



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:29 AM UTC

PDB ID : 3N1Z / pdb_00003n1z
Title : X-ray Crystal Structure of Toluene/o-Xylene Monooxygenase Hydroxylase T201S Mutant
Authors : McCormick, M.S.; Sazinsky, M.H.; Lippard, S.J.
Deposited on : 2010-05-17
Resolution : 2.90 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

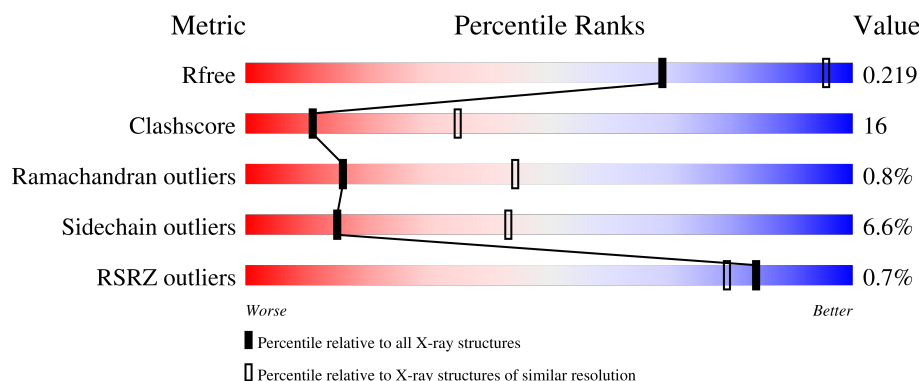
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	498	 64% 30% 5% 1% 0%
2	B	330	 63% 30% 5% 2% 0%
3	C	86	 59% 33% 5% 3% 0%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7491 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 Toluene o-xylene monooxygenase component.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	491	Total	C	N	O	S	0	0	0
			4015	2563	673	753	26			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	201	SER	THR	engineered mutation	UNP Q6IV66

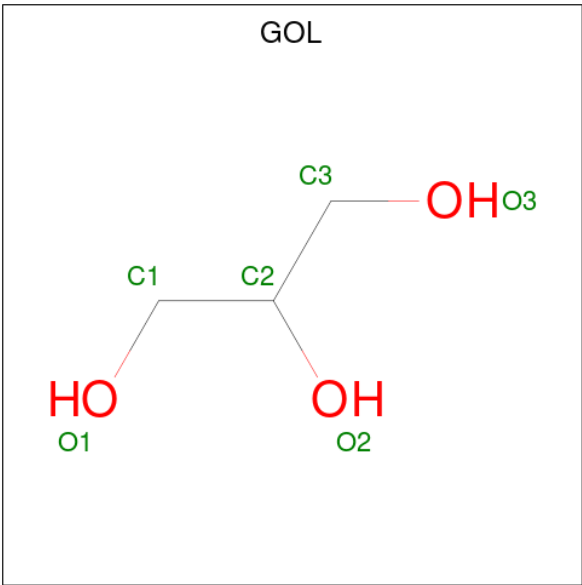
- Molecule 2 is a protein called Toluene o-xylene monooxygenase component.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	322	Total	C	N	O	S	0	0	0
			2641	1674	467	490	10			

- Molecule 3 is a protein called Toluene o-xylene monooxygenase component.

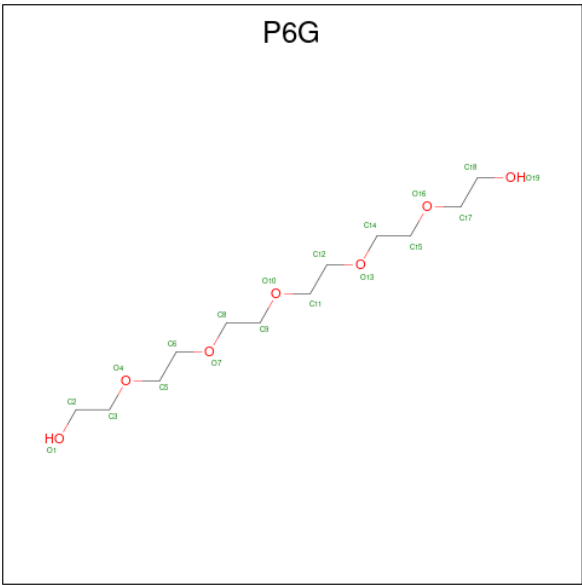
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	83	Total	C	N	O	S	0	0	0
			676	425	120	126	5			

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is HEXAETHYLENE GLYCOL (CCD ID: P6G) (formula: C₁₂H₂₆O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			19	12	7		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			19	12	7		

