



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 12:54 AM EDT

PDB ID : 1PN3 / pdb_00001pn3
Title : Crystal Structure of TDP-epi-Vancosaminyltransferase GtfA in complexes with TDP and the acceptor substrate DVV.
Authors : Mulichak, A.M.; Losey, H.C.; Lu, W.; Wawrzak, Z.; Walsh, C.T.; Garavito, R.M.
Deposited on : 2003-06-12
Resolution : 2.80 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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

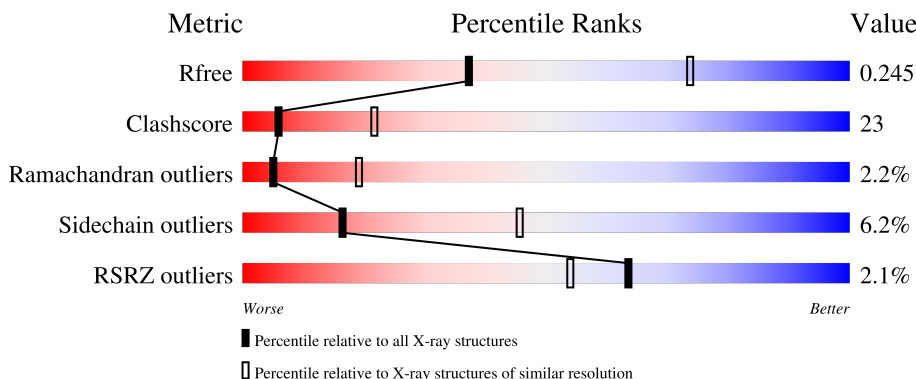
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

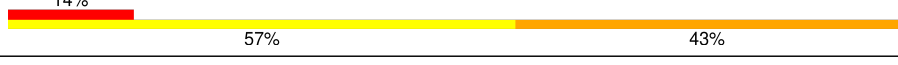
The reported resolution of this entry is 2.80 Å.

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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	404	
1	B	404	
2	C	7	
2	D	7	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6006 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 GLYCOSYLTRANSFERASE GTFA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	391	Total	C	N	O	S	0	0	0
			2834	1781	499	542	12			
1	B	384	Total	C	N	O	S	0	0	0
			2803	1763	497	531	12			

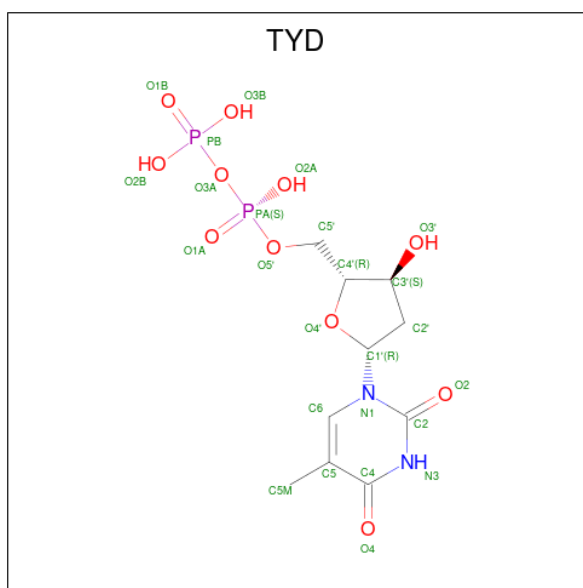
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	397	LEU	-	expression tag	UNP P96558
A	398	GLU	-	expression tag	UNP P96558
A	399	HIS	-	expression tag	UNP P96558
A	400	HIS	-	expression tag	UNP P96558
A	401	HIS	-	expression tag	UNP P96558
A	402	HIS	-	expression tag	UNP P96558
A	403	HIS	-	expression tag	UNP P96558
A	404	HIS	-	expression tag	UNP P96558
B	397	LEU	-	expression tag	UNP P96558
B	398	GLU	-	expression tag	UNP P96558
B	399	HIS	-	expression tag	UNP P96558
B	400	HIS	-	expression tag	UNP P96558
B	401	HIS	-	expression tag	UNP P96558
B	402	HIS	-	expression tag	UNP P96558
B	403	HIS	-	expression tag	UNP P96558
B	404	HIS	-	expression tag	UNP P96558

- Molecule 2 is a protein called DESVANCOSAMINYL VANCOMYCIN.

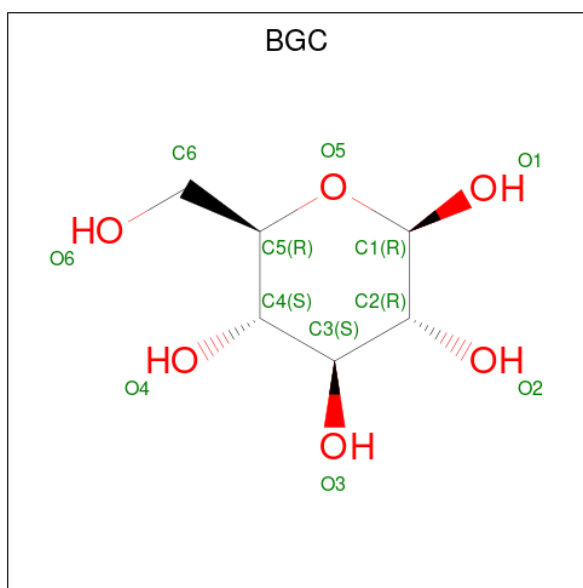
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	7	Total	C	Cl	N	O	0	0	0
			80	53	2	8	17			
2	D	7	Total	C	Cl	N	O	0	0	0
			80	53	2	8	17			

- Molecule 3 is THYMIDINE-5'-DIPHOSPHATE (CCD ID: TYD) (formula: $C_{10}H_{16}N_2O_{11}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			25	10	2	11	2		

- Molecule 4 is beta-D-glucopyranose (CCD ID: BGC) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			11	6	5		
4	D	1	Total	C	O	0	0
			11	6	5		

