



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:34 PM UTC

PDB ID : 4Z77 / pdb_00004z77
Title : Weak TCR binding to an unstable insulin epitope drives type 1 diabetes
Authors : Rizkallah, P.J.; Cole, D.K.
Deposited on : 2015-04-06
Resolution : 1.85 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

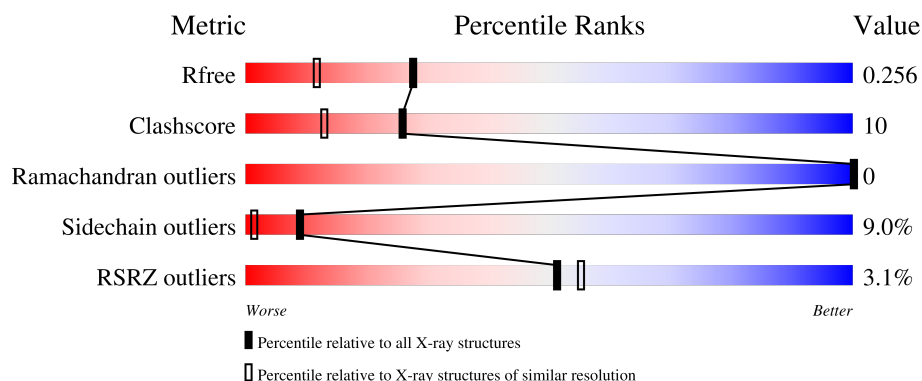
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	277	5% 77% 19% .
1	D	277	3% 78% 17% .
2	B	100	2% 81% 16% ..
2	E	100	% 82% 16% .
3	C	9	78% 11% 11%

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Mol	Chain	Length	Quality of chain
3	F	9	 67% 33%

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
4	GOL	A	301	-	-	X	-
7	SO4	D	308	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6964 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 H-2 class I histocompatibility antigen, K-D alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	277	Total	C	N	O	S	0	0	0
			2287	1449	406	424	8			
1	D	277	Total	C	N	O	S	0	1	0
			2296	1454	407	427	8			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP P01902
A	114	HIS	GLN	conflict	UNP P01902
A	276	PRO	-	expression tag	UNP P01902
D	0	MET	-	initiating methionine	UNP P01902
D	114	HIS	GLN	conflict	UNP P01902
D	276	PRO	-	expression tag	UNP P01902

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			
2	E	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P61769
E	0	MET	-	initiating methionine	UNP P61769

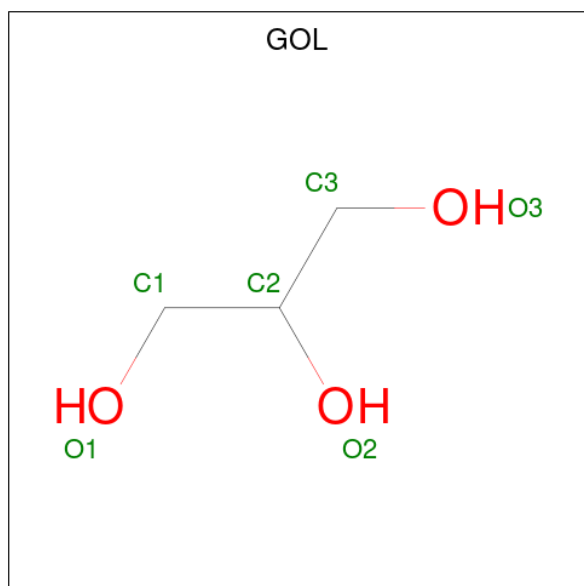
- Molecule 3 is a protein called Insulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	S	0	0	0
			73	47	12	13	1			
3	F	9	Total	C	N	O	S	0	0	0
			73	47	12	13	1			

There are 2 discrepancies between the modelled and reference sequences:

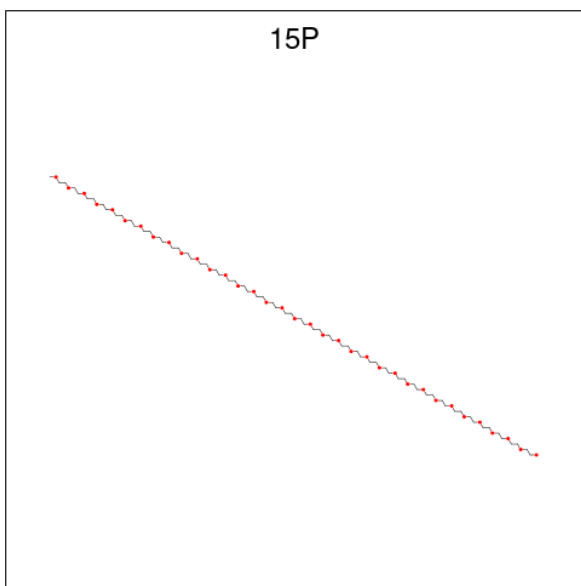
Chain	Residue	Modelled	Actual	Comment	Reference
C	9	VAL	GLY	engineered mutation	UNP P01308
F	9	VAL	GLY	engineered mutation	UNP P01308

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



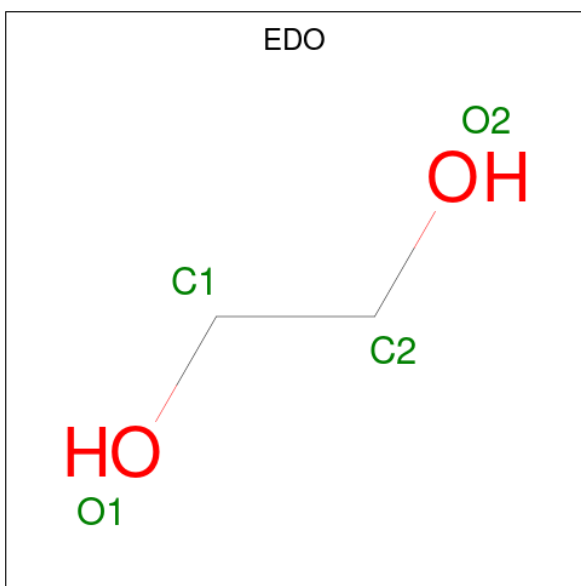
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is POLYETHYLENE GLYCOL (N=34) (CCD ID: 15P) (formula: $C_{69}H_{140}O_{35}$).



