



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 01:30 am BST

PDB ID : 3IF6  
Title : Crystal structure of OXA-46 beta-lactamase from *P. aeruginosa*  
Authors : Docquier, J.D.; Benvenuti, M.; Calderone, V.; Giuliani, F.; Kapetis, D.; De Luca, F.; Rossolini, G.M.; Mangani, S.  
Deposited on : 2009-07-24  
Resolution : 2.40 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

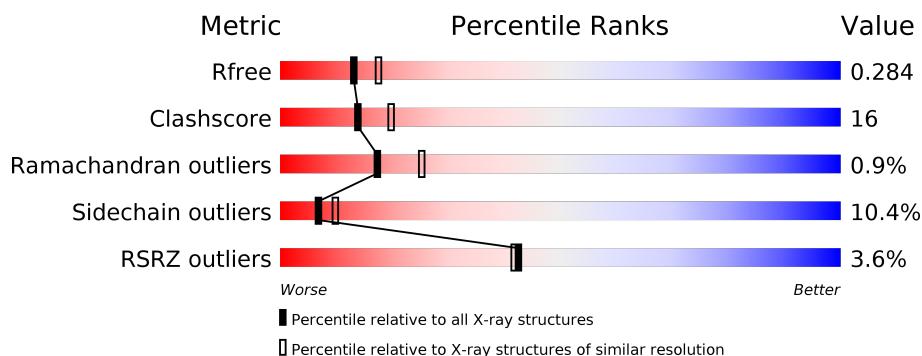
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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))
$R_{free}$	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	266	<div> <div>2%</div> <div> <div></div> <div>62%</div> <div>21%</div> <div>• •</div> <div>14%</div> </div> </div>
2	B	266	<div> <div>2%</div> <div> <div></div> <div>62%</div> <div>24%</div> <div>• •</div> <div>9%</div> </div> </div>
3	C	266	<div> <div>6%</div> <div> <div></div> <div>62%</div> <div>22%</div> <div>•</div> <div>13%</div> </div> </div>

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
5	EDO	B	269	-	-	-	X
5	EDO	B	272	-	-	-	X
6	P6G	B	268	-	-	X	-

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 6286 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 OXA-46 oxacillinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	228	Total	C	N	O	S	0	0	0
			1898	1221	337	338	2			

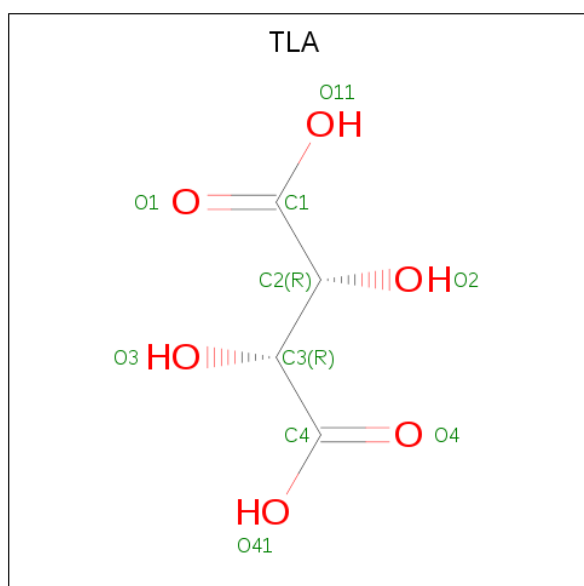
- Molecule 2 is a protein called OXA-46 oxacillinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	242	Total	C	N	O	S	0	0	0
			1996	1280	358	356	2			

- Molecule 3 is a protein called OXA-46 oxacillinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	232	Total	C	N	O	S	0	0	0
			1931	1241	348	340	2			

- Molecule 4 is L(+)-TARTARIC ACID (three-letter code: TLA) (formula: C<sub>4</sub>H<sub>6</sub>O<sub>6</sub>).



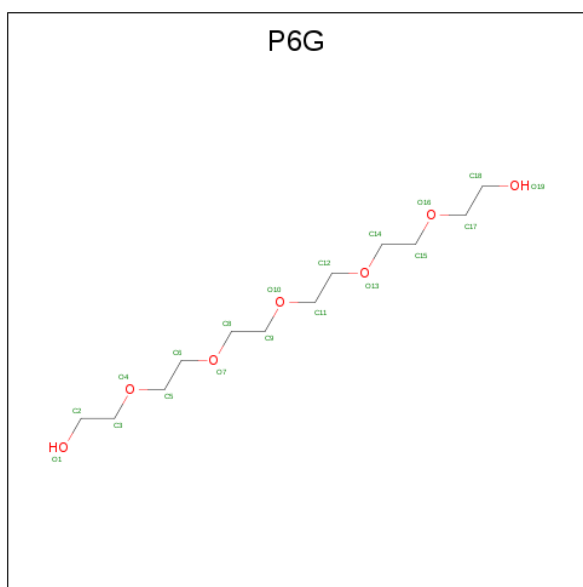
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	4	6		
4	B	1	Total	C	O	0	0
			10	4	6		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