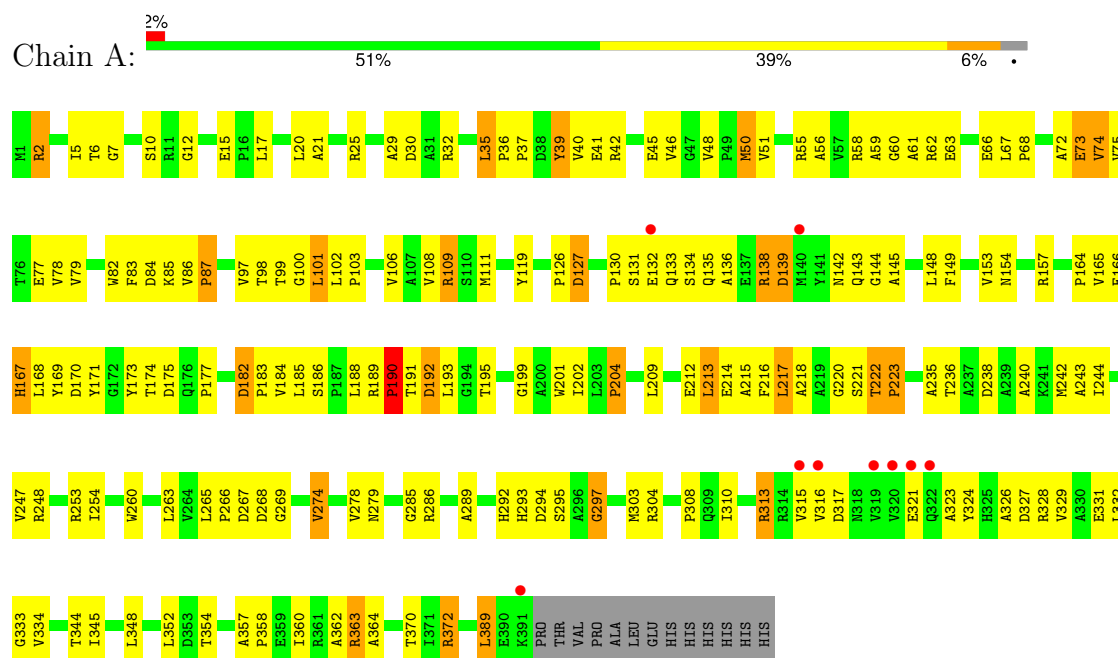
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	67	Total 67	O 67	0	0
5	B	85	Total 85	O 85	0	0
5	C	1	Total 1	O 1	0	0
5	D	9	Total 9	O 9	0	0

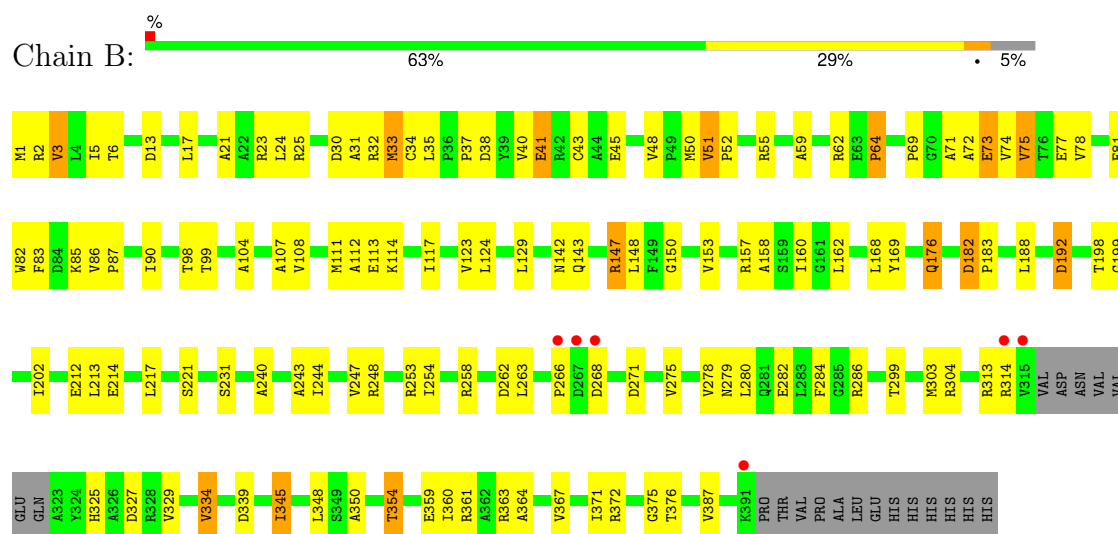
3 Residue-property plots [i](#)

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.

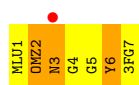
• Molecule 1: GLYCOSYLTRANSFERASE GTFA



• Molecule 1: GLYCOSYLTRANSFERASE GTFA



• Molecule 2: DESVANCOSAMINYL VANCOMYCIN



• Molecule 2: DESVANCOSAMINYL VANCOMYCIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	152.50Å 152.50Å 98.74Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.80 30.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.80) 95.1 (30.00-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.46 (at 2.80Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.212 , 0.249 0.207 , 0.245	Depositor DCC
R_{free} test set	1480 reflections (4.51%)	wwPDB-VP
Wilson B-factor (Å ²)	51.2	Xtriage
Anisotropy	0.239	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 49.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6006	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% 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: OMY, GHP, MLU, 3FG, BGC, OMZ, TYD

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	0.46	0/2891	1.00	13/3963 (0.3%)
1	B	0.48	0/2859	0.98	7/3915 (0.2%)
2	C	1.18	0/7	3.03	1/8 (12.5%)
2	D	0.92	0/7	1.96	0/8
All	All	0.47	0/5764	1.00	21/7894 (0.3%)

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	199	GLY	N-CA-C	-11.34	100.48	112.04
1	B	199	GLY	N-CA-C	-9.67	102.77	111.95
2	C	3	ASN	CA-CB-CG	7.50	120.10	112.60
1	A	222	THR	CA-C-N	7.47	127.38	120.21
1	A	222	THR	C-N-CA	7.47	127.38	120.21
1	A	39	TYR	N-CA-C	7.03	120.73	112.72
1	A	297	GLY	N-CA-C	6.70	120.27	112.50
1	A	148	LEU	N-CA-C	6.63	118.51	111.28
1	B	314	ARG	N-CA-C	-6.21	100.64	109.96
1	A	223	PRO	N-CA-C	6.18	119.88	111.22
1	A	268	ASP	N-CA-C	-5.99	106.06	113.19
1	A	220	GLY	N-CA-C	5.68	118.52	110.74
1	B	182	ASP	CA-C-N	5.66	125.78	119.32
1	B	182	ASP	C-N-CA	5.66	125.78	119.32
1	A	182	ASP	CA-C-N	5.51	125.17	119.05
1	A	182	ASP	C-N-CA	5.51	125.17	119.05
1	B	33	MET	N-CA-C	5.39	118.37	109.85
1	A	74	VAL	N-CA-C	5.30	117.28	111.77
1	B	361	ARG	N-CA-C	-5.09	105.91	111.82
1	A	292	HIS	N-CA-C	5.02	115.16	108.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	262	ASP	N-CA-C	5.01	117.57	110.50

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	2834	0	2770	158	0
1	B	2803	0	2775	104	0
2	C	80	0	44	4	0
2	D	80	0	44	5	0
3	A	25	0	13	5	0
4	C	11	0	10	1	0
4	D	11	0	9	1	0
5	A	67	0	0	4	0
5	B	85	0	0	1	0
5	C	1	0	0	0	0
5	D	9	0	0	0	0
All	All	6006	0	5665	264	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 23.