- Molecule 6 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	Fe	0	0
			2	2		

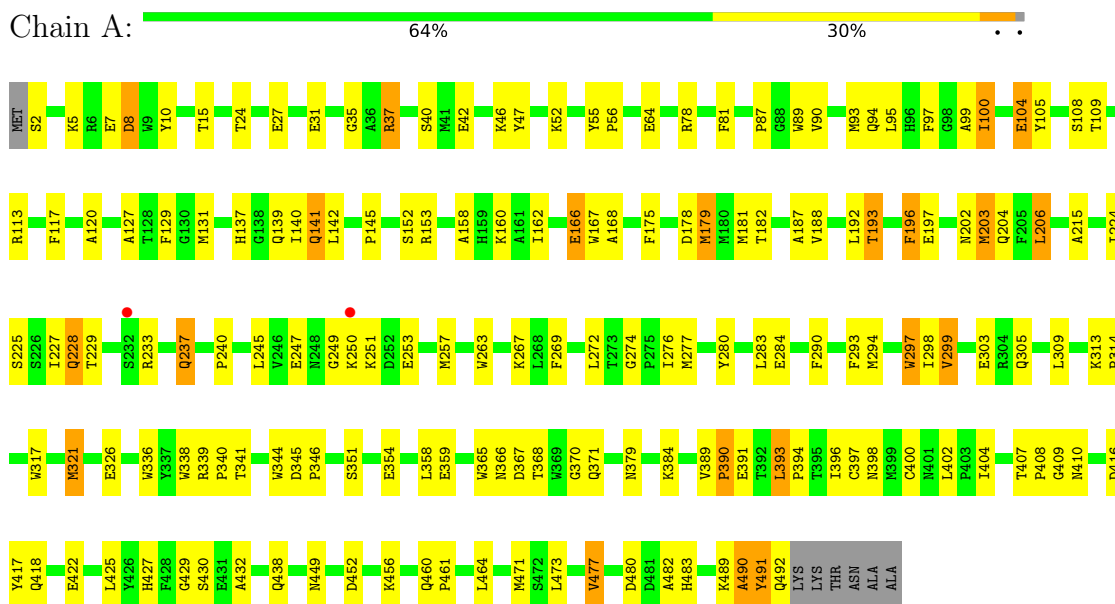
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	48	Total	O	0	0
			48	48		
7	B	44	Total	O	0	0
			44	44		
7	C	9	Total	O	0	0
			9	9		

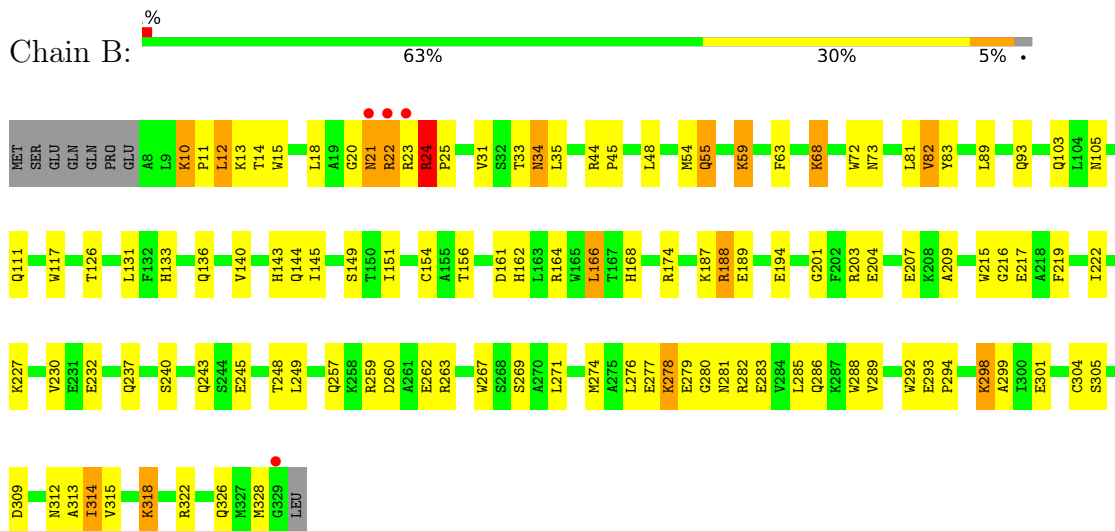
3 Residue-property plots

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: Toluene o-xylene monooxygenase component



- Molecule 2: Toluene o-xylene monooxygenase component



- Molecule 3: Toluene o-xylene monooxygenase component

Chain C:

59%

33%

5%



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	182.83Å 182.83Å 68.86Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.90 50.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (50.00-2.90) 99.9 (50.00-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.28 (at 2.91Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.184 , 0.225 0.181 , 0.219	Depositor DCC
R_{free} test set	1484 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	31.2	Xtriage
Anisotropy	0.988	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 45.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.028 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7491	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% 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: FE, P6G, GOL

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	0.47	0/4139	1.02	26/5625 (0.5%)
2	B	0.48	0/2713	0.98	11/3688 (0.3%)
3	C	0.44	0/690	0.97	1/934 (0.1%)
All	All	0.47	0/7542	1.00	38/10247 (0.4%)

There are no bond length outliers.