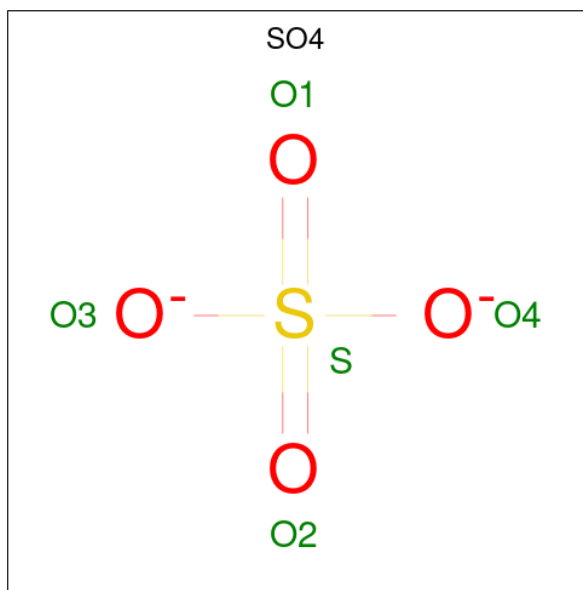
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			10	6	4		
5	D	1	Total	C	O	0	0
			10	6	4		
5	D	1	Total	C	O	0	0
			10	6	4		

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 7 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total O S 5 4 1	0	0
7	A	1	Total O S 5 4 1	0	0
7	D	1	Total O S 5 4 1	0	0
7	E	1	Total O S 5 4 1	0	0
7	E	1	Total O S 5 4 1	0	0
7	E	1	Total O S 5 4 1	0	0

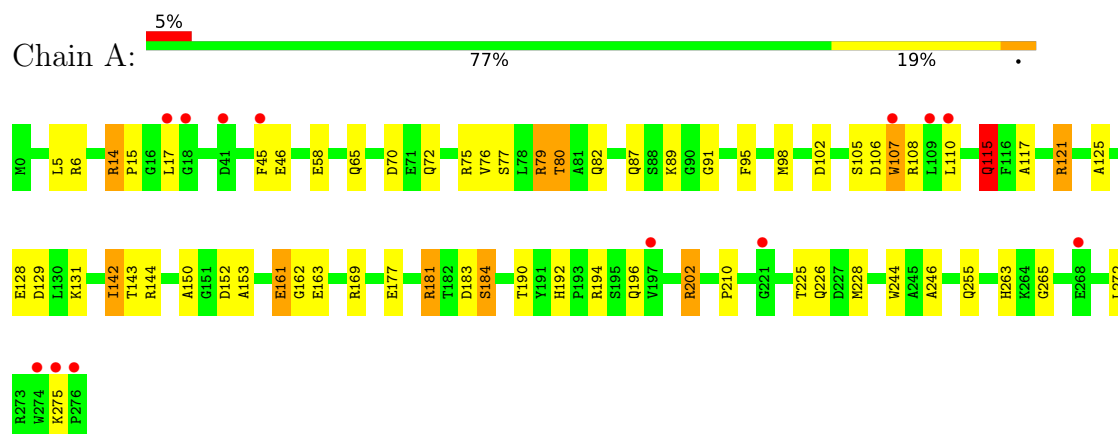
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	117	Total O 117 117	0	0
8	B	71	Total O 71 71	0	0
8	C	4	Total O 4 4	0	0
8	D	147	Total O 147 147	0	0
8	E	65	Total O 65 65	0	0
8	F	7	Total O 7 7	0	0

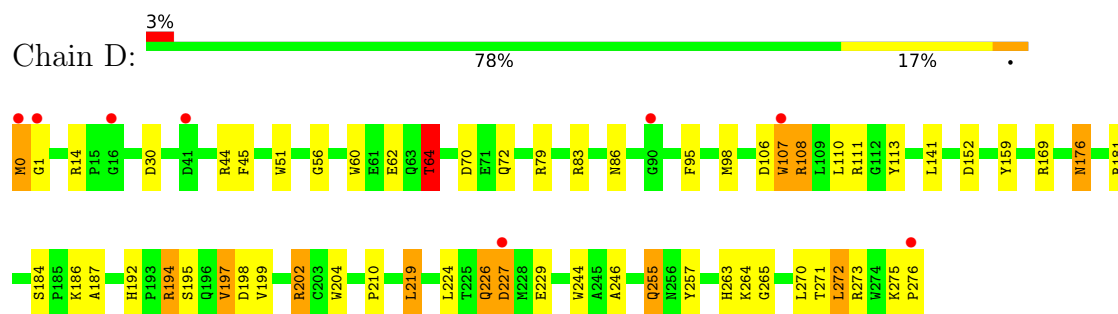
3 Residue-property plots [i](#)

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.

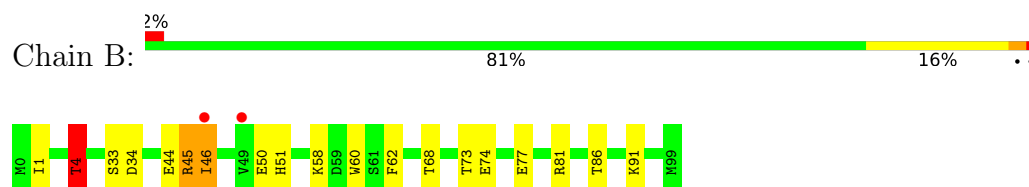
- Molecule 1: H-2 class I histocompatibility antigen, K-D alpha chain



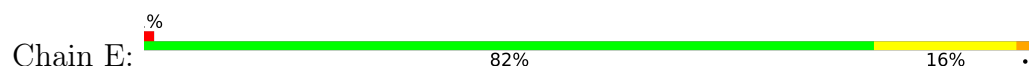
- Molecule 1: H-2 class I histocompatibility antigen, K-D alpha chain