All (264) 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:345:ILE:HD12	1:B:345:ILE:H	1.21	1.02
1:A:265:LEU:HG	1:A:274:VAL:HG22	1.45	0.96
1:A:315:VAL:HG12	1:A:316:VAL:H	1.35	0.91
1:A:327:ASP:O	1:A:331:GLU:HG3	1.71	0.91
1:B:334:VAL:HG22	1:B:364:ALA:HA	1.53	0.91
1:A:372:ARG:HE	1:A:372:ARG:HA	1.35	0.90
1:A:185:LEU:HD13	1:A:303:MET:HE1	1.53	0.90
1:A:329:VAL:HG13	1:A:334:VAL:HG23	1.60	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:345:ILE:HD12	1:B:345:ILE:N	1.96	0.80
1:A:55:ARG:HH21	1:A:74:VAL:HG21	1.49	0.78
1:A:101:LEU:HG	1:A:103:PRO:HD2	1.65	0.78
1:B:90:ILE:HD11	1:B:117:ILE:HD11	1.65	0.77
1:B:143:GLN:HG2	1:B:147:ARG:NH1	1.97	0.77
1:B:3:VAL:HG21	1:B:24:LEU:HD13	1.65	0.77
1:A:6:THR:HG21	1:A:108:VAL:HG21	1.68	0.75
1:B:160:ILE:HD11	1:B:162:LEU:HD12	1.69	0.74
1:B:345:ILE:H	1:B:345:ILE:CD1	1.96	0.73
1:B:240:ALA:O	1:B:244:ILE:HG12	1.91	0.71
1:A:265:LEU:HG	1:A:274:VAL:CG2	2.18	0.70
1:A:244:ILE:HG23	1:A:254:ILE:HD13	1.72	0.70
1:A:86:VAL:HB	1:A:111:MET:HE1	1.74	0.70
1:A:142:ASN:ND2	1:A:169:TYR:HB3	2.06	0.70
1:A:5:ILE:HD12	1:A:21:ALA:HB2	1.74	0.69
1:A:154:ASN:HA	1:A:157:ARG:HD3	1.74	0.69
1:B:5:ILE:HB	1:B:33:MET:HG2	1.76	0.68
1:B:258:ARG:NH1	1:B:263:LEU:O	2.28	0.67
1:B:3:VAL:HG23	1:B:31:ALA:HB2	1.75	0.66
1:A:15:GLU:HG3	3:A:406:TYD:H4'	1.78	0.66
1:A:74:VAL:HG22	1:A:77:GLU:HB3	1.77	0.65
1:A:212:GLU:OE1	1:A:212:GLU:N	2.26	0.65
1:A:130:PRO:HA	1:A:133:GLN:HG2	1.79	0.65
1:A:21:ALA:O	1:A:25:ARG:HG2	1.97	0.65
1:A:188:LEU:HD22	1:A:195:THR:HG21	1.77	0.64
1:A:221:SER:O	1:A:253:ARG:HD3	1.98	0.64
1:A:240:ALA:O	1:A:244:ILE:HG12	1.97	0.63
1:A:242:MET:HE3	1:A:345:ILE:HG13	1.81	0.63
1:A:153:VAL:HG12	1:A:157:ARG:HD2	1.80	0.63
1:A:56:ALA:HB3	1:A:62:ARG:CG	2.30	0.62
1:A:216:PHE:C	1:A:218:ALA:H	2.08	0.62
1:A:248:ARG:NH1	1:A:267:ASP:OD2	2.29	0.61
1:A:56:ALA:HB3	1:A:62:ARG:HG3	1.82	0.61
1:A:109:ARG:HG2	1:A:171:TYR:CZ	2.36	0.61
2:C:6:OMY:CL	4:C:8:BGC:H6C2	2.37	0.61
1:B:244:ILE:HG23	1:B:254:ILE:HD13	1.82	0.61
1:B:2:ARG:HG3	1:B:30:ASP:O	2.01	0.60
1:B:17:LEU:HD11	1:B:99:THR:HG22	1.82	0.60
1:A:62:ARG:HB3	1:A:66:GLU:CD	2.26	0.60
1:A:35:LEU:HB2	1:A:50:MET:HE3	1.83	0.60
1:A:62:ARG:HB3	1:A:66:GLU:CG	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:VAL:HB	1:B:111:MET:HE3	1.83	0.60
1:A:315:VAL:HG12	1:A:316:VAL:N	2.12	0.60
1:A:167:HIS:CD2	1:A:167:HIS:N	2.70	0.59
1:A:360:ILE:C	1:A:362:ALA:H	2.09	0.59
1:A:310:ILE:HD11	1:A:352:LEU:HA	1.83	0.59
1:B:278:VAL:HG22	1:B:279:ASN:N	2.18	0.59
1:A:25:ARG:HA	1:A:29:ALA:O	2.02	0.59
1:B:354:THR:O	1:B:360:ILE:HD12	2.01	0.59
1:B:74:VAL:O	1:B:78:VAL:HG23	2.03	0.59
1:A:109:ARG:HD3	1:A:119:TYR:CD1	2.37	0.59
1:B:72:ALA:O	1:B:75:VAL:HG22	2.03	0.59
1:B:33:MET:HE2	1:B:48:VAL:HG11	1.85	0.58
1:B:202:ILE:HG13	1:B:304:ARG:NH1	2.18	0.58
1:B:55:ARG:HB2	1:B:69:PRO:HG3	1.84	0.58
1:B:278:VAL:HG22	1:B:279:ASN:H	1.69	0.58
1:A:192:ASP:HB2	1:A:195:THR:HG21	1.84	0.58
1:B:350:ALA:O	1:B:354:THR:HG23	2.03	0.57
1:A:372:ARG:HA	1:A:372:ARG:NE	2.12	0.57
1:B:313:ARG:NH1	1:B:327:ASP:OD1	2.37	0.57
1:A:86:VAL:HB	1:A:111:MET:CE	2.35	0.57
1:A:17:LEU:HD11	1:A:99:THR:HG22	1.86	0.57
1:A:36:PRO:HG2	1:A:39:TYR:HE1	1.70	0.56
1:A:266:PRO:HD2	5:A:2040:HOH:O	2.04	0.56
1:B:3:VAL:HG23	1:B:31:ALA:CB	2.35	0.56
1:A:389:LEU:HD11	1:B:212:GLU:HG2	1.86	0.56
1:B:37:PRO:O	1:B:40:VAL:HG23	2.07	0.55
1:A:67:LEU:HB3	1:A:68:PRO:HD2	1.88	0.55
1:A:55:ARG:NH2	1:A:74:VAL:HG21	2.21	0.55
1:B:150:GLY:HA2	1:B:168:LEU:HD11	1.89	0.55
1:A:154:ASN:OD1	1:A:164:PRO:HA	2.07	0.55
1:A:169:TYR:HD1	2:C:2:OMZ:CL	2.27	0.54
1:B:176:GLN:HE21	1:B:176:GLN:HA	1.72	0.54
1:A:131:SER:OG	1:A:192:ASP:HB3	2.07	0.54
1:B:98:THR:HG22	1:B:99:THR:N	2.20	0.54
1:A:102:LEU:HD13	1:A:173:TYR:CE2	2.43	0.54
1:B:243:ALA:O	1:B:247:VAL:HG23	2.08	0.54
1:A:267:ASP:C	1:A:269:GLY:H	2.16	0.53
1:B:33:MET:HE2	1:B:48:VAL:CG1	2.38	0.53
1:B:38:ASP:OD2	1:B:38:ASP:N	2.42	0.53