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

- Molecule 6 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula:  $C_{12}H_{26}O_7$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			19	12	7		

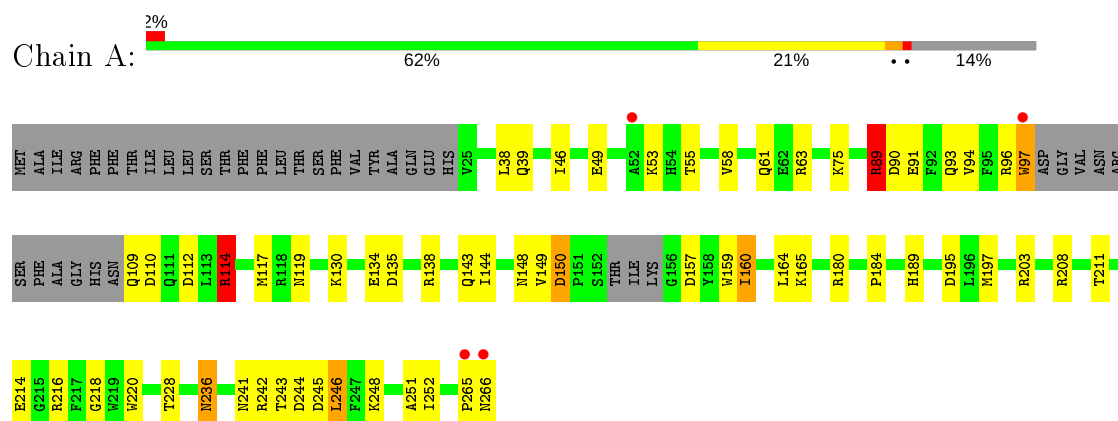
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	154	Total O 154 154	0	0
7	B	120	Total O 120 120	0	0
7	C	124	Total O 124 124	0	0

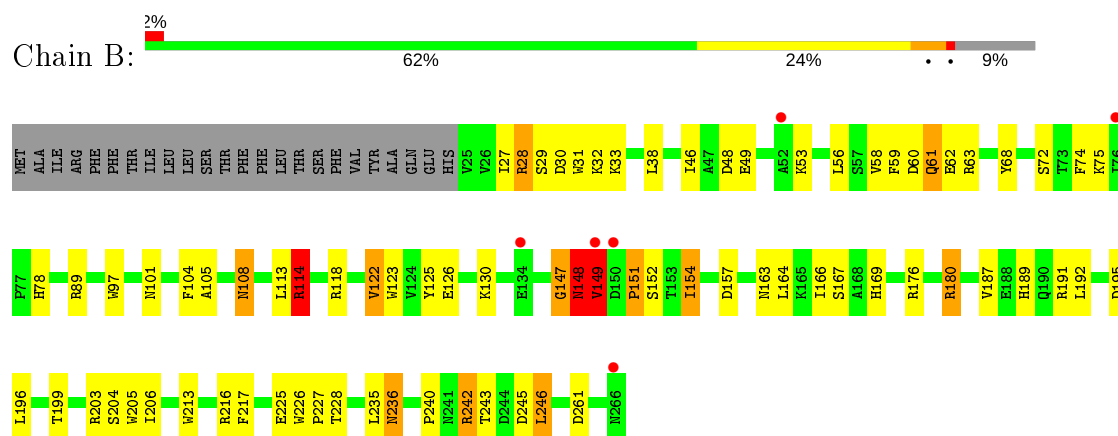
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

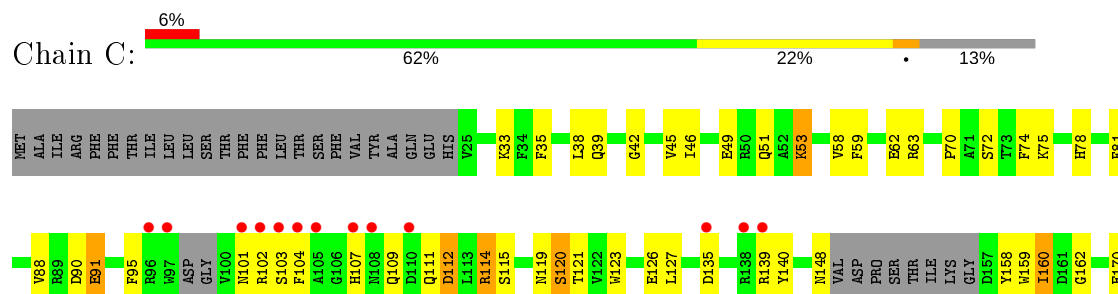
#### • Molecule 1: OXA-46 oxacillinase

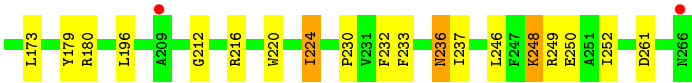


#### • Molecule 2: OXA-46 oxacillinase



#### • Molecule 3: OXA-46 oxacillinase







## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	123.84Å 123.84Å 327.92Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	31.40 – 2.40 31.40 – 2.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (31.40-2.40) 98.0 (31.40-2.40)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.81 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.211 , 0.285 0.211 , 0.284	Depositor DCC
$R_{free}$ test set	3404 reflections (9.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	40.0	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 50.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6286	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: TLA, KCX, P6G, EDO