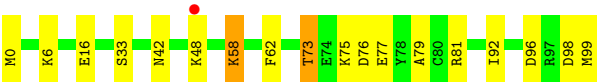


- Molecule 2: Beta-2-microglobulin

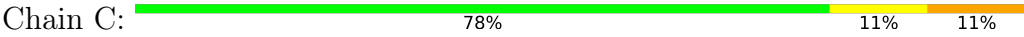


- Molecule 2: Beta-2-microglobulin

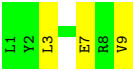




● Molecule 3: Insulin



● Molecule 3: Insulin



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	66.15Å 84.53Å 72.86Å 90.00° 106.86° 90.00°	Depositor
Resolution (Å)	37.10 – 1.85 37.10 – 1.85	Depositor EDS
% Data completeness (in resolution range)	92.6 (37.10-1.85) 92.6 (37.10-1.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.21	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.77 (at 1.85Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.206 , 0.253 0.212 , 0.256	Depositor DCC
R_{free} test set	3073 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	20.1	Xtriage
Anisotropy	0.664	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 46.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6964	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.60% 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: EDO, SO4, GOL, 15P

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.04	3/2357 (0.1%)	1.07	6/3205 (0.2%)
1	D	1.03	2/2366 (0.1%)	1.08	6/3217 (0.2%)
2	B	1.02	0/860	1.05	2/1162 (0.2%)
2	E	0.98	0/860	1.00	0/1162
3	C	1.35	0/73	1.13	0/96
3	F	1.18	0/73	1.29	0/96
All	All	1.03	5/6589 (0.1%)	1.07	14/8938 (0.2%)