1:B:143:GLN:HG2	1:B:147:ARG:HH11	1.68	0.53
1:A:63:GLU:HG2	1:A:66:GLU:OE2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:GLU:OE1	1:A:286:ARG:NH2	2.42	0.53
1:B:75:VAL:HG11	1:B:148:LEU:HG	1.90	0.53
1:B:104:ALA:O	1:B:108:VAL:HG23	2.09	0.53
1:A:278:VAL:HG22	1:A:279:ASN:N	2.24	0.53
1:A:313:ARG:HG3	1:A:323:ALA:HB2	1.91	0.53
1:B:280:LEU:HD22	1:B:284:PHE:CE1	2.44	0.53
1:B:325:HIS:O	1:B:329:VAL:HG23	2.08	0.53
1:A:2:ARG:HE	1:A:32:ARG:HH21	1.57	0.52
1:A:285:GLY:C	1:A:286:ARG:HG3	2.35	0.52
1:A:297:GLY:HA3	3:A:406:TYD:O1A	2.10	0.52
1:A:166:GLU:CB	1:A:167:HIS:HD2	2.22	0.52
1:A:243:ALA:O	1:A:247:VAL:HG23	2.10	0.52
1:A:101:LEU:CG	1:A:103:PRO:HD2	2.38	0.52
1:A:173:TYR:O	1:A:177:PRO:HB3	2.10	0.52
1:B:25:ARG:NH1	1:B:31:ALA:O	2.43	0.52
1:A:363:ARG:HH11	1:A:363:ARG:HG2	1.74	0.52
1:B:6:THR:HG22	1:B:34:CYS:HB2	1.91	0.52
1:B:304:ARG:HD2	5:B:2067:HOH:O	2.11	0.51
2:D:5:GHP:C2	2:D:7:3FG:HN1	2.23	0.51
1:A:85:LYS:HA	5:A:2012:HOH:O	2.10	0.51
1:B:299:THR:O	1:B:303:MET:HB2	2.11	0.51
1:A:72:ALA:HA	1:A:75:VAL:HG23	1.91	0.51
1:A:213:LEU:CD2	1:A:217:LEU:HG	2.41	0.51
1:A:62:ARG:HB3	1:A:66:GLU:HG3	1.93	0.51
1:B:248:ARG:NH1	1:B:271:ASP:OD2	2.44	0.51
1:A:36:PRO:HG2	1:A:39:TYR:CE1	2.45	0.51
1:A:244:ILE:CD1	1:A:254:ILE:HG21	2.40	0.51
1:A:2:ARG:HG3	1:A:30:ASP:HB3	1.92	0.50
1:B:35:LEU:O	1:B:52:PRO:HA	2.12	0.50
1:A:204:PRO:HG2	1:B:41:GLU:HG3	1.93	0.50
1:B:25:ARG:NH1	1:B:25:ARG:HG2	2.25	0.50
1:B:25:ARG:HH11	1:B:25:ARG:HG2	1.75	0.50
1:A:360:ILE:C	1:A:362:ALA:N	2.69	0.50
1:A:166:GLU:O	1:A:167:HIS:C	2.55	0.50
1:A:40:VAL:HG23	1:A:41:GLU:N	2.27	0.50
1:A:83:PHE:HA	1:A:111:MET:HE2	1.93	0.50
1:A:102:LEU:HD22	2:C:2:OMZ:CL	2.49	0.49
1:B:75:VAL:HG21	1:B:148:LEU:HD11	1.93	0.49
1:B:75:VAL:HG21	1:B:148:LEU:CD1	2.42	0.49
1:A:363:ARG:HH11	1:A:363:ARG:CG	2.25	0.49
1:B:1:MET:SD	1:B:387:VAL:HG21	2.53	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:ARG:NE	1:A:165:VAL:HG22	2.28	0.49
1:B:82:TRP:O	1:B:86:VAL:HG23	2.13	0.49
1:A:174:THR:O	1:A:177:PRO:HD3	2.13	0.49
1:B:157:ARG:NH2	1:B:162:LEU:HB3	2.28	0.49
1:A:72:ALA:O	1:A:73:GLU:C	2.56	0.48
1:A:149:PHE:HE1	1:A:168:LEU:HD23	1.77	0.48
1:A:332:LEU:O	1:A:363:ARG:NH1	2.46	0.48
1:B:198:THR:O	1:B:375:GLY:HA2	2.13	0.48
1:B:83:PHE:HA	1:B:111:MET:HE2	1.95	0.48
1:B:86:VAL:N	1:B:87:PRO:CD	2.76	0.48
1:A:6:THR:O	1:A:98:THR:HA	2.13	0.48
1:A:59:ALA:C	1:A:61:ALA:H	2.21	0.48
1:A:145:ALA:HB1	1:A:149:PHE:CZ	2.49	0.48
1:A:153:VAL:O	1:A:157:ARG:HG3	2.13	0.48
1:B:275:VAL:CG1	1:B:278:VAL:HB	2.44	0.48
1:B:303:MET:HE3	1:B:371:ILE:HD11	1.94	0.48
1:B:359:GLU:O	1:B:363:ARG:HG3	2.13	0.48
1:A:186:SER:HA	1:A:324:TYR:OH	2.14	0.48
1:A:293:HIS:CD2	1:A:295:SER:HB2	2.49	0.48
1:A:149:PHE:CE1	1:A:168:LEU:HD23	2.49	0.48
1:A:223:PRO:HB3	1:A:253:ARG:HB2	1.96	0.48
1:B:248:ARG:HH12	1:B:271:ASP:CG	2.21	0.48
1:A:134:SER:C	1:A:136:ALA:N	2.69	0.48
1:A:59:ALA:O	1:A:61:ALA:N	2.47	0.47
1:B:5:ILE:HD12	1:B:21:ALA:HB2	1.96	0.47
1:B:142:ASN:CG	1:B:169:TYR:HB3	2.39	0.47
1:B:188:LEU:HD22	1:B:192:ASP:HB2	1.95	0.47
1:A:12:GLY:HA3	3:A:406:TYD:O3A	2.14	0.47
1:A:102:LEU:HD13	1:A:173:TYR:HE2	1.80	0.47
1:A:149:PHE:O	1:A:153:VAL:HG23	2.15	0.47
1:A:238:ASP:O	1:A:242:MET:HG2	2.14	0.47
1:A:12:GLY:HA2	3:A:406:TYD:H5'2	1.97	0.47
1:A:62:ARG:NH1	1:A:68:PRO:N	2.63	0.47
1:A:86:VAL:N	1:A:87:PRO:CD	2.77	0.47
1:A:7:GLY:HA2	1:A:99:THR:O	2.15	0.47
2:D:5:GHP:C2	2:D:7:3FG:N	2.77	0.47
1:B:3:VAL:CG2	1:B:24:LEU:HD13	2.40	0.47
1:A:42:ARG:O	1:A:45:GLU:HB3	2.15	0.46
1:A:130:PRO:HA	1:A:133:GLN:CG	2.42	0.46
1:B:40:VAL:HA	1:B:50:MET:HE3	1.96	0.46
1:A:78:VAL:O	1:A:79:VAL:C	2.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:TYR:CD1	2:C:2:OMZ:CL	3.05	0.46
1:A:55:ARG:NH1	1:A:66:GLU:HB2	2.31	0.46
1:A:75:VAL:O	1:A:78:VAL:HB	2.15	0.46
1:B:43:CYS:SG	1:B:50:MET:HG3	2.55	0.46
1:A:132:GLU:HG2	1:A:192:ASP:OD1	2.16	0.46
1:A:334:VAL:HG12	1:A:364:ALA:HA	1.96	0.46
2:D:6:OMY:CL	4:D:8:BGC:H6C2	2.52	0.46