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	0.85	0/1935	0.90	6/2617 (0.2%)
2	B	0.84	0/2050	0.87	3/2776 (0.1%)
3	C	0.81	0/1969	0.79	0/2661
All	All	0.83	0/5954	0.85	9/8054 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	1
All	All	0	2

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	208	ARG	NE-CZ-NH2	-9.66	115.47	120.30
1	A	208	ARG	NE-CZ-NH1	7.85	124.23	120.30
1	A	114	ARG	NE-CZ-NH2	-7.48	116.56	120.30
2	B	148	ASN	N-CA-C	-6.80	92.64	111.00
2	B	149	VAL	CB-CA-C	-6.05	99.90	111.40
2	B	114	ARG	NE-CZ-NH2	-5.91	117.35	120.30
1	A	112	ASP	CB-CG-OD2	5.29	123.06	118.30
1	A	244	ASP	CB-CG-OD1	5.24	123.02	118.30
1	A	114	ARG	NE-CZ-NH1	5.04	122.82	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	89	ARG	Peptide
2	B	147	GLY	Peptide

## 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	1898	0	1858	42	0
2	B	1996	0	1951	101	0
3	C	1931	0	1884	45	0
4	A	10	0	4	1	0
4	B	10	0	4	1	0
5	A	8	0	12	2	1
5	B	16	0	24	2	0
6	B	19	0	26	21	0
7	A	154	0	0	2	2
7	B	120	0	0	9	0
7	C	124	0	0	4	0
All	All	6286	0	5763	184	2