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	491	TYR	N-CA-C	-9.20	101.75	113.72
1	A	8	ASP	N-CA-C	9.00	121.09	111.28
1	A	100	ILE	N-CA-C	8.39	118.70	111.90
1	A	142	LEU	N-CA-C	-8.22	102.00	112.93
2	B	189	GLU	N-CA-C	8.00	120.00	111.28
1	A	196	PHE	N-CA-C	7.37	119.21	111.03
1	A	160	LYS	N-CA-C	7.36	119.38	111.36
2	B	31	VAL	N-CA-C	6.86	119.48	112.90
1	A	117	PHE	N-CA-C	6.28	121.11	113.38
1	A	407	THR	N-CA-C	6.26	118.60	109.71
2	B	68	LYS	N-CA-C	6.14	119.71	109.95
2	B	151	ILE	N-CA-C	-6.11	104.89	110.82
1	A	104	GLU	N-CA-C	-6.11	104.55	111.14
1	A	297	TRP	N-CA-C	6.08	120.77	113.23
1	A	158	ALA	N-CA-C	-5.89	104.99	111.82
1	A	249	GLY	N-CA-C	5.88	119.76	112.64
1	A	37	ARG	N-CA-C	5.86	119.47	111.39
2	B	126	THR	N-CA-C	5.82	121.55	113.45
1	A	193	THR	N-CA-C	5.80	117.68	111.36
1	A	299	VAL	N-CA-C	5.76	115.95	110.53
1	A	129	PHE	N-CA-C	-5.73	105.00	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	326	GLU	N-CA-C	5.72	119.79	112.12
1	A	166	GLU	N-CA-C	-5.69	101.43	109.96
1	A	298	ILE	N-CA-C	5.67	116.43	111.56
2	B	222	ILE	N-CA-C	5.61	116.67	111.45
1	A	15	THR	N-CA-C	-5.55	98.20	108.24
2	B	309	ASP	N-CA-C	-5.51	105.86	112.58
2	B	103	GLN	N-CA-C	5.48	117.06	111.14
1	A	40	SER	N-CA-C	5.37	117.80	110.55
1	A	224	ILE	N-CA-C	5.29	115.43	110.30
1	A	179	MET	N-CA-C	5.25	118.15	111.69
2	B	10	LYS	CA-C-N	5.23	126.38	119.84
2	B	10	LYS	C-N-CA	5.23	126.38	119.84
1	A	490	ALA	N-CA-C	-5.11	99.92	110.80
3	C	26	THR	N-CA-C	-5.09	103.68	110.55
2	B	55	GLN	N-CA-C	-5.09	105.65	111.14
1	A	438	GLN	N-CA-C	5.07	117.70	111.82
1	A	233	ARG	N-CA-C	5.04	118.20	111.75

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	4015	0	3764	143	0
2	B	2641	0	2537	89	0
3	C	676	0	667	33	0
4	A	12	0	16	1	0
4	B	6	0	8	1	0
5	A	38	0	52	8	0
6	A	2	0	0	0	0
7	A	48	0	0	2	0
7	B	44	0	0	0	0
7	C	9	0	0	0	0
All	All	7491	0	7044	237	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 16.