1:A:189:ARG:O	1:A:190:PRO:C	2.57	0.45
1:A:267:ASP:C	1:A:269:GLY:N	2.74	0.45
1:A:333:GLY:HA2	5:A:2053:HOH:O	2.16	0.45
1:A:130:PRO:HB3	1:A:169:TYR:OH	2.16	0.45
1:B:73:GLU:H	1:B:73:GLU:CD	2.24	0.45
1:B:221:SER:O	1:B:253:ARG:HD3	2.17	0.45
1:A:216:PHE:C	1:A:218:ALA:N	2.74	0.45
1:B:367:VAL:O	1:B:371:ILE:HD12	2.17	0.45
1:B:72:ALA:HB2	2:D:1:MLU:HD12	1.99	0.45
1:A:354:THR:O	1:A:357:ALA:HB3	2.17	0.45
1:A:2:ARG:HE	1:A:32:ARG:NH2	2.14	0.44
1:A:324:TYR:O	1:A:328:ARG:HG2	2.17	0.44
1:A:82:TRP:C	1:A:84:ASP:N	2.72	0.44
1:A:143:GLN:O	1:A:144:GLY:C	2.59	0.44
1:A:184:VAL:HG21	1:A:370:THR:OG1	2.17	0.44
1:B:2:ARG:HD3	1:B:32:ARG:CZ	2.47	0.44
1:B:158:ALA:C	1:B:160:ILE:H	2.26	0.44
1:B:202:ILE:HG13	1:B:304:ARG:HH12	1.82	0.44
1:A:289:ALA:HB2	1:A:308:PRO:HG2	2.00	0.44
1:B:107:ALA:O	1:B:111:MET:HG2	2.18	0.44
1:A:46:VAL:HG12	1:A:46:VAL:O	2.17	0.44
1:B:111:MET:O	1:B:112:ALA:C	2.61	0.44
1:B:13:ASP:HA	1:B:124:LEU:HD11	2.00	0.44
1:A:50:MET:HG2	1:A:51:VAL:N	2.32	0.43
1:A:202:ILE:O	1:A:204:PRO:HD3	2.18	0.43
1:A:215:ALA:O	1:A:218:ALA:HB3	2.19	0.43
1:B:142:ASN:OD1	1:B:169:TYR:HB3	2.17	0.43
1:A:109:ARG:HG2	1:A:171:TYR:CE2	2.53	0.43
1:B:87:PRO:HD3	1:B:111:MET:HE3	2.00	0.43
1:B:275:VAL:HG13	1:B:278:VAL:HB	2.00	0.43
1:A:189:ARG:HD3	5:A:2017:HOH:O	2.19	0.43
1:B:111:MET:O	1:B:114:LYS:N	2.52	0.43
1:A:235:ALA:O	1:A:236:THR:C	2.62	0.43
1:B:3:VAL:O	1:B:31:ALA:HA	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:LEU:O	1:B:217:LEU:HG	2.19	0.43
1:A:58:ARG:HG3	1:A:260:TRP:CD2	2.53	0.43
1:B:87:PRO:HD3	1:B:111:MET:CE	2.49	0.43
1:B:98:THR:CG2	1:B:99:THR:N	2.82	0.43
1:B:243:ALA:HA	1:B:348:LEU:HD13	2.00	0.43
1:A:142:ASN:HD21	1:A:170:ASP:H	1.66	0.43
1:B:111:MET:C	1:B:113:GLU:N	2.73	0.43
1:B:41:GLU:O	1:B:45:GLU:HG3	2.19	0.42
1:B:81:GLU:CD	1:B:85:LYS:HD3	2.44	0.42
1:B:153:VAL:HG12	1:B:157:ARG:HD2	2.00	0.42
1:A:209:LEU:HD12	1:A:286:ARG:NH1	2.33	0.42
1:A:328:ARG:O	1:A:332:LEU:HG	2.19	0.42
1:A:243:ALA:HA	1:A:348:LEU:HD13	2.01	0.42
1:B:5:ILE:HD11	1:B:24:LEU:HD12	2.00	0.42
1:A:182:ASP:HA	1:A:183:PRO:HD3	1.86	0.42
1:B:23:ARG:HG2	1:B:376:THR:HB	2.02	0.42
1:B:71:ALA:O	1:B:74:VAL:HG22	2.19	0.42
1:A:74:VAL:HG22	1:A:74:VAL:O	2.19	0.42
1:A:190:PRO:O	1:A:191:THR:C	2.63	0.42
1:A:244:ILE:HG23	1:A:254:ILE:CD1	2.43	0.42
1:A:5:ILE:HA	1:A:97:VAL:O	2.20	0.42
1:A:153:VAL:HG12	1:A:157:ARG:CD	2.50	0.42
1:A:106:VAL:HG13	1:A:171:TYR:CD2	2.55	0.42
1:B:33:MET:O	1:B:51:VAL:HG12	2.20	0.42
1:B:143:GLN:C	1:B:147:ARG:NH1	2.78	0.41
1:A:126:PRO:HD3	1:A:186:SER:HB3	2.02	0.41
1:A:127:ASP:HA	1:A:132:GLU:OE1	2.20	0.41
1:A:2:ARG:NE	1:A:32:ARG:HH21	2.16	0.41
1:A:100:GLY:O	1:A:101:LEU:C	2.64	0.41
1:A:135:GLN:O	1:A:139:ASP:OD1	2.39	0.41
1:A:2:ARG:HB2	1:A:2:ARG:HH11	1.84	0.41
1:A:37:PRO:O	1:A:40:VAL:HG13	2.19	0.41
1:A:363:ARG:HD2	1:A:363:ARG:HA	1.83	0.41
1:B:2:ARG:HA	1:B:30:ASP:O	2.20	0.41
1:A:20:LEU:HD22	1:A:201:TRP:CZ3	2.56	0.41
1:A:294:ASP:OD1	1:A:326:ALA:N	2.43	0.41
1:B:123:VAL:HG21	1:B:129:LEU:HD23	2.03	0.41
1:B:214:GLU:OE1	1:B:286:ARG:NH1	2.54	0.41
1:A:12:GLY:HA2	3:A:406:TYD:C5'	2.51	0.41
1:A:193:LEU:O	1:A:195:THR:N	2.47	0.41
1:B:59:ALA:HA	1:B:62:ARG:CZ	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:282:GLU:O	1:B:286:ARG:HG2	2.21	0.41
1:A:25:ARG:HD2	1:A:48:VAL:HG22	2.03	0.40
1:B:17:LEU:HD11	1:B:99:THR:CG2	2.50	0.40
2:D:1:MLU:HD23	2:D:1:MLU:HA	1.93	0.40
1:A:6:THR:HG23	1:A:82:TRP:CZ3	2.56	0.40
1:B:182:ASP:HA	1:B:183:PRO:HD3	1.83	0.40
1:A:389:LEU:CD1	1:B:212:GLU:HG2	2.49	0.40
1:A:40:VAL:CG2	1:A:41:GLU:N	2.85	0.40
1:A:242:MET:CE	1:A:345:ILE:HG13	2.50	0.40
1:B:313:ARG:HE	1:B:339:ASP:HB3	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	389/404 (96%)	335 (86%)	42 (11%)	12 (3%)	3	12
1	B	380/404 (94%)	355 (93%)	20 (5%)	5 (1%)	9	31
2	C	1/7 (14%)	0	1 (100%)	0	100	100
2	D	1/7 (14%)	1 (100%)	0	0	100	100
All	All	771/822 (94%)	691 (90%)	63 (8%)	17 (2%)	5	19