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 (184) 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)
2:B:123:TRP:HB3	6:B:268:P6G:H122	1.35	1.08
2:B:122:VAL:H	6:B:268:P6G:H61	1.18	1.06
1:A:134:GLU:O	1:A:138:ARG:HG3	1.57	1.05
2:B:206:ILE:CD1	3:C:114:ARG:HH21	1.72	1.03
2:B:148:ASN:ND2	2:B:149:VAL:H	1.55	1.03
2:B:242:ARG:NH1	7:B:335:HOH:O	1.88	1.02
1:A:157:ASP:HB2	1:A:160:ILE:CD1	1.98	0.94
1:A:157:ASP:HB2	1:A:160:ILE:HD11	1.52	0.90
2:B:147:GLY:C	2:B:149:VAL:HG23	1.92	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:58:VAL:HG12	2:B:59:PHE:N	1.86	0.89
2:B:148:ASN:HD22	2:B:149:VAL:H	1.18	0.88
2:B:147:GLY:HA3	2:B:149:VAL:CA	2.02	0.88
2:B:148:ASN:HD22	2:B:148:ASN:N	1.65	0.88
3:C:224:ILE:H	3:C:224:ILE:HD12	1.41	0.84
1:A:96:ARG:O	1:A:97:TRP:HB2	1.77	0.84
2:B:206:ILE:CD1	3:C:114:ARG:NH2	2.40	0.84
1:A:63:ARG:HE	1:A:236:ASN:HD21	1.27	0.83
2:B:147:GLY:HA3	2:B:149:VAL:HA	1.58	0.82
2:B:149:VAL:O	2:B:149:VAL:HG12	1.78	0.81
2:B:148:ASN:HD22	2:B:148:ASN:H	1.29	0.81
3:C:42:GLY:HA3	3:C:237:ILE:HD12	1.61	0.80
2:B:147:GLY:N	2:B:149:VAL:HG22	1.97	0.80
3:C:63:ARG:HE	3:C:236:ASN:HD21	1.30	0.79
1:A:243:THR:HA	1:A:246:LEU:HD22	1.65	0.78
3:C:38:LEU:HD13	3:C:248:LYS:HB3	1.65	0.78
1:A:63:ARG:HE	1:A:236:ASN:ND2	1.79	0.78
2:B:203:ARG:HG2	7:C:324:HOH:O	1.85	0.76
6:B:268:P6G:H121	7:B:356:HOH:O	1.86	0.76
2:B:147:GLY:CA	2:B:149:VAL:HG22	2.16	0.76
2:B:147:GLY:CA	2:B:149:VAL:CG2	2.64	0.75
1:A:49:GLU:OE1	1:A:180:ARG:NH2	2.19	0.74
2:B:242:ARG:HH11	2:B:242:ARG:CG	1.99	0.74
2:B:148:ASN:ND2	2:B:149:VAL:N	2.34	0.74
2:B:147:GLY:O	2:B:149:VAL:HG23	1.87	0.74
2:B:147:GLY:H	2:B:149:VAL:HG22	1.53	0.73
2:B:123:TRP:H	6:B:268:P6G:H92	1.54	0.72
2:B:148:ASN:HD22	2:B:149:VAL:N	1.87	0.71
2:B:49:GLU:OE2	2:B:176:ARG:CZ	2.38	0.70
2:B:108:ASN:H	2:B:108:ASN:HD22	1.40	0.70
3:C:224:ILE:HD12	3:C:224:ILE:N	2.06	0.70
2:B:242:ARG:HH11	2:B:242:ARG:HG2	1.55	0.69
1:A:157:ASP:HB2	1:A:160:ILE:HD12	1.74	0.69
2:B:122:VAL:N	6:B:268:P6G:H61	2.01	0.69
2:B:58:VAL:HG12	2:B:59:PHE:H	1.56	0.69
1:A:114:ARG:NH2	1:A:195:ASP:O	2.26	0.68
2:B:206:ILE:HD13	3:C:114:ARG:HH21	1.58	0.68
2:B:63:ARG:HE	2:B:236:ASN:HD21	1.43	0.67
2:B:148:ASN:ND2	2:B:148:ASN:H	1.92	0.67
2:B:68:TYR:HB3	2:B:217:PHE:CE1	2.29	0.67
1:A:39:GLN:HE22	6:B:268:P6G:H171	1.58	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:180:ARG:CG	2:B:180:ARG:HH11	2.07	0.67
3:C:63:ARG:HE	3:C:236:ASN:ND2	1.93	0.67
2:B:154:ILE:O	2:B:154:ILE:HG23	1.94	0.67
2:B:63:ARG:HE	2:B:236:ASN:ND2	1.93	0.65
2:B:148:ASN:HD21	2:B:164:LEU:HD12	1.62	0.65
2:B:187:VAL:O	2:B:191:ARG:HG3	1.95	0.65
2:B:148:ASN:ND2	2:B:148:ASN:N	2.39	0.64
2:B:58:VAL:CG1	2:B:59:PHE:N	2.57	0.64
1:A:63:ARG:HH21	1:A:236:ASN:HD22	1.45	0.64
1:A:189:HIS:HD2	7:A:278:HOH:O	1.80	0.64
1:A:89:ARG:H	1:A:93:GLN:NE2	1.95	0.64
2:B:154:ILE:O	2:B:154:ILE:CG2	2.46	0.64
1:A:248:KCX:CX	7:B:356:HOH:O	2.46	0.63
3:C:114:ARG:HD3	3:C:196:LEU:HD23	1.81	0.62
3:C:261:ASP:HB3	7:C:306:HOH:O	1.99	0.62
3:C:38:LEU:HB3	3:C:248:LYS:HD3	1.81	0.61
2:B:147:GLY:C	2:B:149:VAL:CG2	2.67	0.61
2:B:149:VAL:CG1	2:B:149:VAL:O	2.47	0.61
3:C:53:LYS:H	3:C:53:LYS:HZ2	1.47	0.61
2:B:147:GLY:HA3	2:B:149:VAL:N	2.15	0.61
2:B:114:ARG:HD3	7:C:278:HOH:O	2.01	0.60
2:B:48:ASP:C	2:B:48:ASP:OD1	2.39	0.60
2:B:206:ILE:HD11	3:C:114:ARG:HH21	1.64	0.58
2:B:180:ARG:HG2	2:B:180:ARG:HH11	1.66	0.58
1:A:245:ASP:OD1	1:A:248:KCX:HE2	2.03	0.58
1:A:265:PRO:O	1:A:266:ASN:HB2	2.04	0.58
2:B:206:ILE:HD13	3:C:114:ARG:NH2	2.16	0.58
1:A:241:ASN:ND2	2:B:157:ASP:HB2	2.19	0.57
2:B:28:ARG:HG3	2:B:30:ASP:OD1	2.04	0.57
2:B:147:GLY:HA3	2:B:149:VAL:CG2	2.34	0.57
2:B:206:ILE:HD12	3:C:114:ARG:NH2	2.19	0.55
2:B:180:ARG:NH1	2:B:180:ARG:CG	2.69	0.55
2:B:58:VAL:CG1	2:B:59:PHE:H	2.19	0.55
1:A:157:ASP:CB	1:A:160:ILE:HD11	2.30	0.55
1:A:148:ASN:OD1	1:A:150:ASP:HB3	2.07	0.55
1:A:94:VAL:HG13	1:A:110:ASP:HB3	1.89	0.55
2:B:74:PHE:O	2:B:78:HIS:HB2	2.06	0.55
2:B:226:TRP:HB3	2:B:227:PRO:HD2	1.89	0.54
6:B:268:P6G:C12	7:B:356:HOH:O	2.52	0.54
2:B:226:TRP:HB3	2:B:227:PRO:CD	2.37	0.54