All (237) 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:367:ASP:HB3	1:A:410:ASN:ND2	1.65	1.09
3:C:63:PRO:HD2	3:C:66:MET:HE3	1.35	1.03
2:B:21:ASN:O	2:B:22:ARG:HB2	1.60	0.99
2:B:318:LYS:O	2:B:322:ARG:HG3	1.67	0.93
1:A:464:LEU:HD22	5:A:502:P6G:H111	1.53	0.91
1:A:393:LEU:HD22	5:A:502:P6G:H121	1.50	0.90
1:A:2:SER:N	2:B:105:ASN:HD22	1.72	0.88
1:A:416:ASP:OD2	1:A:427:HIS:HD2	1.57	0.87
1:A:425:LEU:HD23	3:C:76:THR:HG22	1.55	0.87
1:A:367:ASP:HB3	1:A:410:ASN:HD21	1.40	0.86
1:A:113:ARG:HH11	2:B:144:GLN:HE21	1.23	0.85
1:A:427:HIS:CE1	3:C:76:THR:HG23	2.12	0.85
1:A:427:HIS:HE1	3:C:76:THR:HG23	1.41	0.84
2:B:188:ARG:HG2	2:B:188:ARG:HH11	1.45	0.81
2:B:188:ARG:HH11	2:B:188:ARG:CG	1.95	0.80
1:A:427:HIS:HE1	3:C:76:THR:CG2	1.93	0.79
2:B:168:HIS:HD2	2:B:257:GLN:HE21	1.30	0.77
1:A:351:SER:OG	1:A:354:GLU:HG3	1.85	0.76
1:A:394:PRO:HG3	5:A:502:P6G:H182	1.67	0.76
1:A:47:TYR:CE1	1:A:240:PRO:HB2	2.22	0.74
1:A:78:ARG:HH11	1:A:78:ARG:HG3	1.52	0.73
2:B:21:ASN:O	2:B:22:ARG:CB	2.38	0.71
1:A:338:TRP:CD1	1:A:390:PRO:HG3	2.25	0.71
1:A:398:ASN:HD22	1:A:427:HIS:H	1.38	0.69
1:A:113:ARG:HH11	2:B:144:GLN:NE2	1.91	0.68
1:A:416:ASP:OD2	1:A:427:HIS:CD2	2.45	0.68
1:A:139:GLN:HE22	2:B:83:TYR:H	1.42	0.67
2:B:24:ARG:O	2:B:24:ARG:HG2	1.94	0.67
3:C:39:ILE:CG2	3:C:45:PRO:HG3	2.25	0.67
2:B:34:ASN:N	2:B:34:ASN:HD22	1.93	0.66
3:C:63:PRO:CD	3:C:66:MET:HE3	2.20	0.65
1:A:460:GLN:HA	1:A:461:PRO:C	2.22	0.65
2:B:301:GLU:HA	2:B:314:ILE:HD13	1.79	0.65
2:B:162:HIS:HE1	2:B:227:LYS:HZ2	1.46	0.64
1:A:182:THR:HA	2:B:54:MET:HG2	1.79	0.64
2:B:168:HIS:CD2	2:B:257:GLN:HE21	2.15	0.63
1:A:491:TYR:O	1:A:492:GLN:HB2	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:ASP:O	2:B:174:ARG:NH2	2.32	0.63
1:A:140:ILE:HG21	1:A:227:ILE:HD11	1.81	0.63
1:A:314:PRO:HD2	1:A:317:TRP:CE3	2.34	0.62
1:A:398:ASN:ND2	1:A:427:HIS:H	1.98	0.62
2:B:21:ASN:OD1	2:B:21:ASN:N	2.31	0.62
1:A:2:SER:N	2:B:105:ASN:ND2	2.46	0.62
1:A:137:HIS:CD2	1:A:227:ILE:HD12	2.34	0.62
1:A:336:TRP:O	1:A:339:ARG:HB2	1.99	0.62
1:A:489:LYS:O	1:A:489:LYS:HG3	2.00	0.61
2:B:305:SER:HB3	2:B:314:ILE:HD11	1.82	0.61
1:A:367:ASP:CB	1:A:410:ASN:HD21	2.12	0.61
1:A:417:TYR:CE2	1:A:430:SER:HA	2.36	0.61
2:B:20:GLY:C	2:B:21:ASN:OD1	2.44	0.60
2:B:164:ARG:NH2	2:B:260:ASP:OD2	2.35	0.60
1:A:339:ARG:HB3	1:A:340:PRO:CD	2.30	0.60
1:A:339:ARG:HG2	1:A:480:ASP:HA	1.82	0.60
2:B:14:THR:HG23	2:B:15:TRP:O	2.01	0.59
1:A:253:GLU:OE1	1:A:253:GLU:N	2.33	0.59
1:A:294:MET:O	1:A:299:VAL:HG23	2.02	0.59
1:A:391:GLU:HA	1:A:464:LEU:HD11	1.85	0.59
1:A:203:MET:HG2	1:A:297:TRP:HB3	1.84	0.59
1:A:339:ARG:HB3	1:A:340:PRO:HD3	1.85	0.59
1:A:137:HIS:O	1:A:141:GLN:HB2	2.02	0.58
1:A:203:MET:HA	1:A:203:MET:HE2	1.83	0.58
2:B:269:SER:OG	2:B:328:MET:HE2	2.04	0.58
1:A:368:THR:HA	1:A:409:GLY:HA3	1.84	0.58
1:A:344:TRP:O	1:A:346:PRO:HD3	2.04	0.58
1:A:89:TRP:CD1	1:A:93:MET:HE2	2.39	0.58
1:A:95:LEU:HD13	1:A:344:TRP:CZ3	2.39	0.57
1:A:203:MET:HE2	1:A:203:MET:CA	2.34	0.57
1:A:7:GLU:CD	1:A:7:GLU:H	2.12	0.57
1:A:95:LEU:HD23	1:A:276:ILE:HD11	1.86	0.57
1:A:416:ASP:H	3:C:56:HIS:CE1	2.22	0.57
2:B:204:GLU:OE1	2:B:298:LYS:NZ	2.37	0.57
2:B:81:LEU:HD11	2:B:263:ARG:HD2	1.87	0.57
2:B:162:HIS:HE1	2:B:227:LYS:NZ	2.03	0.57
1:A:47:TYR:HB3	1:A:120:ALA:HB1	1.86	0.56
2:B:23:ARG:O	2:B:23:ARG:HG2	2.05	0.56
2:B:314:ILE:O	2:B:318:LYS:HB2	2.06	0.56
1:A:272:LEU:O	1:A:276:ILE:HD13	2.05	0.56
1:A:345:ASP:O	1:A:482:ALA:HB2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:33:THR:HB	2:B:34:ASN:HD22	1.71	0.56
2:B:34:ASN:N	2:B:34:ASN:ND2	2.54	0.55
2:B:166:LEU:O	2:B:166:LEU:HD22	2.06	0.55
2:B:188:ARG:CG	2:B:188:ARG:NH1	2.61	0.55
1:A:418:GLN:HE22	3:C:78:THR:H	1.53	0.55
1:A:416:ASP:H	3:C:56:HIS:HE1	1.55	0.55
2:B:45:PRO:HG2	2:B:55:GLN:OE1	2.07	0.55
1:A:93:MET:SD	4:A:500:GOL:H12	2.46	0.55
2:B:304:CYS:HB2	2:B:314:ILE:HG12	1.89	0.55
1:A:35:GLY:O	1:A:37:ARG:HG3	2.08	0.54
2:B:59:LYS:HA	2:B:63:PHE:HD2	1.72	0.54
2:B:174:ARG:O	2:B:174:ARG:HD3	2.07	0.54
2:B:282:ARG:O	2:B:286:GLN:HG3	2.07	0.54
1:A:299:VAL:O	1:A:303:GLU:HG3	2.08	0.54
1:A:24:THR:OG1	1:A:27:GLU:HG3	2.07	0.54
1:A:153:ARG:NH1	2:B:12:LEU:HD22	2.23	0.53
1:A:366:ASN:HA	1:A:370:GLY:HA3	1.90	0.53
1:A:105:TYR:O	1:A:108:SER:HB3	2.08	0.53
3:C:9:ASN:HB2	3:C:16:ILE:HG12	1.90	0.53
2:B:24:ARG:O	2:B:24:ARG:CG	2.56	0.53
3:C:27:MET:HE2	3:C:66:MET:HG2	1.89	0.52
3:C:23:THR:HA	3:C:68:VAL:HB	1.92	0.52
1:A:139:GLN:HE22	2:B:82:VAL:HG13	1.74	0.52
1:A:359:GLU:HB2	1:A:366:ASN:ND2	2.24	0.52
1:A:339:ARG:CG	1:A:480:ASP:HA	2.40	0.51
1:A:379:ASN:HD22	1:A:384:LYS:HE3	1.74	0.51
1:A:400:CYS:O	1:A:402:LEU:HG	2.10	0.51
1:A:339:ARG:CD	1:A:480:ASP:HA	2.41	0.51
1:A:100:ILE:HD11	5:A:501:P6G:H91	1.92	0.51
2:B:203:ARG:O	2:B:207:GLU:HG3	2.10	0.51
2:B:194:GLU:HA	2:B:203:ARG:NH1	2.26	0.51
3:C:47:PRO:C	3:C:49:LYS:H	2.18	0.51
3:C:56:HIS:HD2	3:C:80:ASP:OD1	1.93	0.51
1:A:277:MET:HE1	1:A:293:PHE:HB2	1.92	0.51
1:A:139:GLN:NE2	2:B:82:VAL:HG13	2.27	0.50
1:A:37:ARG:NH2	1:A:257:MET:HE1	2.27	0.50
1:A:89:TRP:NE1	1:A:93:MET:HE2	2.26	0.50
1:A:166:GLU:HA	1:A:471:MET:HB3	1.92	0.50
3:C:10:PHE:CE1	3:C:81:ILE:HG21	2.46	0.50
1:A:99:ALA:O	1:A:100:ILE:HD13	2.12	0.50
1:A:303:GLU:OE2	1:A:313:LYS:HE2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:35:LEU:HB2	2:B:149:SER:CB	2.43	0.49