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	64	PRO
1	A	60	GLY
1	A	138	ARG
1	A	10	SER
1	A	190	PRO

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Mol	Chain	Res	Type
1	A	321	GLU
1	A	389	LEU
1	B	266	PRO
1	A	73	GLU
1	A	101	LEU
1	A	127	ASP
1	A	217	LEU
1	A	263	LEU
1	B	268	ASP
1	A	204	PRO
1	B	73	GLU
1	B	231	SER

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	280/311 (90%)	259 (92%)	21 (8%)	12	37
1	B	281/311 (90%)	268 (95%)	13 (5%)	24	58
2	C	1/1 (100%)	0	1 (100%)	0	0
2	D	1/1 (100%)	1 (100%)	0	100	100
All	All	563/624 (90%)	528 (94%)	35 (6%)	16	45

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	35	LEU
1	A	50	MET
1	A	87	PRO
1	A	109	ARG
1	A	138	ARG
1	A	139	ASP
1	A	167	HIS
1	A	175	ASP

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Mol	Chain	Res	Type
1	A	190	PRO
1	A	192	ASP
1	A	213	LEU
1	A	222	THR
1	A	274	VAL
1	A	304	ARG
1	A	313	ARG
1	A	317	ASP
1	A	344	THR
1	A	358	PRO
1	A	363	ARG
1	A	372	ARG
1	B	3	VAL
1	B	41	GLU
1	B	51	VAL
1	B	64	PRO
1	B	75	VAL
1	B	77	GLU
1	B	147	ARG
1	B	176	GLN
1	B	192	ASP
1	B	334	VAL
1	B	345	ILE
1	B	354	THR
1	B	372	ARG
2	C	3	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	133	GLN
1	A	142	ASN
1	A	167	HIS
1	A	176	GLN
1	A	197	GLN
1	A	381	GLN
1	B	133	GLN
1	B	176	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

12 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
2	GHP	C	4	2,4	10,11,12	2.30	4 (40%)	11,14,16	1.57	2 (18%)
2	MLU	C	1	2	7,8,9	1.07	0	7,9,11	1.14	1 (14%)
2	OMY	C	6	2	12,14,15	2.49	5 (41%)	17,19,21	2.14	2 (11%)
2	GHP	D	4	2,4	10,11,12	1.56	2 (20%)	11,14,16	1.08	1 (9%)
2	GHP	C	5	2	10,11,12	2.00	2 (20%)	11,14,16	2.04	5 (45%)
2	OMZ	C	2	2	12,14,15	1.71	3 (25%)	17,19,21	1.32	1 (5%)
2	OMY	D	6	2	12,14,15	2.17	5 (41%)	17,19,21	1.67	2 (11%)
2	3FG	D	7	2	12,13,13	2.70	7 (58%)	14,18,18	1.46	2 (14%)
2	MLU	D	1	2	7,8,9	1.02	0	7,9,11	1.14	1 (14%)
2	3FG	C	7	2	12,13,13	4.03	8 (66%)	14,18,18	1.90	2 (14%)
2	OMZ	D	2	2	12,14,15	1.37	1 (8%)	17,19,21	1.30	1 (5%)
2	GHP	D	5	2	10,11,12	1.93	3 (30%)	11,14,16	1.85	5 (45%)

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	GHP	C	4	2,4	-	0/4/6/8	0/1/1/1
2	MLU	C	1	2	-	2/5/8/10	-
2	OMY	C	6	2	-	1/9/10/12	0/1/1/1
2	GHP	D	4	2,4	-	0/4/6/8	0/1/1/1
2	GHP	C	5	2	-	0/4/6/8	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OMZ	C	2	2	-	0/9/10/12	0/1/1/1
2	OMY	D	6	2	-	0/9/10/12	0/1/1/1
2	3FG	D	7	2	-	3/8/8/8	0/1/1/1
2	MLU	D	1	2	-	4/5/8/10	-
2	3FG	C	7	2	-	5/8/8/8	0/1/1/1
2	OMZ	D	2	2	-	1/9/10/12	0/1/1/1
2	GHP	D	5	2	-	0/4/6/8	0/1/1/1