2:B:240:PRO:HD2	2:B:245:ASP:OD2	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:PRO:O	1:A:266:ASN:CB	2.56	0.53
2:B:105:ALA:HB3	6:B:268:P6G:H21	1.89	0.53
2:B:49:GLU:OE2	2:B:176:ARG:NH1	2.41	0.53
1:A:242:ARG:HH22	2:B:216:ARG:HG3	1.73	0.53
2:B:89:ARG:HG3	7:B:288:HOH:O	2.09	0.53
3:C:212:GLY:O	3:C:249:ARG:NH1	2.41	0.52
3:C:35:PHE:CD2	3:C:237:ILE:HD11	2.44	0.52
1:A:117:MET:HG3	5:A:268:EDO:H22	1.91	0.52
3:C:38:LEU:HD12	3:C:252:ILE:HG13	1.92	0.52
3:C:112:ASP:HB3	3:C:115:SER:H	1.75	0.52
1:A:38:LEU:HD12	1:A:252:ILE:HG13	1.92	0.51
3:C:111:GLN:HG3	3:C:121:THR:HG21	1.93	0.51
3:C:179:TYR:CE2	3:C:230:PRO:HG3	2.45	0.51
2:B:72:SER:HB2	4:B:267:TLA:O2	2.09	0.51
1:A:251:ALA:HB1	2:B:101:ASN:HD21	1.76	0.51
2:B:151:PRO:HB3	2:B:163:ASN:HB3	1.93	0.51
2:B:189:HIS:HD2	7:B:289:HOH:O	1.94	0.50
2:B:105:ALA:HB3	6:B:268:P6G:C2	2.41	0.50
3:C:261:ASP:CB	7:C:306:HOH:O	2.58	0.50
3:C:74:PHE:O	3:C:78:HIS:HB2	2.11	0.50
3:C:58:VAL:HG12	3:C:59:PHE:N	2.26	0.49
1:A:75:LYS:NZ	1:A:119:ASN:O	2.45	0.49
2:B:205:TRP:HA	2:B:225:GLU:O	2.13	0.48
1:A:63:ARG:HH21	1:A:236:ASN:ND2	2.10	0.48
2:B:123:TRP:H	6:B:268:P6G:C9	2.25	0.48
3:C:236:ASN:HD22	3:C:236:ASN:C	2.17	0.48
2:B:123:TRP:HD1	6:B:268:P6G:C8	2.27	0.48
2:B:122:VAL:H	6:B:268:P6G:C6	2.07	0.47
6:B:268:P6G:H32	7:B:393:HOH:O	2.14	0.47
2:B:118:ARG:HA	5:B:270:EDO:H11	1.96	0.47
1:A:148:ASN:HB3	1:A:164:LEU:HD12	1.97	0.47
2:B:147:GLY:C	2:B:149:VAL:N	2.63	0.47
2:B:123:TRP:HB2	6:B:268:P6G:H181	1.97	0.47
2:B:196:LEU:O	5:B:270:EDO:O1	2.33	0.47
1:A:143:GLN:NE2	7:A:368:HOH:O	2.47	0.47
3:C:35:PHE:HD2	3:C:237:ILE:HD11	1.80	0.47
2:B:123:TRP:HB3	6:B:268:P6G:C12	2.24	0.46
2:B:147:GLY:HA3	2:B:149:VAL:HG22	1.95	0.46
2:B:108:ASN:HD22	2:B:108:ASN:N	2.11	0.46
2:B:147:GLY:CA	2:B:149:VAL:N	2.78	0.46
3:C:88:VAL:HG23	3:C:95:PHE:HZ	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:176:ARG:HG2	2:B:180:ARG:HE	1.79	0.46
2:B:97:TRP:CH2	6:B:268:P6G:H142	2.51	0.46
2:B:123:TRP:HD1	6:B:268:P6G:H92	1.82	0.45
1:A:211:THR:HG22	1:A:220:TRP:CD1	2.50	0.45
1:A:89:ARG:H	1:A:93:GLN:HE21	1.61	0.45
2:B:213:TRP:CG	2:B:246:LEU:HD11	2.52	0.45
1:A:148:ASN:HB2	1:A:165:LYS:O	2.17	0.45
3:C:104:PHE:HB3	3:C:107:HIS:CD2	2.51	0.45
3:C:81:PHE:CE1	3:C:140:TYR:HB3	2.52	0.45
2:B:123:TRP:CD1	6:B:268:P6G:H92	2.51	0.44
2:B:60:ASP:O	2:B:62:GLU:N	2.51	0.44
2:B:204:SER:HB2	7:B:336:HOH:O	2.17	0.44
3:C:107:HIS:HE1	3:C:119:ASN:O	2.01	0.44
3:C:90:ASP:HB2	3:C:91:GLU:OE1	2.17	0.44
3:C:70:PRO:HB2	3:C:74:PHE:HB2	2.00	0.44
1:A:135:ASP:O	1:A:138:ARG:HB2	2.18	0.43
2:B:60:ASP:O	2:B:61:GLN:C	2.56	0.43
1:A:157:ASP:HB3	1:A:159:TRP:CZ2	2.54	0.43
2:B:199:THR:HG21	7:B:299:HOH:O	2.18	0.43
3:C:159:TRP:CD1	3:C:160:ILE:HG13	2.54	0.43
2:B:123:TRP:HD1	6:B:268:P6G:C9	2.32	0.43
3:C:224:ILE:H	3:C:224:ILE:CD1	2.22	0.43
2:B:166:ILE:HG12	2:B:167:SER:H	1.84	0.43
2:B:126:GLU:OE2	2:B:157:ASP:OD1	2.37	0.43
3:C:75:KCX:HE3	3:C:120:SER:HA	2.01	0.42
3:C:45:VAL:O	3:C:233:PHE:HA	2.19	0.42
2:B:28:ARG:HG2	2:B:31:TRP:CE2	2.55	0.42
2:B:75:LYS:HE2	2:B:125:TYR:CE1	2.55	0.42
3:C:46:ILE:HD13	3:C:233:PHE:HB3	2.01	0.42
2:B:114:ARG:NH2	2:B:195:ASP:O	2.48	0.42
2:B:104:PHE:CE2	6:B:268:P6G:H82	2.55	0.41
2:B:176:ARG:CG	2:B:180:ARG:HE	2.33	0.41
3:C:170:GLU:HA	3:C:173:LEU:HD12	2.03	0.41
1:A:197:MET:HA	5:A:268:EDO:H21	2.02	0.41
3:C:158:TYR:HA	3:C:162:GLY:HA3	2.01	0.41
3:C:220:TRP:CD2	3:C:250:GLU:HG2	2.56	0.41
3:C:49:GLU:OE1	3:C:180:ARG:NH2	2.53	0.41
4:A:267:TLA:O3	4:A:267:TLA:O11	2.37	0.41
3:C:88:VAL:HG23	3:C:95:PHE:CZ	2.55	0.41
2:B:192:LEU:O	2:B:196:LEU:HG	2.21	0.41
6:B:268:P6G:H61	6:B:268:P6G:H91	1.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:VAL:HG11	1:A:61:GLN:HA	2.03	0.41
3:C:230:PRO:HG2	3:C:232:PHE:CE1	2.56	0.41
1:A:144:ILE:HG22	1:A:184:PRO:HD2	2.03	0.40
1:A:218:GLY:O	1:A:236:ASN:HA	2.20	0.40
2:B:61:GLN:HE22	2:B:169:HIS:CE1	2.40	0.40
3:C:123:TRP:HA	3:C:126:GLU:HB2	2.03	0.40
1:A:214:GLU:OE2	1:A:216:ARG:NH1	2.54	0.40
2:B:108:ASN:H	2:B:108:ASN:ND2	2.15	0.40
1:A:96:ARG:O	1:A:97:TRP:CB	2.60	0.40
1:A:94:VAL:CG1	1:A:110:ASP:HB3	2.52	0.40
2:B:243:THR:HA	2:B:246:LEU:HD22	2.04	0.40