3:C:54:ARG:HG3	3:C:80:ASP:HB2	1.93	0.49
1:A:358:LEU:HD13	1:A:365:TRP:CZ2	2.48	0.49
1:A:449:ASN:OD1	1:A:449:ASN:C	2.54	0.49
2:B:143:HIS:C	2:B:143:HIS:CD2	2.91	0.49
1:A:55:TYR:HB3	1:A:56:PRO:HD3	1.94	0.48
2:B:145:ILE:HG13	2:B:145:ILE:O	2.13	0.48
1:A:197:GLU:O	1:A:202:ASN:HB2	2.13	0.48
2:B:161:ASP:O	2:B:164:ARG:HB3	2.13	0.48
2:B:219:PHE:CZ	2:B:271:LEU:HD23	2.49	0.48
1:A:225:SER:O	1:A:229:THR:HG23	2.14	0.48
1:A:153:ARG:HB3	1:A:477:VAL:HG12	1.96	0.47
1:A:206:LEU:HD13	1:A:228:GLN:CD	2.40	0.47
2:B:285:LEU:O	2:B:289:VAL:HG23	2.14	0.47
1:A:317:TRP:CD1	1:A:321:MET:HE1	2.50	0.47
2:B:154:CYS:HB3	2:B:267:TRP:CE2	2.48	0.47
3:C:75:PRO:O	3:C:76:THR:HB	2.15	0.47
1:A:10:TYR:CZ	1:A:52:LYS:HB3	2.50	0.47
1:A:393:LEU:HD22	5:A:502:P6G:C12	2.35	0.47
1:A:109:THR:HG23	2:B:144:GLN:HB2	1.97	0.47
1:A:393:LEU:N	1:A:393:LEU:HD23	2.30	0.47
2:B:18:LEU:O	2:B:21:ASN:OD1	2.33	0.47
2:B:93:GLN:HE22	2:B:259:ARG:HD3	1.80	0.47
1:A:491:TYR:O	1:A:492:GLN:CB	2.63	0.46
3:C:54:ARG:NH1	3:C:80:ASP:OD2	2.48	0.46
1:A:139:GLN:NE2	7:A:523:HOH:O	2.45	0.46
1:A:47:TYR:CD1	1:A:240:PRO:HB2	2.51	0.46
1:A:78:ARG:HG3	1:A:78:ARG:NH1	2.27	0.46
2:B:276:LEU:HD22	2:B:282:ARG:HB2	1.98	0.46
1:A:187:ALA:HB2	1:A:257:MET:HE1	1.98	0.46
1:A:367:ASP:HB3	1:A:410:ASN:HD22	1.68	0.46
1:A:427:HIS:CE1	3:C:76:THR:CG2	2.80	0.46
3:C:74:ARG:O	3:C:75:PRO:C	2.56	0.45
2:B:201:GLY:HA3	2:B:299:ALA:HA	1.97	0.45
2:B:35:LEU:HB2	2:B:149:SER:HB3	1.99	0.45
2:B:293:GLU:N	2:B:294:PRO:CD	2.79	0.45
1:A:196:PHE:CZ	5:A:501:P6G:H61	2.52	0.45
2:B:44:ARG:NH1	2:B:48:LEU:O	2.49	0.45
1:A:204:GLN:HB2	1:A:269:PHE:HZ	1.82	0.45
1:A:263:TRP:CE2	1:A:432:ALA:HB3	2.52	0.45
2:B:131:LEU:HD21	2:B:230:VAL:HG22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:304:CYS:HB3	2:B:313:ALA:HB3	1.98	0.45
1:A:338:TRP:NE1	1:A:390:PRO:HG3	2.32	0.45
3:C:76:THR:HG23	3:C:76:THR:O	2.16	0.45
1:A:305:GLN:HG3	7:A:547:HOH:O	2.17	0.45
1:A:345:ASP:HB3	1:A:482:ALA:HA	1.98	0.45
3:C:52:ARG:HG3	3:C:52:ARG:HH11	1.81	0.45
1:A:47:TYR:OH	1:A:237:GLN:HA	2.17	0.44
1:A:78:ARG:HH11	1:A:78:ARG:CG	2.22	0.44
1:A:167:TRP:CD1	5:A:502:P6G:H172	2.52	0.44
1:A:203:MET:CG	1:A:297:TRP:HB3	2.45	0.44
1:A:396:ILE:HG22	1:A:397:CYS:O	2.16	0.44
2:B:322:ARG:O	2:B:326:GLN:HG3	2.17	0.44
1:A:178:ASP:HA	2:B:48:LEU:HD11	2.00	0.44
1:A:250:LYS:HB3	1:A:253:GLU:HB2	2.00	0.44
1:A:131:MET:HE3	2:B:156:THR:HG23	1.98	0.44
1:A:452:ASP:O	1:A:456:LYS:HG3	2.18	0.44
2:B:117:TRP:CE3	2:B:245:GLU:HG3	2.53	0.44
2:B:133:HIS:O	2:B:136:GLN:HB3	2.17	0.44
1:A:109:THR:HB	1:A:181:MET:HE1	1.99	0.44
2:B:12:LEU:HD12	2:B:12:LEU:HA	1.83	0.44
1:A:166:GLU:OE1	1:A:168:ALA:HB3	2.18	0.44
1:A:389:VAL:HG21	5:A:502:P6G:H21	1.99	0.44
2:B:72:TRP:HA	2:B:274:MET:HE1	2.00	0.44
1:A:404:ILE:HG12	1:A:429:GLY:HA2	2.00	0.43
1:A:90:VAL:O	1:A:94:GLN:HG3	2.18	0.43
1:A:113:ARG:HD3	2:B:144:GLN:NE2	2.33	0.43
2:B:215:TRP:HE1	4:B:331:GOL:C1	2.31	0.43
1:A:153:ARG:CZ	2:B:12:LEU:HD22	2.48	0.43
1:A:379:ASN:ND2	1:A:384:LYS:HE3	2.34	0.43
3:C:8:SER:O	3:C:16:ILE:HA	2.18	0.43
1:A:152:SER:HA	2:B:11:PRO:HG3	2.01	0.43
1:A:100:ILE:HG22	1:A:104:GLU:HG3	2.01	0.43
1:A:274:GLY:HA2	1:A:290:PHE:CD1	2.53	0.43
1:A:100:ILE:HG22	1:A:104:GLU:CG	2.49	0.43
3:C:52:ARG:HG3	3:C:52:ARG:NH1	2.34	0.43
1:A:245:LEU:HD23	1:A:245:LEU:HA	1.76	0.42
1:A:339:ARG:HB2	1:A:339:ARG:HE	1.54	0.42
2:B:174:ARG:NE	2:B:174:ARG:HA	2.34	0.42
3:C:6:ILE:C	3:C:6:ILE:HD12	2.44	0.42
3:C:75:PRO:O	3:C:76:THR:CB	2.67	0.42
1:A:97:PHE:CD2	1:A:145:PRO:HB3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:ALA:HB2	1:A:237:GLN:HE22	1.85	0.42
1:A:396:ILE:HD13	1:A:396:ILE:N	2.35	0.42
3:C:23:THR:O	3:C:68:VAL:HB	2.19	0.42
1:A:341:THR:O	1:A:473:LEU:HD11	2.19	0.42
1:A:47:TYR:CB	1:A:120:ALA:HB1	2.48	0.42
1:A:87:PRO:HG2	1:A:483:HIS:CD2	2.55	0.42
1:A:131:MET:HE3	2:B:156:THR:CG2	2.49	0.42
2:B:68:LYS:HB2	2:B:278:LYS:HE2	2.01	0.42
2:B:217:GLU:HG3	2:B:288:TRP:CD1	2.55	0.42
1:A:267:LYS:HD2	1:A:267:LYS:HA	1.83	0.41
3:C:6:ILE:HG13	3:C:19:VAL:O	2.19	0.41
1:A:162:ILE:HG22	1:A:162:ILE:O	2.20	0.41
1:A:227:ILE:HD13	1:A:227:ILE:HA	1.88	0.41
2:B:249:LEU:C	2:B:249:LEU:HD23	2.45	0.41
1:A:139:GLN:NE2	2:B:83:TYR:H	2.12	0.41
3:C:7:MET:HB2	3:C:78:THR:HA	2.02	0.41
1:A:206:LEU:HD12	1:A:206:LEU:HA	1.94	0.41
2:B:188:ARG:HH11	2:B:188:ARG:HG3	1.83	0.41
2:B:232:GLU:O	2:B:237:GLN:HG2	2.21	0.41
1:A:193:THR:HG22	1:A:197:GLU:OE1	2.21	0.41
2:B:166:LEU:HD22	2:B:166:LEU:C	2.45	0.41
2:B:215:TRP:CG	2:B:216:GLY:N	2.89	0.41
2:B:280:GLY:HA2	2:B:283:GLU:OE1	2.20	0.41
3:C:11:GLU:HG2	3:C:12:ARG:HG3	2.01	0.41
1:A:404:ILE:O	3:C:15:VAL:HG23	2.21	0.41
1:A:81:PHE:HZ	1:A:215:ALA:O	2.03	0.41
2:B:278:LYS:HG2	2:B:281:ASN:ND2	2.36	0.40
3:C:66:MET:HG3	3:C:67:ILE:N	2.36	0.40
1:A:188:VAL:O	1:A:192:LEU:HB3	2.21	0.40
1:A:228:GLN:HE21	1:A:228:GLN:HB3	1.69	0.40
2:B:34:ASN:HA	2:B:73:ASN:OD1	2.21	0.40
2:B:209:ALA:HA	2:B:292:TRP:CH2	2.57	0.40
2:B:274:MET:O	2:B:277:GLU:HG3	2.20	0.40
1:A:153:ARG:NH1	2:B:12:LEU:HD13	2.36	0.40
1:A:175:PHE:CE1	1:A:179:MET:HG3	2.56	0.40
2:B:194:GLU:O	2:B:203:ARG:NH1	2.55	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	489/498 (98%)	454 (93%)	32 (6%)	3 (1%)	21	51
2	B	320/330 (97%)	301 (94%)	16 (5%)	3 (1%)	14	41
3	C	81/86 (94%)	72 (89%)	8 (10%)	1 (1%)	10	34
All	All	890/914 (97%)	827 (93%)	56 (6%)	7 (1%)	16	44