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	7	3FG	CB-CA	9.38	1.62	1.52
2	C	7	3FG	CG1-CB	7.30	1.49	1.39
2	D	7	3FG	CG1-CB	5.47	1.47	1.39
2	C	6	OMY	CZ-CE1	4.93	1.44	1.39
2	D	6	OMY	CZ-CE1	4.48	1.44	1.39
2	C	4	GHP	C3-C2	4.39	1.45	1.38
2	C	5	GHP	CA-C	4.36	1.58	1.51
2	D	5	GHP	CA-C	3.84	1.57	1.51
2	C	2	OMZ	CD2-CG	3.71	1.45	1.39
2	D	2	OMZ	CD2-CG	3.41	1.44	1.39
2	D	7	3FG	CG2-CD2	3.35	1.44	1.39
2	C	7	3FG	CG1-CD1	3.33	1.44	1.39
2	C	4	GHP	C1-CA	3.33	1.55	1.52
2	D	7	3FG	OXT-C	-3.29	1.20	1.30
2	C	6	OMY	OCZ-CZ	3.25	1.42	1.36
2	C	7	3FG	CG2-CD2	3.22	1.43	1.39
2	C	7	3FG	CG2-CB	3.18	1.43	1.39
2	D	7	3FG	CB-CA	3.16	1.56	1.52
2	C	6	OMY	CD2-CG	3.02	1.43	1.39
2	C	5	GHP	C3-C4	2.91	1.44	1.39
2	D	7	3FG	CZ-CD1	2.88	1.43	1.39
2	D	4	GHP	C3-C2	2.80	1.43	1.38
2	C	7	3FG	OXT-C	-2.77	1.21	1.30
2	C	2	OMZ	CE2-CZ	2.76	1.44	1.39
2	C	4	GHP	C3-C4	2.72	1.44	1.39
2	D	6	OMY	CD2-CG	2.69	1.43	1.39
2	D	5	GHP	C1-CA	2.67	1.55	1.52
2	C	6	OMY	CD1-CG	2.54	1.42	1.39
2	D	6	OMY	CA-N	-2.48	1.40	1.47
2	D	7	3FG	CG1-CD1	2.47	1.42	1.39
2	D	6	OMY	OCZ-CZ	2.47	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	6	OMY	CD1-CE1	2.36	1.42	1.38
2	C	2	OMZ	OH-CZ	2.25	1.40	1.36
2	C	7	3FG	CA-C	2.24	1.60	1.54
2	D	6	OMY	CD1-CG	2.21	1.42	1.39
2	C	4	GHP	O4-C4	2.19	1.41	1.37
2	C	7	3FG	O-C	2.18	1.28	1.22
2	D	7	3FG	CG2-CB	2.14	1.42	1.39
2	D	5	GHP	C3-C4	2.04	1.42	1.39
2	D	4	GHP	O4-C4	2.02	1.41	1.37

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	6	OMY	CG-CB-CA	-7.69	101.48	111.58
2	D	6	OMY	CG-CB-CA	-5.47	104.40	111.58
2	C	7	3FG	CG1-CB-CA	4.22	126.26	119.79
2	C	7	3FG	CD2-CG2-CB	3.48	123.09	120.09
2	C	2	OMZ	O-C-CA	-3.44	115.94	124.77
2	C	5	GHP	C2-C1-CA	-3.34	115.45	120.64
2	C	4	GHP	C5-C6-C1	3.22	124.39	121.18
2	D	7	3FG	CB-CA-C	3.02	116.62	110.10
2	D	5	GHP	C2-C3-C4	-2.88	116.83	119.88
2	C	4	GHP	C2-C1-CA	2.75	124.91	120.64
2	D	2	OMZ	O-C-CA	-2.73	117.76	124.77
2	C	5	GHP	C6-C1-CA	2.70	124.84	120.64
2	C	5	GHP	C3-C2-C1	2.70	123.88	121.18
2	C	5	GHP	C5-C6-C1	-2.59	118.60	121.18
2	D	5	GHP	C2-C1-CA	-2.58	116.63	120.64
2	C	5	GHP	C2-C3-C4	-2.56	117.17	119.88
2	D	5	GHP	C5-C6-C1	-2.40	118.78	121.18
2	D	4	GHP	C5-C6-C1	2.34	123.52	121.18
2	D	5	GHP	C3-C2-C1	2.28	123.45	121.18
2	C	6	OMY	OCZ-CZ-CE1	2.20	124.55	119.25
2	C	1	MLU	CB-CA-C	-2.19	107.62	110.99
2	D	7	3FG	CD1-CG1-CB	-2.17	118.21	120.09
2	D	5	GHP	C6-C1-CA	2.13	123.96	120.64
2	D	1	MLU	CB-CA-C	-2.09	107.78	110.99
2	D	6	OMY	OCZ-CZ-CE1	2.08	124.27	119.25

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1	MLU	C-CA-CB-CG
2	C	7	3FG	C-CA-CB-CG1
2	C	7	3FG	C-CA-CB-CG2
2	C	7	3FG	OXT-C-CA-N
2	D	7	3FG	C-CA-CB-CG1
2	D	7	3FG	C-CA-CB-CG2
2	D	7	3FG	OXT-C-CA-N
2	D	1	MLU	N-CA-CB-CG
2	C	1	MLU	CA-CB-CG-CD1
2	C	1	MLU	CA-CB-CG-CD2
2	D	1	MLU	CA-CB-CG-CD2
2	D	1	MLU	CA-CB-CG-CD1
2	C	7	3FG	O-C-CA-CB
2	C	7	3FG	OXT-C-CA-CB
2	D	2	OMZ	O-C-CA-CB
2	C	6	OMY	O-C-CA-CB

There are no ring outliers.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	6	OMY	1	0
2	C	2	OMZ	3	0
2	D	6	OMY	1	0
2	D	7	3FG	2	0
2	D	1	MLU	2	0
2	D	5	GHP	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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	$\# Z > 2$
4	BGC	C	8	2	11,11,12	1.00	1 (9%)	15,15,17	1.79	3 (20%)
3	TYD	A	406	-	25,26,26	0.96	1 (4%)	38,40,40	0.74	1 (2%)
4	BGC	D	8	2	11,11,12	1.17	1 (9%)	15,15,17	1.84	3 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BGC	C	8	2	-	2/2/19/22	0/1/1/1
3	TYD	A	406	-	-	3/16/28/28	0/2/2/2
4	BGC	D	8	2	-	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)
3	A	406	TYD	PA-O3A	4.16	1.64	1.59
4	C	8	BGC	C6-C5	2.13	1.59	1.51
4	D	8	BGC	O5-C1	-2.01	1.40	1.43

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	8	BGC	O6-C6-C5	5.04	128.51	111.33
4	D	8	BGC	O6-C6-C5	4.89	127.97	111.33
4	D	8	BGC	C1-C2-C3	2.79	113.70	109.64
3	A	406	TYD	O3A-PA-O1A	-2.51	103.15	110.70
4	C	8	BGC	C1-C2-C3	2.34	113.06	109.64
4	D	8	BGC	O5-C5-C6	-2.31	103.16	107.66
4	C	8	BGC	C6-C5-C4	2.03	118.00	113.02