All (2) 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)
7:A:305:HOH:O	7:A:360:HOH:O[5_555]	2.15	0.05
5:A:268:EDO:O1	7:A:286:HOH:O[5_555]	2.18	0.02

## 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	221/266 (83%)	210 (95%)	10 (4%)	1 (0%)	29	41
2	B	240/266 (90%)	222 (92%)	13 (5%)	5 (2%)	7	8
3	C	225/266 (85%)	207 (92%)	18 (8%)	0	100	100
All	All	686/798 (86%)	639 (93%)	41 (6%)	6 (1%)	17	25

All (6) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
2	B	149	VAL
2	B	29	SER
2	B	32	LYS
2	B	61	GLN
2	B	151	PRO
1	A	149	VAL

### 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	195/228 (86%)	179 (92%)	16 (8%)	11	17
2	B	206/229 (90%)	184 (89%)	22 (11%)	6	9
3	C	196/228 (86%)	172 (88%)	24 (12%)	5	6
All	All	597/685 (87%)	535 (90%)	62 (10%)	7	10

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	ILE
1	A	53	LYS
1	A	55	THR
1	A	89	ARG
1	A	90	ASP
1	A	91	GLU
1	A	97	TRP
1	A	109	GLN
1	A	114	ARG
1	A	130	LYS
1	A	150	ASP
1	A	160	ILE
1	A	203	ARG
1	A	228	THR
1	A	236	ASN
1	A	246	LEU
2	B	27	ILE

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Mol	Chain	Res	Type
2	B	28	ARG
2	B	33	LYS
2	B	38	LEU
2	B	46	ILE
2	B	53	LYS
2	B	56	LEU
2	B	108	ASN
2	B	113	LEU
2	B	114	ARG
2	B	122	VAL
2	B	130	LYS
2	B	148	ASN
2	B	152	SER
2	B	154	ILE
2	B	180	ARG
2	B	228	THR
2	B	235	LEU
2	B	236	ASN
2	B	242	ARG
2	B	246	LEU
2	B	261	ASP
3	C	33	LYS
3	C	39	GLN
3	C	51	GLN
3	C	53	LYS
3	C	62	GLU
3	C	72	SER
3	C	91	GLU
3	C	101	ASN
3	C	102	ARG
3	C	103	SER
3	C	109	GLN
3	C	112	ASP
3	C	114	ARG
3	C	120	SER
3	C	127	LEU
3	C	135	ASP
3	C	139	ARG
3	C	148	ASN
3	C	160	ILE
3	C	216	ARG
3	C	224	ILE