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	22	ARG
1	A	237	GLN
1	A	408	PRO
3	C	48	GLU
1	A	490	ALA
2	B	24	ARG
2	B	25	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	416/422 (99%)	395 (95%)	21 (5%)	22	53
2	B	274/282 (97%)	249 (91%)	25 (9%)	9	28
3	C	77/79 (98%)	72 (94%)	5 (6%)	15	44
All	All	767/783 (98%)	716 (93%)	51 (7%)	15	43

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	A	31	GLU
1	A	42	GLU
1	A	46	LYS
1	A	64	GLU
1	A	141	GLN
1	A	203	MET
1	A	206	LEU
1	A	228	GLN
1	A	247	GLU
1	A	251	LYS
1	A	280	TYR
1	A	283	LEU
1	A	284	GLU
1	A	309	LEU
1	A	321	MET
1	A	371	GLN
1	A	390	PRO
1	A	393	LEU
1	A	422	GLU
1	A	477	VAL
2	B	10	LYS
2	B	12	LEU
2	B	13	LYS
2	B	21	ASN
2	B	24	ARG
2	B	34	ASN
2	B	59	LYS
2	B	82	VAL
2	B	89	LEU
2	B	111	GLN
2	B	140	VAL
2	B	166	LEU
2	B	187	LYS
2	B	188	ARG
2	B	240	SER
2	B	243	GLN
2	B	248	THR
2	B	262	GLU
2	B	278	LYS
2	B	279	GLU
2	B	298	LYS