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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	1	GLY	N-CA	6.76	1.53	1.44
1	A	115	GLN	CA-C	-6.57	1.44	1.52
1	A	142	ILE	N-CA	-5.60	1.40	1.46
1	A	115	GLN	N-CA	5.45	1.52	1.45
1	D	227	ASP	CB-CG	5.32	1.65	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	163	GLU	N-CA-C	7.85	120.53	111.11
1	A	161	GLU	O-C-N	-7.01	113.50	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	202	ARG	NE-CZ-NH2	-6.64	113.22	119.20
1	D	56	GLY	CA-C-N	6.62	126.87	119.32
1	D	56	GLY	C-N-CA	6.62	126.87	119.32
1	A	161	GLU	N-CA-C	-6.57	100.18	110.36
1	A	128	GLU	N-CA-CB	-6.20	100.34	110.14
1	A	202	ARG	NE-CZ-NH2	-5.92	113.88	119.20
1	D	64	THR	N-CA-CB	5.57	118.31	110.12
1	D	152	ASP	N-CA-C	5.33	117.84	111.71
2	B	73	THR	CB-CA-C	-5.32	99.77	110.30
1	D	202	ARG	NE-CZ-NH1	5.17	126.67	121.50
2	B	4	THR	CB-CA-C	5.15	116.13	108.87
1	A	142	ILE	CA-CB-CG2	5.11	119.19	110.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	17	LEU	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	2287	0	2153	47	1
1	D	2296	0	2158	47	0
2	B	837	0	803	15	1
2	E	837	0	803	12	0
3	C	73	0	78	3	0
3	F	73	0	78	2	0
4	A	12	0	16	5	0
4	B	12	0	16	3	0
4	D	12	0	16	1	0
4	E	6	0	8	0	0
5	A	10	0	13	3	0
5	D	20	0	26	5	0
6	A	12	0	17	3	0
6	B	12	0	18	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	4	0	6	0	0
6	D	12	0	18	1	0
6	E	8	0	12	1	0
7	A	10	0	0	0	0
7	D	5	0	0	4	0
7	E	15	0	0	0	0
8	A	117	0	0	10	0
8	B	71	0	0	4	0
8	C	4	0	0	0	0
8	D	147	0	0	9	0
8	E	65	0	0	1	0
8	F	7	0	0	0	0
All	All	6964	0	6239	122	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (122) 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)
8:A:455:HOH:O	1:D:227:ASP:HB2	1.67	0.95
1:D:202:ARG:HD2	1:D:244:TRP:CD2	2.07	0.90
1:A:202:ARG:HD2	1:A:244:TRP:CD2	2.08	0.88
1:A:75:ARG:O	1:A:79:ARG:NH1	2.08	0.86
1:D:86:ASN:ND2	7:D:308:SO4:O3	2.12	0.83
1:A:6:ARG:NH2	1:A:102:ASP:OD1	2.16	0.78
1:A:202:ARG:HD2	1:A:244:TRP:CE3	2.22	0.75
1:D:255:GLN:O	1:D:273:ARG:NH1	2.22	0.72
2:B:51:HIS:HE1	4:B:302:GOL:H32	1.54	0.72
1:D:194:ARG:HG2	1:D:194:ARG:HH11	1.55	0.71
2:B:81:ARG:NH1	8:B:402:HOH:O	2.26	0.69
1:D:202:ARG:HD2	1:D:244:TRP:CE3	2.26	0.69
1:A:263:HIS:CD2	1:A:265:GLY:H	2.11	0.68
1:A:115:GLN:HG2	1:A:125:ALA:HB1	1.77	0.67
8:D:430:HOH:O	2:E:58:LYS:HD3	1.95	0.66
1:D:86:ASN:ND2	7:D:308:SO4:S	2.67	0.65
1:D:62[A]:GLU:HG3	8:D:517:HOH:O	1.96	0.65
1:D:263:HIS:CD2	1:D:265:GLY:H	2.16	0.63
1:A:121:ARG:HD3	8:A:478:HOH:O	1.98	0.63
1:D:108:ARG:HA	1:D:108:ARG:HE	1.63	0.63
1:A:5:LEU:HD21	6:A:306:EDO:H22	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:306:EDO:H12	3:C:1:LEU:C	2.25	0.62
1:A:115:GLN:HG2	1:A:125:ALA:CB	2.30	0.62
8:D:430:HOH:O	2:E:58:LYS:CD	2.48	0.61
1:D:106:ASP:O	1:D:107:TRP:HB2	2.01	0.60
5:D:304:15P:C4	5:D:304:15P:OXT	2.48	0.60
1:D:51:TRP:HA	4:D:301:GOL:H2	1.82	0.60
1:D:108:ARG:HA	1:D:108:ARG:NE	2.17	0.60
5:D:303:15P:C3	3:F:7:GLU:OE1	2.50	0.60
1:A:131:LYS:HA	1:A:153:ALA:HB1	1.83	0.59
2:B:51:HIS:CE1	4:B:302:GOL:H32	2.37	0.59
1:A:150:ALA:HB1	4:A:301:GOL:H32	1.84	0.59
2:B:34:ASP:HB2	8:B:453:HOH:O	2.02	0.59
1:A:150:ALA:CB	4:A:301:GOL:H12	2.31	0.59
1:A:202:ARG:CD	1:A:244:TRP:CE3	2.85	0.59
1:D:60:TRP:O	1:D:64:THR:HG23	2.03	0.59
2:E:42:ASN:OD1	2:E:77:GLU:HG2	2.03	0.58
1:D:62[A]:GLU:CG	8:D:517:HOH:O	2.52	0.58
2:B:46:ILE:HD13	2:B:68:THR:HG21	1.84	0.58
2:B:51:HIS:HE1	4:B:302:GOL:C3	2.16	0.58
1:D:192:HIS:CE1	2:E:98:ASP:HB3	2.39	0.58
1:D:275:LYS:O	1:D:276:PRO:C	2.47	0.57
2:B:46:ILE:CD1	2:B:68:THR:HG21	2.36	0.56
1:A:14:ARG:NH2	8:A:404:HOH:O	2.39	0.56
1:A:106:ASP:O	1:A:107:TRP:HB2	2.05	0.55
1:A:263:HIS:HD2	1:A:265:GLY:H	1.53	0.55
2:E:79:ALA:HB3	6:E:103:EDO:H21	1.88	0.54
1:A:77:SER:HA	1:A:80:THR:CG2	2.38	0.54
2:E:96:ASP:HB3	2:E:99:MET:HE2	1.90	0.54
1:A:150:ALA:HB1	4:A:301:GOL:H12	1.91	0.53
1:D:202:ARG:CD	1:D:244:TRP:CE3	2.91	0.53
1:D:210:PRO:O	1:D:263:HIS:HE1	1.92	0.52
1:D:195:SER:OG	1:D:198:ASP:HB2	2.10	0.52
1:D:270:LEU:HD23	1:D:271:THR:N	2.26	0.51
1:A:161:GLU:O	1:A:162:GLY:C	2.50	0.51
1:A:210:PRO:O	1:A:263:HIS:HE1	1.93	0.51
1:D:226:GLN:HE21	1:D:226:GLN:H	1.59	0.51
1:A:58:GLU:OE2	1:D:226:GLN:HA	2.10	0.50
1:D:229:GLU:OE2	8:D:401:HOH:O	2.20	0.50
1:A:115:GLN:HG3	8:A:431:HOH:O	2.10	0.50
1:A:255:GLN:H	1:A:255:GLN:CD	2.18	0.50
1:A:46:GLU:HG2	5:A:303:15P:C2	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:86:ASN:ND2	7:D:308:SO4:O2	2.45	0.50
1:D:30:ASP:OD1	6:D:305:EDO:H12	2.11	0.49
1:D:202:ARG:HD3	1:D:246:ALA:HB2	1.95	0.49
2:E:0:MET:N	8:E:205:HOH:O	2.45	0.49
1:D:219:LEU:HG	1:D:257:TYR:CE2	2.47	0.49
5:D:304:15P:H14	5:D:304:15P:O3	2.12	0.49
1:D:219:LEU:HG	1:D:257:TYR:CZ	2.48	0.48
1:A:196:GLN:H	1:A:196:GLN:CD	2.22	0.48
1:D:159:TYR:CD2	3:F:3:LEU:HD22	2.48	0.48
1:D:270:LEU:HD22	1:D:272:LEU:CD1	2.44	0.48
1:A:76:VAL:O	1:A:80:THR:HG22	2.13	0.48
1:A:91:GLY:HA3	8:A:423:HOH:O	2.13	0.48
1:D:169:ARG:HD2	1:D:169:ARG:O	2.14	0.48
1:A:225:THR:HA	1:A:228:MET:HE2	1.96	0.48
1:A:194:ARG:HD3	8:A:489:HOH:O	2.13	0.48
1:D:60:TRP:O	1:D:64:THR:CG2	2.62	0.48
1:A:181:ARG:HD2	1:A:183:ASP:OD1	2.13	0.47
1:A:177:GLU:OE2	2:E:6:LYS:NZ	2.48	0.47
1:D:83:ARG:O	7:D:308:SO4:S	2.72	0.47
1:A:121:ARG:HG3	8:A:478:HOH:O	2.14	0.47
2:B:50:GLU:OE1	8:B:401:HOH:O	2.20	0.47
1:A:150:ALA:O	4:A:301:GOL:O2	2.20	0.47
1:A:190:THR:OG1	1:A:192:HIS:HE1	1.98	0.47
2:B:81:ARG:HH11	2:B:81:ARG:HG2	1.79	0.46
1:D:195:SER:HG	1:D:198:ASP:HB2	1.80	0.46
1:D:0:MET:HG2	1:D:264:LYS:NZ	2.31	0.46
1:D:111:ARG:HG2	1:D:113:TYR:CZ	2.51	0.45
1:D:263:HIS:HD2	1:D:265:GLY:H	1.63	0.45
2:B:4:THR:HB	2:B:86:THR:OG1	2.16	0.45
1:A:121:ARG:HB3	2:B:1:ILE:HD12	1.98	0.45
6:A:306:EDO:H12	3:C:1:LEU:O	2.14	0.45
5:D:304:15P:OXT	5:D:304:15P:H14	2.15	0.45
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.52	0.45
5:D:304:15P:H25	8:D:485:HOH:O	2.17	0.44
1:D:83:ARG:NH1	8:D:405:HOH:O	2.40	0.44
1:D:0:MET:HG3	1:D:264:LYS:HE2	1.99	0.44
1:D:197:VAL:O	1:D:197:VAL:CG2	2.65	0.44
1:A:202:ARG:HD3	1:A:246:ALA:HB2	1.99	0.44
1:A:46:GLU:HG2	5:A:303:15P:H12	2.00	0.44
2:B:46:ILE:HD11	2:B:68:THR:OG1	2.18	0.44
1:A:144:ARG:CZ	8:A:427:HOH:O	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:33:SER:HB3	2:B:62:PHE:CE2	2.54	0.42
2:B:91:LYS:HE2	8:B:439:HOH:O	2.20	0.42
2:E:73:THR:HG23	2:E:76:ASP:OD2	2.20	0.42
2:E:81:ARG:HG3	2:E:92:ILE:CD1	2.49	0.42
1:D:176:ASN:ND2	8:D:402:HOH:O	2.32	0.42
1:A:82:GLN:NE2	8:A:412:HOH:O	2.52	0.42
1:A:46:GLU:HG2	5:A:303:15P:H22	2.00	0.42
1:A:115:GLN:HE21	1:A:115:GLN:HB2	1.33	0.42
1:D:255:GLN:NE2	1:D:255:GLN:H	2.17	0.42
1:A:143:THR:OG1	3:C:9:VAL:HG13	2.20	0.42
1:D:176:ASN:ND2	1:D:176:ASN:C	2.78	0.41
1:A:184:SER:HB2	2:E:0:MET:O	2.21	0.41
2:E:33:SER:HB3	2:E:62:PHE:CE2	2.55	0.41
1:D:192:HIS:O	1:D:199:VAL:HG23	2.20	0.41
1:A:87:GLN:NE2	8:A:414:HOH:O	2.53	0.41
1:A:14:ARG:HA	1:A:15:PRO:HD3	2.00	0.41
1:A:152:ASP:OD1	4:A:301:GOL:H32	2.21	0.40
1:D:14:ARG:NH2	8:D:414:HOH:O	2.55	0.40
1:D:187:ALA:HA	1:D:204:TRP:O	2.20	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:ASP:O	2:B:45:ARG:NH1[2_645]	2.19	0.01