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Mol	Chain	Res	Type
3	C	236	ASN
3	C	246	LEU
3	C	248	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	GLN
1	A	143	GLN
1	A	169	HIS
1	A	189	HIS
1	A	236	ASN
1	A	241	ASN
2	B	101	ASN
2	B	108	ASN
2	B	109	GLN
2	B	148	ASN
2	B	169	HIS
2	B	236	ASN
3	C	39	GLN
3	C	107	HIS
3	C	109	GLN
3	C	169	HIS
3	C	189	HIS
3	C	236	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	KCX	C	75	3	7,11,12	0.95	0	4,12,14	1.63	1 (25%)
1	KCX	A	248	1	7,11,12	0.67	0	4,12,14	0.56	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
3	KCX	C	75	3	-	1/7/10/12	-
1	KCX	A	248	1	-	1/7/10/12	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	75	KCX	CE-NZ-CX	3.15	128.28	122.95

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	248	KCX	CG-CD-CE-NZ
3	C	75	KCX	CG-CD-CE-NZ

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	75	KCX	1	0
1	A	248	KCX	2	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

9 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	TLA	A	267	-	3,9,9	0.86	0	6,12,12	1.09	0
5	EDO	A	268	-	3,3,3	0.59	0	2,2,2	0.24	0
4	TLA	B	267	-	3,9,9	0.51	0	6,12,12	1.27	1 (16%)
5	EDO	B	270	-	3,3,3	0.30	0	2,2,2	0.85	0
5	EDO	A	269	-	3,3,3	0.57	0	2,2,2	0.61	0
5	EDO	B	269	-	3,3,3	0.49	0	2,2,2	0.27	0
5	EDO	B	272	-	3,3,3	0.52	0	2,2,2	0.18	0
5	EDO	B	271	-	3,3,3	0.44	0	2,2,2	0.38	0
6	P6G	B	268	-	18,18,18	0.70	0	17,17,17	0.78	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
4	TLA	A	267	-	-	4/4/12/12	-
5	EDO	A	268	-	-	0/1/1/1	-
4	TLA	B	267	-	-	0/4/12/12	-
5	EDO	B	270	-	-	1/1/1/1	-
5	EDO	A	269	-	-	0/1/1/1	-
5	EDO	B	269	-	-	1/1/1/1	-
5	EDO	B	272	-	-	1/1/1/1	-
5	EDO	B	271	-	-	1/1/1/1	-
6	P6G	B	268	-	-	13/16/16/16	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	267	TLA	O2-C2-C1	-2.48	105.14	111.10

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	267	TLA	C1-C2-C3-O3
4	A	267	TLA	O2-C2-C3-C4
6	B	268	P6G	C9-C8-O7-C6
6	B	268	P6G	O16-C17-C18-O19
6	B	268	P6G	O10-C11-C12-O13
5	B	269	EDO	O1-C1-C2-O2
4	A	267	TLA	C1-C2-C3-C4
4	A	267	TLA	O2-C2-C3-O3
6	B	268	P6G	O4-C5-C6-O7
5	B	272	EDO	O1-C1-C2-O2
6	B	268	P6G	C8-C9-O10-C11
6	B	268	P6G	C14-C15-O16-C17
6	B	268	P6G	C15-C14-O13-C12
6	B	268	P6G	C5-C6-O7-C8
6	B	268	P6G	C2-C3-O4-C5
5	B	270	EDO	O1-C1-C2-O2
6	B	268	P6G	C12-C11-O10-C9
6	B	268	P6G	C6-C5-O4-C3
6	B	268	P6G	O13-C14-C15-O16
5	B	271	EDO	O1-C1-C2-O2
6	B	268	P6G	C11-C12-O13-C14

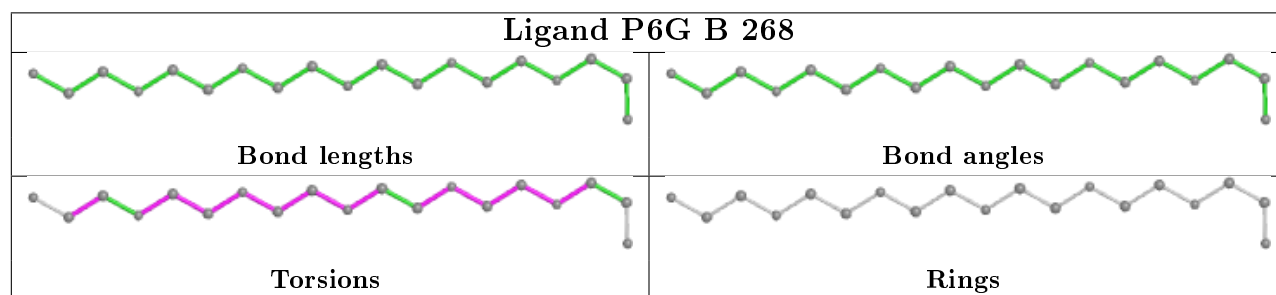
There are no ring outliers.