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	406	TYD	PA-O3A-PB-O2B

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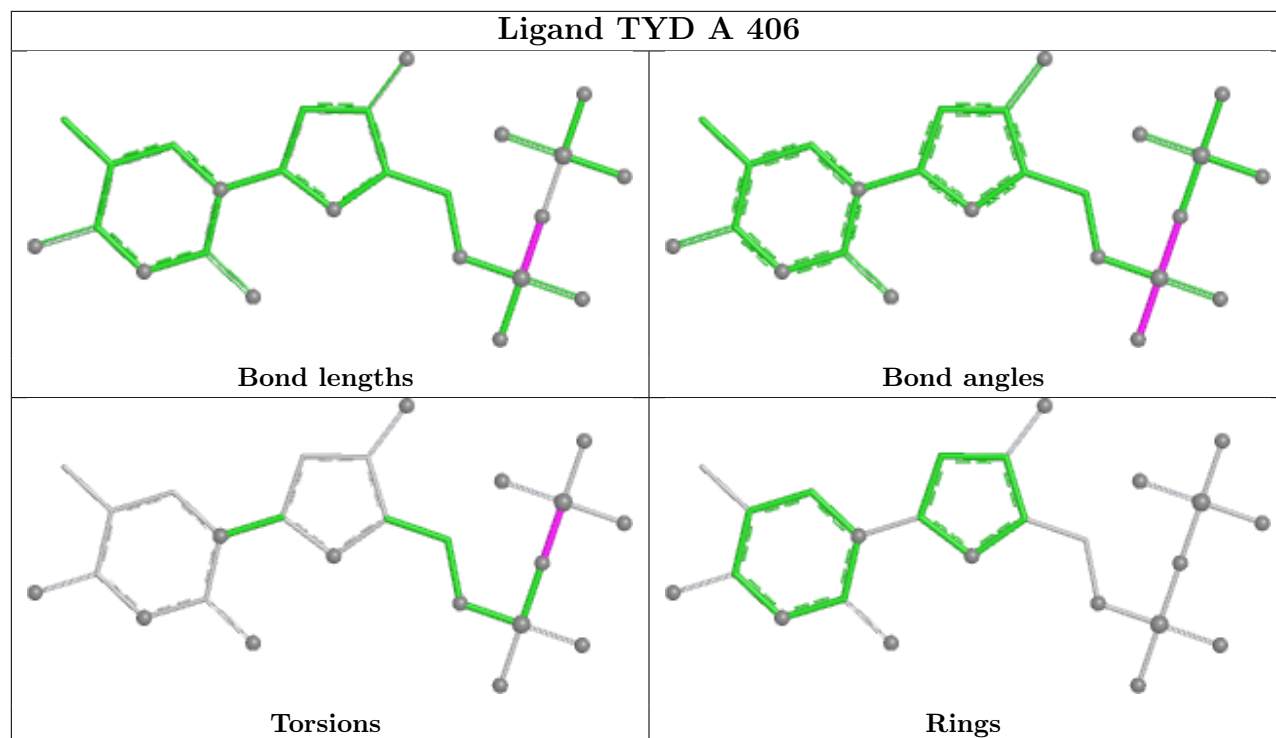
Mol	Chain	Res	Type	Atoms
3	A	406	TYD	PA-O3A-PB-O3B
4	C	8	BGC	C4-C5-C6-O6
4	C	8	BGC	O5-C5-C6-O6
3	A	406	TYD	PA-O3A-PB-O1B

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	8	BGC	1	0
3	A	406	TYD	5	0
4	D	8	BGC	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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	391/404 (96%)	0.06	9 (2%) 61 51	29, 46, 68, 74	1 (0%)
1	B	384/404 (95%)	-0.16	6 (1%) 70 61	25, 40, 54, 71	0
2	C	1/7 (14%)	2.76	1 (100%) 0 0	42, 42, 42, 42	1 (100%)
2	D	1/7 (14%)	0.91	0 100 100	38, 38, 38, 38	0
All	All	777/822 (94%)	-0.05	16 (2%) 63 54	25, 43, 65, 74	2 (0%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	315	VAL	5.1
1	A	321	GLU	3.8
1	A	320	VAL	3.3
1	A	391	LYS	2.8
1	B	268	ASP	2.8
2	C	3	ASN	2.8
1	B	266	PRO	2.8
1	A	132	GLU	2.7
1	A	322	GLN	2.7
1	B	391	LYS	2.6
1	B	314	ARG	2.5
1	A	315	VAL	2.3
1	A	140	MET	2.2
1	A	319	VAL	2.2
1	A	316	VAL	2.1
1	B	267	ASP	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
2	OMZ	C	2	14/15	0.51	0.28	57,59,61,62	14
2	OMZ	D	2	14/15	0.61	0.17	28,30,34,35	0
2	OMY	C	6	14/15	0.61	0.24	56,57,58,58	14
2	OMY	D	6	14/15	0.71	0.16	25,27,32,37	0
2	3FG	C	7	13/13	0.76	0.21	57,58,61,63	13
2	MLU	C	1	9/10	0.83	0.28	59,60,62,62	9
2	GHP	C	4	11/12	0.86	0.13	54,55,57,58	11
2	GHP	C	5	11/12	0.93	0.13	55,57,58,59	11
2	MLU	D	1	9/10	0.93	0.14	33,35,40,42	0
2	GHP	D	5	11/12	0.95	0.07	26,29,30,34	0
2	3FG	D	7	13/13	0.95	0.09	31,33,37,42	0
2	GHP	D	4	11/12	0.96	0.06	29,30,33,33	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

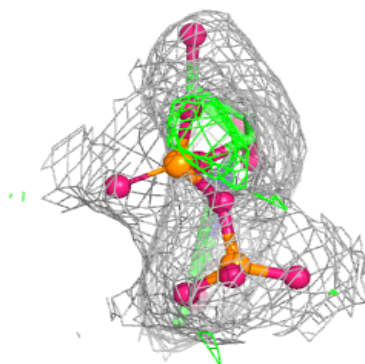
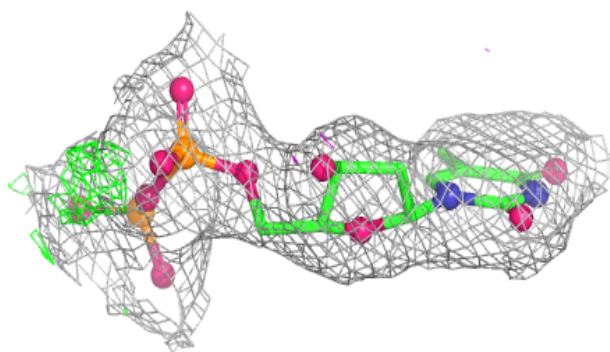
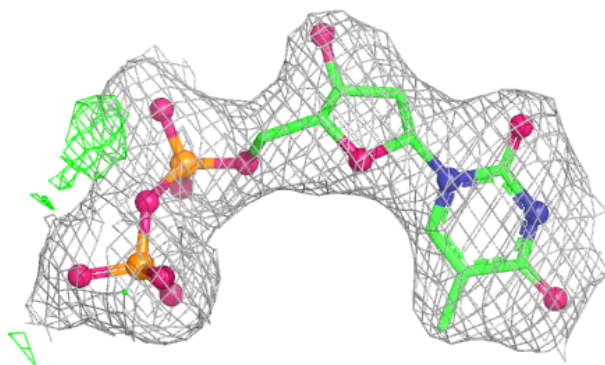
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	BGC	C	8	11/12	0.69	0.17	60,61,63,65	11
4	BGC	D	8	11/12	0.94	0.08	32,33,34,36	0
3	TYD	A	406	25/25	0.96	0.08	35,39,41,42	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around TYD A 406:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.