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	275/277 (99%)	268 (98%)	7 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	276/277 (100%)	268 (97%)	8 (3%)	0	100	100
2	B	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
2	E	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
3	C	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
3	F	7/9 (78%)	7 (100%)	0	0	100	100
All	All	761/772 (99%)	743 (98%)	18 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	236/236 (100%)	213 (90%)	23 (10%)	8	1
1	D	237/236 (100%)	213 (90%)	24 (10%)	7	1
2	B	95/95 (100%)	88 (93%)	7 (7%)	13	3
2	E	95/95 (100%)	90 (95%)	5 (5%)	20	7
3	C	8/8 (100%)	7 (88%)	1 (12%)	4	0
3	F	8/8 (100%)	7 (88%)	1 (12%)	4	0
All	All	679/678 (100%)	618 (91%)	61 (9%)	9	1

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ARG
1	A	45	PHE
1	A	65	GLN
1	A	70	ASP
1	A	72	GLN
1	A	79	ARG
1	A	80	THR
1	A	89	LYS

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Mol	Chain	Res	Type
1	A	95	PHE
1	A	98	MET
1	A	105	SER
1	A	107	TRP
1	A	108	ARG
1	A	110	LEU
1	A	115	GLN
1	A	121	ARG
1	A	142	ILE
1	A	169	ARG
1	A	181	ARG
1	A	184	SER
1	A	226	GLN
1	A	272	LEU
1	A	275	LYS
2	B	4	THR
2	B	44	GLU
2	B	45	ARG
2	B	46	ILE
2	B	58	LYS
2	B	74	GLU
2	B	77	GLU
3	C	1	LEU
1	D	0	MET
1	D	44	ARG
1	D	45	PHE
1	D	64	THR
1	D	70	ASP
1	D	72	GLN
1	D	79	ARG
1	D	95	PHE
1	D	98	MET
1	D	107	TRP
1	D	108	ARG
1	D	110	LEU
1	D	141	LEU
1	D	176	ASN
1	D	181	ARG
1	D	184	SER
1	D	186	LYS
1	D	194	ARG
1	D	197	VAL

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Mol	Chain	Res	Type
1	D	219	LEU
1	D	224	LEU
1	D	226	GLN
1	D	255	GLN
1	D	272	LEU
2	E	16	GLU
2	E	48	LYS
2	E	58	LYS
2	E	73	THR
2	E	75	LYS
3	F	9	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	GLN
1	A	86	ASN
1	A	114	HIS
1	A	115	GLN
1	A	192	HIS
1	A	220	ASN
1	A	263	HIS
2	B	51	HIS
1	D	114	HIS
1	D	226	GLN
1	D	255	GLN
1	D	263	HIS
2	E	17	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

28 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	GOL	D	301	-	5,5,5	0.40	0	5,5,5	0.68	0
4	GOL	D	302	-	5,5,5	0.37	0	5,5,5	0.78	0
4	GOL	A	302	-	5,5,5	0.46	0	5,5,5	0.46	0
5	15P	D	304	-	9,9,103	1.14	0	8,8,102	1.20	0
7	SO4	E	106	-	4,4,4	0.46	0	6,6,6	0.23	0
4	GOL	A	301	-	5,5,5	1.11	0	5,5,5	2.33	2 (40%)
6	EDO	C	101	-	3,3,3	0.38	0	2,2,2	0.42	0
5	15P	D	303	-	9,9,103	0.73	0	8,8,102	0.87	0
5	15P	A	303	-	9,9,103	0.49	0	8,8,102	0.48	0
7	SO4	E	104	-	4,4,4	0.51	0	6,6,6	0.20	0
4	GOL	B	302	-	5,5,5	0.37	0	5,5,5	1.06	0
6	EDO	A	306	-	3,3,3	0.78	0	2,2,2	0.62	0
6	EDO	A	304	-	3,3,3	0.49	0	2,2,2	0.43	0
6	EDO	B	303	-	3,3,3	0.52	0	2,2,2	0.26	0
6	EDO	B	304	-	3,3,3	0.71	0	2,2,2	0.11	0
4	GOL	B	301	-	5,5,5	1.24	0	5,5,5	1.35	0
4	GOL	E	101	-	5,5,5	0.73	0	5,5,5	0.58	0
6	EDO	D	305	-	3,3,3	0.51	0	2,2,2	0.50	0
6	EDO	D	307	-	3,3,3	0.40	0	2,2,2	0.38	0
6	EDO	E	103	-	3,3,3	0.39	0	2,2,2	0.62	0
6	EDO	D	306	-	3,3,3	0.60	0	2,2,2	0.48	0
6	EDO	B	305	-	3,3,3	0.73	0	2,2,2	0.37	0
7	SO4	E	105	-	4,4,4	0.43	0	6,6,6	0.33	0
6	EDO	E	102	-	3,3,3	0.22	0	2,2,2	0.64	0
7	SO4	D	308	-	4,4,4	0.64	0	6,6,6	0.75	0
6	EDO	A	305	-	3,3,3	0.45	0	2,2,2	0.38	0
7	SO4	A	307	-	4,4,4	0.56	0	6,6,6	0.50	0
7	SO4	A	308	-	4,4,4	0.49	0	6,6,6	0.11	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	GOL	D	301	-	-	4/4/4/4	-
4	GOL	D	302	-	-	4/4/4/4	-
4	GOL	A	302	-	-	2/4/4/4	-
5	15P	D	304	-	-	7/7/7/101	-
4	GOL	A	301	-	-	2/4/4/4	-
6	EDO	C	101	-	-	1/1/1/1	-
5	15P	D	303	-	-	4/7/7/101	-
5	15P	A	303	-	-	6/7/7/101	-
4	GOL	B	302	-	-	0/4/4/4	-
6	EDO	A	306	-	-	1/1/1/1	-
6	EDO	A	304	-	-	1/1/1/1	-
6	EDO	B	303	-	-	1/1/1/1	-
6	EDO	B	304	-	-	0/1/1/1	-
4	GOL	B	301	-	-	0/4/4/4	-
4	GOL	E	101	-	-	4/4/4/4	-
6	EDO	D	305	-	-	1/1/1/1	-
6	EDO	D	307	-	-	0/1/1/1	-
6	EDO	E	103	-	-	1/1/1/1	-
6	EDO	D	306	-	-	1/1/1/1	-
6	EDO	B	305	-	-	1/1/1/1	-
6	EDO	E	102	-	-	1/1/1/1	-
6	EDO	A	305	-	-	0/1/1/1	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	301	GOL	O2-C2-C3	-3.34	95.34	109.18
4	A	301	GOL	C3-C2-C1	3.14	123.31	111.80