5 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	267	TLA	1	0
5	A	268	EDO	2	1
4	B	267	TLA	1	0
5	B	270	EDO	2	0
6	B	268	P6G	21	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 ⓘ

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	227/266 (85%)	-0.14	4 (1%) 68 66	17, 32, 51, 65	0
2	B	242/266 (90%)	-0.02	6 (2%) 57 55	27, 41, 58, 68	0
3	C	231/266 (86%)	0.25	15 (6%) 18 17	27, 43, 71, 90	0
All	All	700/798 (87%)	0.03	25 (3%) 42 42	17, 38, 62, 90	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	104	PHE	6.2
2	B	266	ASN	4.4
2	B	52	ALA	3.9
3	C	139	ARG	3.8
3	C	96	ARG	3.7
3	C	107	HIS	3.2
1	A	52	ALA	3.1
3	C	101	ASN	3.1
3	C	266	ASN	3.0
3	C	103	SER	3.0
3	C	110	ASP	3.0
3	C	108	ASN	2.8
2	B	150	ASP	2.8
1	A	265	PRO	2.8
3	C	105	ALA	2.7
1	A	97	TRP	2.7
3	C	102	ARG	2.6
1	A	266	ASN	2.6
3	C	209	ALA	2.6
2	B	134	GLU	2.1
3	C	135	ASP	2.1
3	C	138	ARG	2.1
2	B	76	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	149	VAL	2.0
3	C	97	TRP	2.0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	KCX	C	75	12/13	0.79	0.27	39,44,60,60	0
1	KCX	A	248	12/13	0.86	0.23	27,27,48,48	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

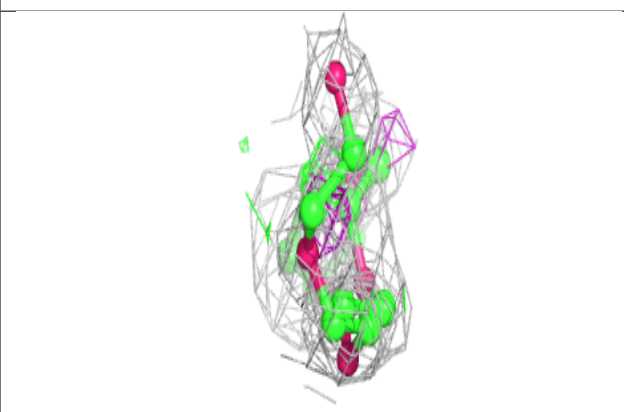
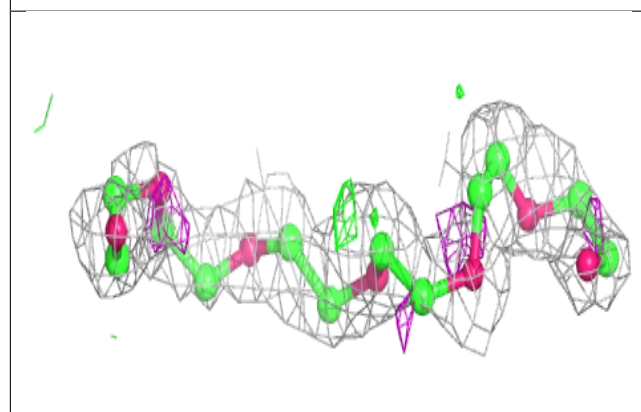
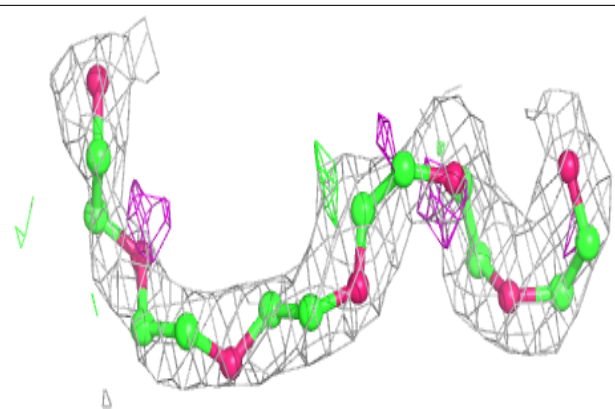
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	EDO	B	269	4/4	0.57	0.49	89,91,91,91	0
5	EDO	B	272	4/4	0.67	0.45	67,69,71,73	0
6	P6G	B	268	19/19	0.81	0.29	40,45,50,50	0
5	EDO	A	269	4/4	0.81	0.38	42,43,46,48	0
5	EDO	B	270	4/4	0.83	0.31	45,45,46,50	0
4	TLA	A	267	10/10	0.91	0.21	53,59,61,61	0
5	EDO	A	268	4/4	0.91	0.21	33,35,35,41	0
5	EDO	B	271	4/4	0.94	0.16	52,52,53,53	0
4	TLA	B	267	10/10	0.97	0.13	28,33,36,38	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 B 268:**

$2mF_o - DF_c$  (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.