GLY	4.6
1	B	288	GLU	4.5
1	A	216	ALA	4.5
1	A	217	HIS	4.5
1	B	219	LEU	4.4
1	A	246	GLY	4.3
1	B	365	GLN	4.3
1	A	368	TYR	4.2
1	B	217	HIS	4.1
1	B	220	TYR	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	213	GLU	3.8
1	A	258	ARG	3.7
1	B	110	TRP	3.7
1	A	218	ARG	3.7
1	B	46	VAL	3.6
1	B	255	HIS	3.5
1	B	210	TYR	3.5
1	A	120	PHE	3.5
1	A	211	ILE	3.4
1	B	332	GLY	3.3
1	B	361	ASP	3.3
1	B	209	CYS	3.2
1	B	248	PRO	3.2
1	A	287	VAL	3.2
1	B	48	ARG	3.2
1	B	382	ASN	3.2
1	A	213	GLU	3.2
1	B	43	TYR	3.1
1	A	210	TYR	3.1
1	B	364	GLN	3.1
1	B	21	ARG	3.1
1	B	256	PRO	3.0
1	B	103	ILE	3.0
1	A	256	PRO	3.0
1	B	254	GLU	3.0
1	B	377	GLN	3.0
1	B	214	GLY	2.9
1	A	331	PRO	2.9
1	B	218	ARG	2.9
1	B	107	GLY	2.9
1	B	259	VAL	2.9
1	A	209	CYS	2.9
1	B	120	PHE	2.9
1	B	212	PRO	2.8
1	A	365	GLN	2.8
1	A	107	GLY	2.8
1	B	216	ALA	2.8
1	B	117	ALA	2.8
1	B	215	LYS	2.8
1	B	8	PHE	2.8
1	A	284	PRO	2.7
1	A	3	LEU	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	309	ALA	2.7
1	B	55	ARG	2.6
1	A	11	GLU	2.6
1	B	360	TYR	2.6
1	A	301	LEU	2.6
1	A	91	THR	2.6
1	A	360	TYR	2.6
1	A	51	PRO	2.5
1	B	75	GLY	2.5
1	A	90	GLU	2.5
1	B	39	ARG	2.5
1	B	99	TYR	2.5
1	A	106	PHE	2.5
1	A	364	GLN	2.5
1	B	363	ALA	2.5
1	B	2	SER	2.5
1	A	314	ASP	2.5
1	A	50	ALA	2.5
1	A	244	VAL	2.4
1	A	300	GLY	2.4
1	A	149	LEU	2.4
1	A	290	LEU	2.4
1	B	285	ARG	2.4
1	A	43	TYR	2.4
1	A	351	TYR	2.4
1	B	183	VAL	2.4
1	A	14	GLU	2.4
1	A	75	GLY	2.3
1	B	316	MET	2.3
1	A	212	PRO	2.3
1	A	321	THR	2.3
1	B	331	PRO	2.3
1	B	128	TYR	2.3
1	A	111	ILE	2.3
1	A	359	GLY	2.2
1	B	266	ARG	2.2
1	A	30	HIS	2.2
1	A	47	GLU	2.2
1	B	381	GLU	2.2
1	A	109	ASP	2.2
1	A	369	ARG	2.2
1	B	330	GLN	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	104	THR	2.2
1	B	74	PRO	2.2
1	A	274	THR	2.1
1	B	36	GLY	2.1
1	A	316	MET	2.1
1	A	285	ARG	2.1
1	B	51	PRO	2.1
1	B	35	ILE	2.1
1	B	49	ALA	2.1
1	A	357	LEU	2.1
1	A	268	GLY	2.1
1	B	237	ILE	2.1
1	B	311	ASN	2.0
1	B	268	GLY	2.0
1	B	37	TYR	2.0
1	A	26	HIS	2.0
1	B	369	ARG	2.0
1	B	181	GLU	2.0
1	A	248	PRO	2.0
1	B	335	ASP	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 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	DGY	B	1382	7/7	0.83	0.23	28,30,32,33	0
2	DGY	A	1382	7/7	0.87	0.22	34,36,38,41	0
3	MN	A	1383	1/1	0.93	0.20	47,47,47,47	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MN	B	1383	1/1	0.97	0.25	50,50,50,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.