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	302	GOL	O1-C1-C2-C3
4	E	101	GOL	C1-C2-C3-O3
5	D	304	15P	C1-C2-O1-C3
5	A	303	15P	O1-C3-C4-O2
5	D	304	15P	O1-C3-C4-O2

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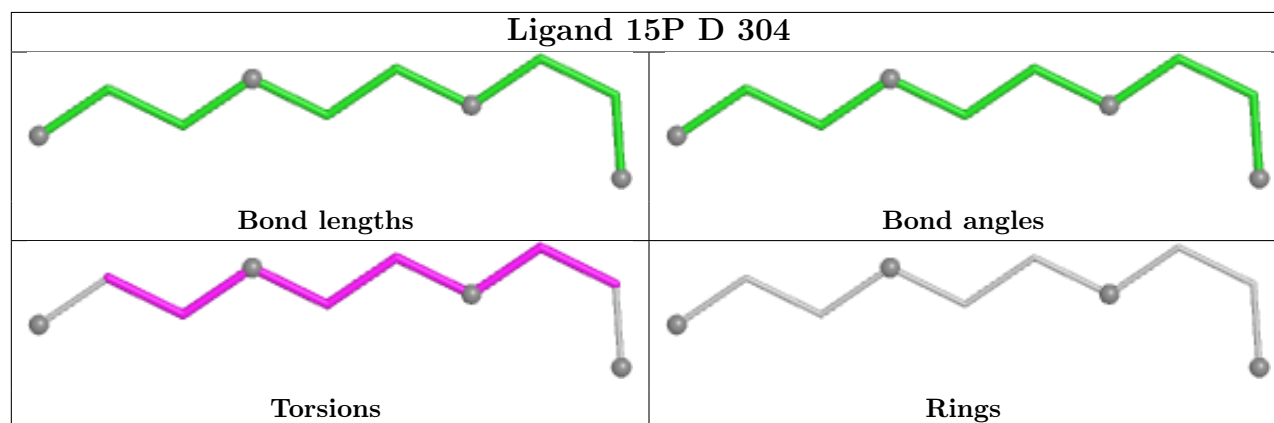
Mol	Chain	Res	Type	Atoms
4	D	302	GOL	O1-C1-C2-O2
5	A	303	15P	OXT-C1-C2-O1
5	A	303	15P	O2-C5-C6-O3
5	D	304	15P	C3-C4-O2-C5
4	A	301	GOL	O1-C1-C2-C3
4	A	302	GOL	O1-C1-C2-C3
4	D	301	GOL	C1-C2-C3-O3
4	D	302	GOL	C1-C2-C3-O3
4	E	101	GOL	O1-C1-C2-C3
5	D	304	15P	O2-C5-C6-O3
5	D	303	15P	O2-C5-C6-O3
6	B	303	EDO	O1-C1-C2-O2
6	B	305	EDO	O1-C1-C2-O2
5	D	304	15P	C6-C5-O2-C4
4	A	302	GOL	O1-C1-C2-O2
6	A	306	EDO	O1-C1-C2-O2
6	E	102	EDO	O1-C1-C2-O2
4	D	302	GOL	O2-C2-C3-O3
6	D	305	EDO	O1-C1-C2-O2
4	E	101	GOL	O2-C2-C3-O3
5	D	303	15P	C3-C4-O2-C5
5	A	303	15P	C3-C4-O2-C5
4	A	301	GOL	C1-C2-C3-O3
5	A	303	15P	C4-C3-O1-C2
5	A	303	15P	C1-C2-O1-C3
5	D	304	15P	OXT-C1-C2-O1
6	D	306	EDO	O1-C1-C2-O2
6	E	103	EDO	O1-C1-C2-O2
4	E	101	GOL	O1-C1-C2-O2
4	D	301	GOL	O1-C1-C2-O2
4	D	301	GOL	O2-C2-C3-O3
6	C	101	EDO	O1-C1-C2-O2
5	D	303	15P	C4-C3-O1-C2
5	D	304	15P	C4-C3-O1-C2
5	D	303	15P	O1-C3-C4-O2
6	A	304	EDO	O1-C1-C2-O2
4	D	301	GOL	O1-C1-C2-C3