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Mol	Chain	Res	Type
2	B	312	ASN
2	B	314	ILE
2	B	315	VAL
2	B	318	LYS
3	C	3	THR
3	C	48	GLU
3	C	54	ARG
3	C	66	MET
3	C	76	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	139	GLN
1	A	141	GLN
1	A	165	ASN
1	A	228	GLN
1	A	237	GLN
1	A	248	ASN
1	A	305	GLN
1	A	379	ASN
1	A	398	ASN
1	A	418	GLN
1	A	427	HIS
2	B	17	HIS
2	B	34	ASN
2	B	51	ASN
2	B	87	ASN
2	B	93	GLN
2	B	144	GLN
2	B	153	ASN
2	B	162	HIS
2	B	168	HIS
2	B	223	ASN
2	B	236	GLN
2	B	286	GLN
3	C	56	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 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	$\# Z > 2$
5	P6G	A	502	-	18,18,18	0.65	0	17,17,17	1.08	1 (5%)
4	GOL	A	500	-	5,5,5	0.27	0	5,5,5	0.34	0
5	P6G	A	501	6	18,18,18	0.55	0	17,17,17	0.79	0
4	GOL	A	499	-	5,5,5	0.29	0	5,5,5	0.32	0
4	GOL	B	331	-	5,5,5	0.38	0	5,5,5	0.83	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
5	P6G	A	502	-	-	5/16/16/16	-
4	GOL	A	500	-	-	0/4/4/4	-
5	P6G	A	501	6	-	4/16/16/16	-
4	GOL	A	499	-	-	0/4/4/4	-
4	GOL	B	331	-	-	0/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	502	P6G	C11-O10-C9	-2.17	103.75	113.26

There are no chirality outliers.

All (9) torsion outliers are listed below:

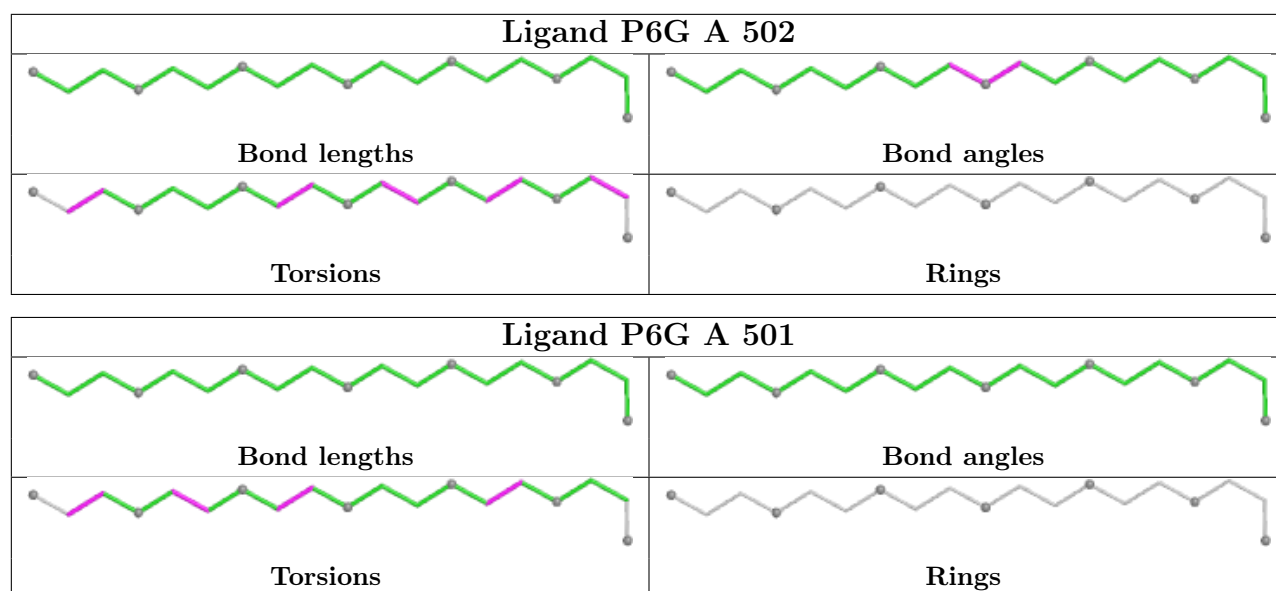
Mol	Chain	Res	Type	Atoms
5	A	502	P6G	O4-C5-C6-O7
5	A	501	P6G	O4-C5-C6-O7
5	A	501	P6G	O16-C17-C18-O19
5	A	502	P6G	O1-C2-C3-O4
5	A	502	P6G	O10-C11-C12-O13
5	A	501	P6G	O10-C11-C12-O13
5	A	502	P6G	O16-C17-C18-O19
5	A	501	P6G	O13-C14-C15-O16
5	A	502	P6G	O7-C8-C9-O10

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	502	P6G	6	0
4	A	500	GOL	1	0
5	A	501	P6G	2	0
4	B	331	GOL	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	491/498 (98%)	-0.43	2 (0%) 88 85	12, 25, 39, 55	0
2	B	322/330 (97%)	-0.43	4 (1%) 76 69	14, 23, 41, 78	0
3	C	83/86 (96%)	-0.35	0 100 100	21, 29, 39, 50	0
All	All	896/914 (98%)	-0.43	6 (0%) 84 79	12, 25, 40, 78	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	23	ARG	3.8
2	B	22	ARG	3.7
2	B	329	GLY	3.4
1	A	250	LYS	2.4
1	A	232	SER	2.3
2	B	21	ASN	2.3

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](#)

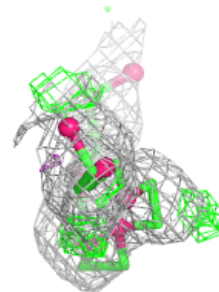
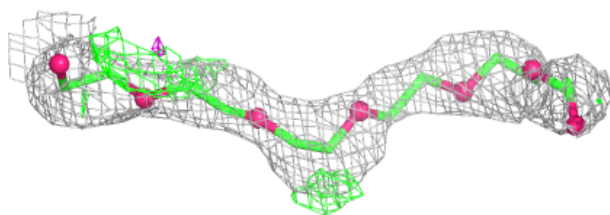
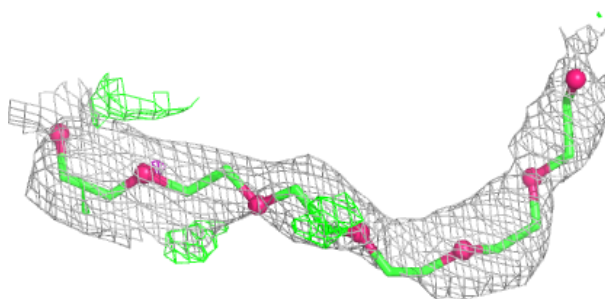
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists 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
4	GOL	A	499	6/6	0.86	0.18	43,45,45,46	0
4	GOL	A	500	6/6	0.88	0.16	38,39,40,44	0
5	P6G	A	501	19/19	0.88	0.22	44,59,64,64	0
5	P6G	A	502	19/19	0.89	0.18	38,47,75,75	0
4	GOL	B	331	6/6	0.90	0.13	28,28,31,32	0
6	FE	A	503	1/1	0.99	0.05	24,24,24,24	0
6	FE	A	504	1/1	1.00	0.04	29,29,29,29	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.

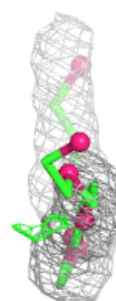
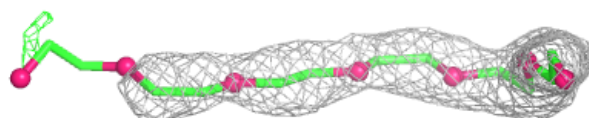
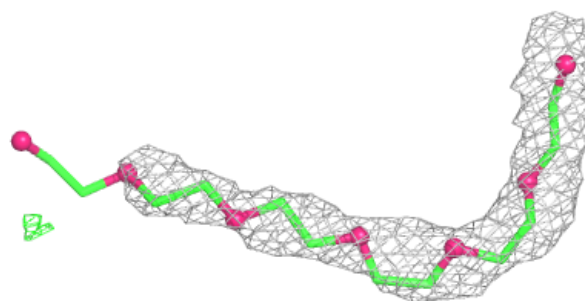
Electron density around P6G A 501:

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



Electron density around P6G A 502:

$2mF_o-DF_c$ (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.