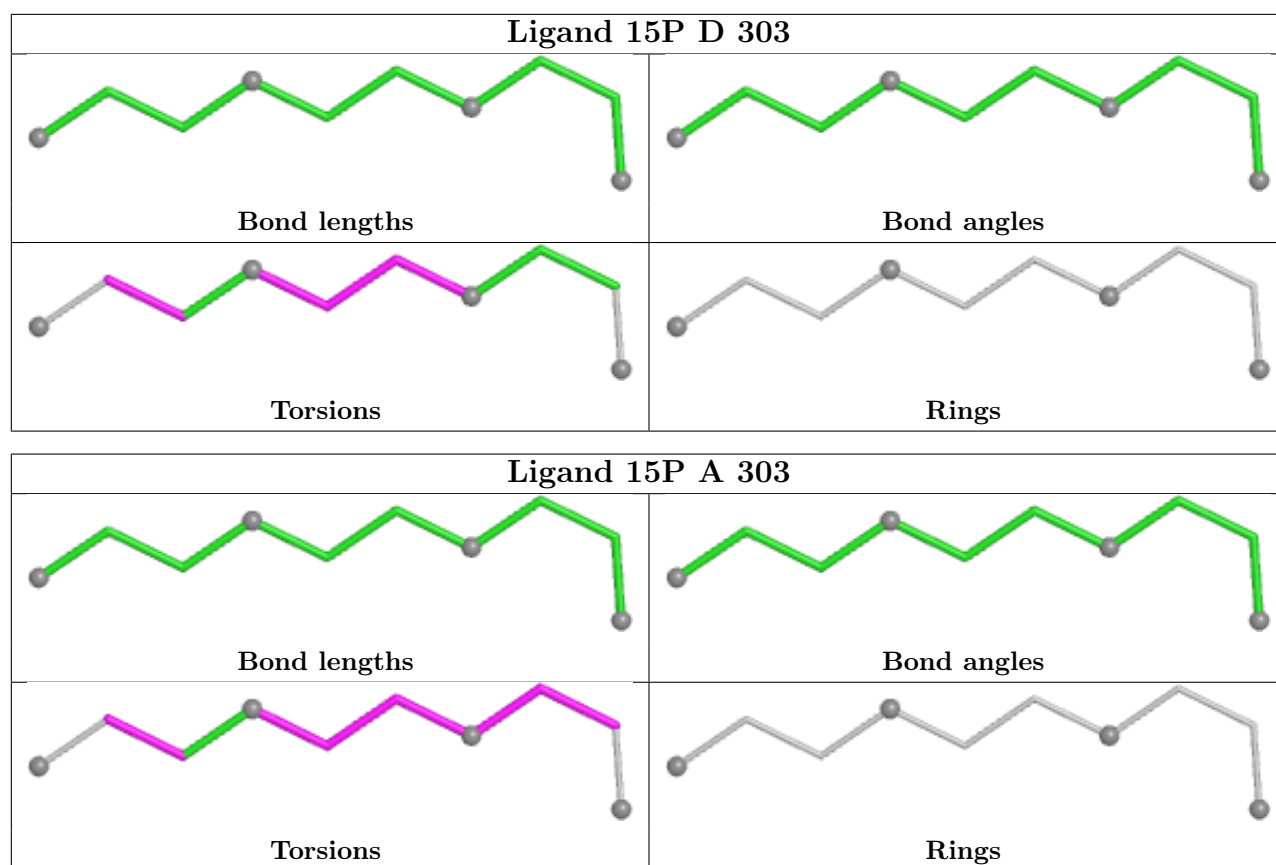
There are no ring outliers.

10 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	301	GOL	1	0
5	D	304	15P	4	0
4	A	301	GOL	5	0
5	D	303	15P	1	0
5	A	303	15P	3	0
4	B	302	GOL	3	0
6	A	306	EDO	3	0
6	D	305	EDO	1	0
6	E	103	EDO	1	0
7	D	308	SO4	4	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, 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	277/277 (100%)	0.46	13 (4%) 36 39	15, 29, 55, 72	0
1	D	277/277 (100%)	0.24	8 (2%) 53 57	15, 26, 45, 66	1 (0%)
2	B	100/100 (100%)	0.24	2 (2%) 65 68	15, 26, 44, 52	0
2	E	100/100 (100%)	0.18	1 (1%) 79 83	16, 27, 46, 52	0
3	C	9/9 (100%)	0.31	0 100 100	20, 23, 30, 31	0
3	F	9/9 (100%)	0.28	0 100 100	22, 24, 27, 28	0
All	All	772/772 (100%)	0.31	24 (3%) 51 55	15, 27, 48, 72	1 (0%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	276	PRO	4.6
1	D	276	PRO	4.0
1	A	107	TRP	4.0
1	A	17	LEU	4.0
1	A	274	TRP	3.4
1	A	18	GLY	3.0
1	D	0	MET	2.9
1	D	16	GLY	2.8
1	A	109	LEU	2.7
1	A	110	LEU	2.6
1	D	90	GLY	2.6
1	D	107	TRP	2.5
1	A	268	GLU	2.5
2	B	46	ILE	2.5
1	D	227	ASP	2.5
1	A	275	LYS	2.4
2	E	48	LYS	2.4
1	D	1	GLY	2.3
2	B	49	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	41	ASP	2.2
1	A	45	PHE	2.2
1	A	197	VAL	2.2
1	D	41	ASP	2.2
1	A	221	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	SO4	A	308	5/5	0.68	0.15	80,90,92,98	0
4	GOL	A	302	6/6	0.70	0.18	52,63,65,68	0
5	15P	A	303	10/104	0.71	0.18	50,55,59,60	0
4	GOL	D	302	6/6	0.71	0.16	49,53,53,56	0
4	GOL	E	101	6/6	0.72	0.17	49,56,57,57	0
6	EDO	B	305	4/4	0.74	0.17	38,39,42,43	0
7	SO4	E	106	5/5	0.78	0.17	76,79,95,96	0
7	SO4	E	104	5/5	0.79	0.14	39,40,42,43	5
6	EDO	A	304	4/4	0.80	0.15	48,48,48,50	0
6	EDO	A	305	4/4	0.80	0.14	47,48,49,58	0
5	15P	D	303	10/104	0.82	0.13	36,41,44,47	0
4	GOL	D	301	6/6	0.82	0.13	45,48,50,50	0
7	SO4	E	105	5/5	0.82	0.12	76,76,80,81	0
6	EDO	D	305	4/4	0.82	0.12	38,39,40,40	0
5	15P	D	304	10/104	0.85	0.14	20,25,36,37	0
6	EDO	B	304	4/4	0.85	0.14	37,44,45,48	0
6	EDO	B	303	4/4	0.86	0.13	43,47,48,48	0
6	EDO	D	307	4/4	0.86	0.13	30,32,33,36	0

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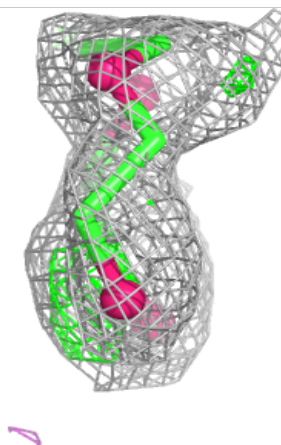
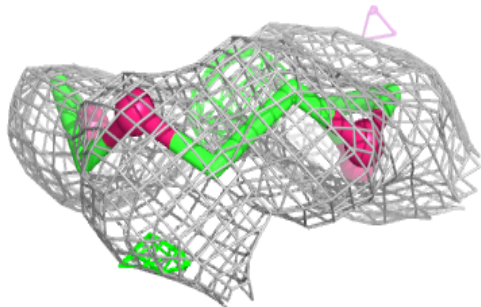
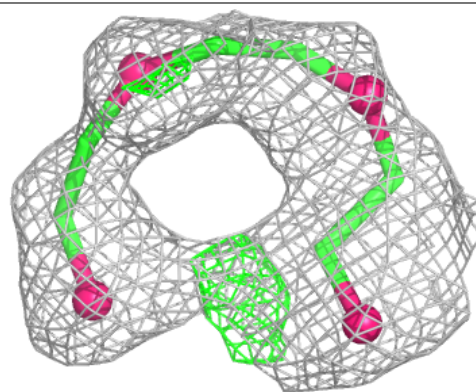
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GOL	B	302	6/6	0.88	0.11	32,36,38,40	0
6	EDO	C	101	4/4	0.88	0.12	33,33,34,34	0
6	EDO	D	306	4/4	0.89	0.09	32,35,35,36	0
4	GOL	B	301	6/6	0.89	0.11	24,32,37,41	0
7	SO4	D	308	5/5	0.90	0.13	18,21,25,28	5
4	GOL	A	301	6/6	0.90	0.15	27,28,29,32	0
7	SO4	A	307	5/5	0.91	0.10	57,59,62,63	0
6	EDO	E	103	4/4	0.91	0.10	33,33,34,37	0
6	EDO	E	102	4/4	0.93	0.08	18,20,20,24	0
6	EDO	A	306	4/4	0.93	0.11	8,9,13,16	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.

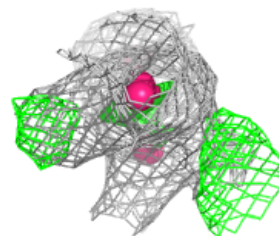
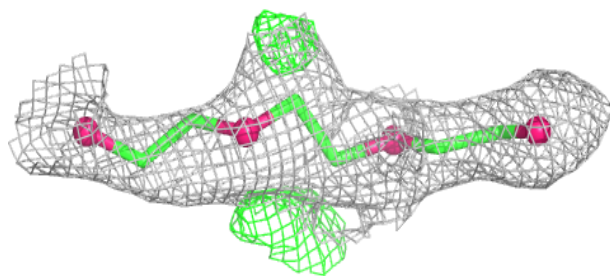
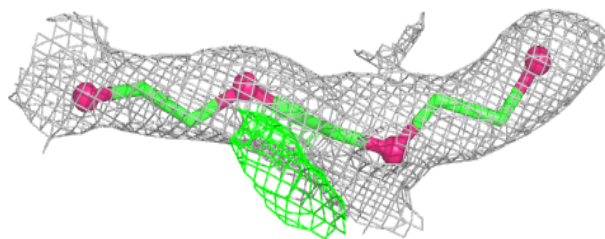
Electron density around 15P A 303:

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

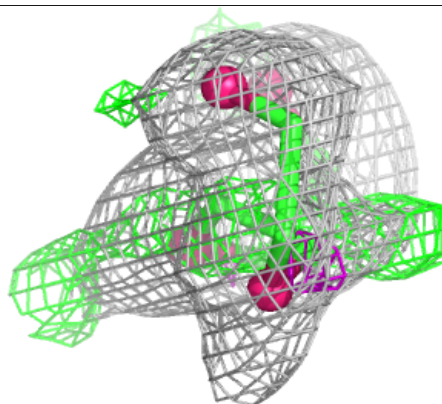
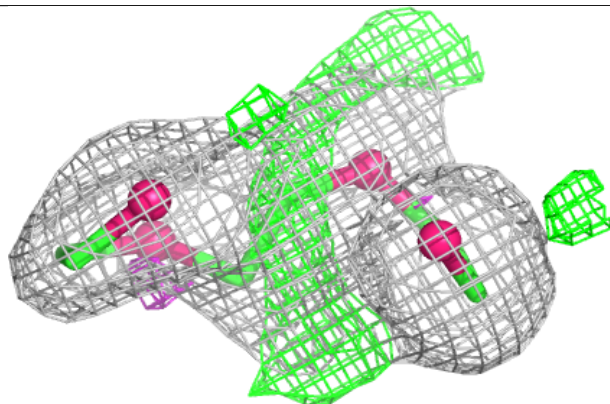
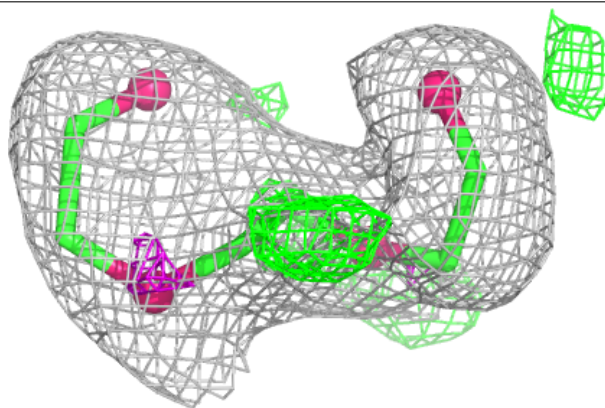


Electron density around 15P D 303:

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

**Electron density around 15P D 304:**

$2mF_o-DF_c$ (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.