



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:50 AM UTC

PDB ID : 4E7E / pdb\_00004e7e  
Title : E. cloacae C115D MurA in complex with UDP-glucose  
Authors : Zhu, J.-Y.; Yang, Y.; Schonbrunn, E.  
Deposited on : 2012-03-16  
Resolution : 2.30 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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

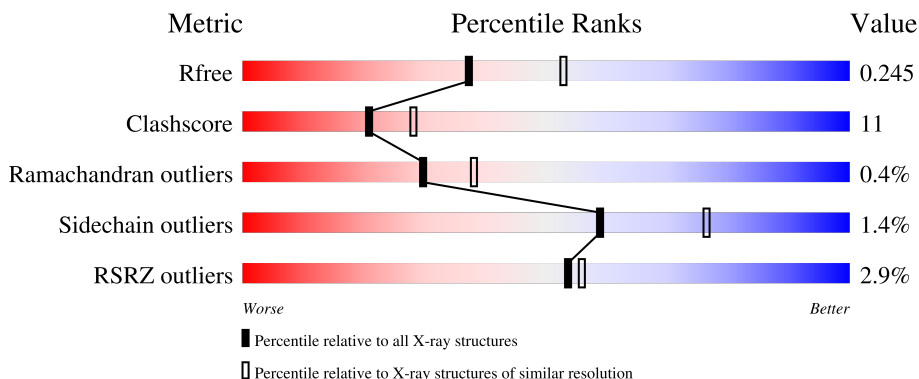
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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  $\geq 3$ , 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	419	 4% 76% 22%
1	B	419	 3% 77% 19%
1	C	419	 4% 72% 25%
1	D	419	 % 76% 21%

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 13403 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 UDP-N-acetylglucosamine 1-carboxyvinyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	419	3144	1977	554	600	13	0	0	0
1	B	419	3144	1977	554	600	13	0	0	0
1	C	419	3145	1977	554	601	13	0	0	0
1	D	419	3144	1977	554	600	13	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	67	IAS	ASN	SEE REMARK 999	UNP P33038
A	115	ASP	CYS	engineered mutation	UNP P33038
B	67	IAS	ASN	SEE REMARK 999	UNP P33038
B	115	ASP	CYS	engineered mutation	UNP P33038
C	67	IAS	ASN	SEE REMARK 999	UNP P33038
C	115	ASP	CYS	engineered mutation	UNP P33038
D	67	IAS	ASN	SEE REMARK 999	UNP P33038
D	115	ASP	CYS	engineered mutation	UNP P33038

- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



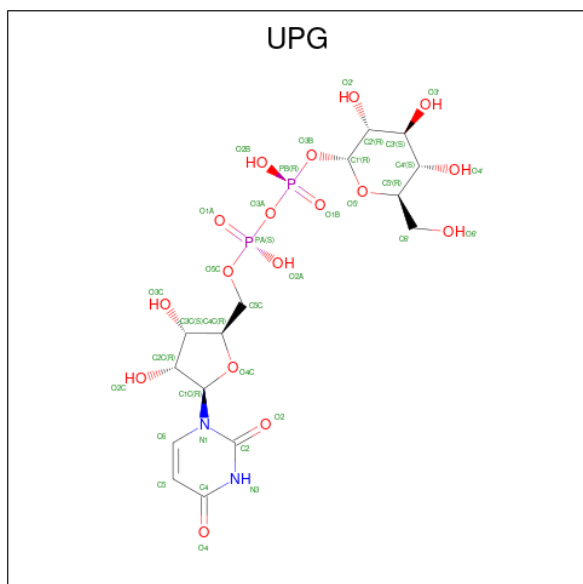
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0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

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



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

- Molecule 4 is URIDINE-5'-DIPHOSPHATE-GLUCOSE (CCD ID: UPG) (formula:  $C_{15}H_{24}N_2O_{17}P_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
4	A	1	Total	C	N	O	P	0	0
			36	15	2	17	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	D	1	36	15	2	17	2	0	0

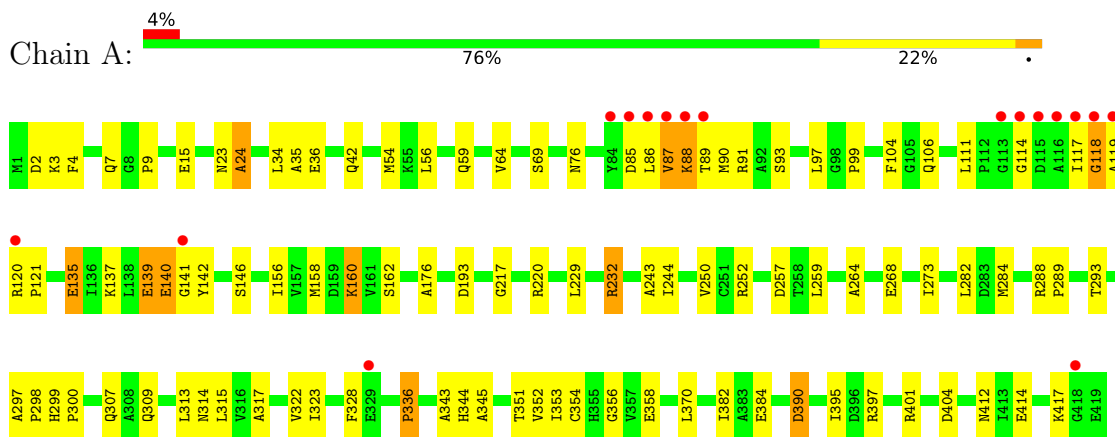
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	180	Total 180	O 180	0	0
5	B	168	Total 168	O 168	0	0
5	C	171	Total 171	O 171	0	0
5	D	183	Total 183	O 183	0	0

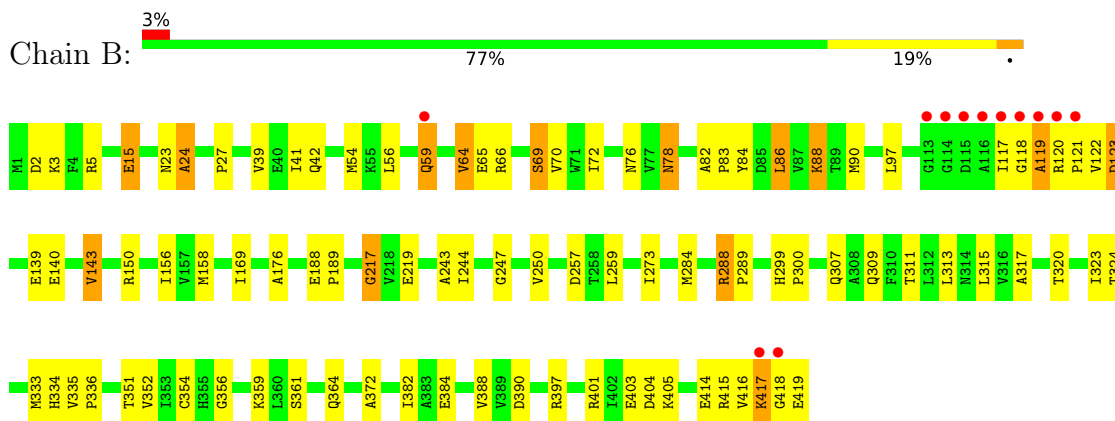
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

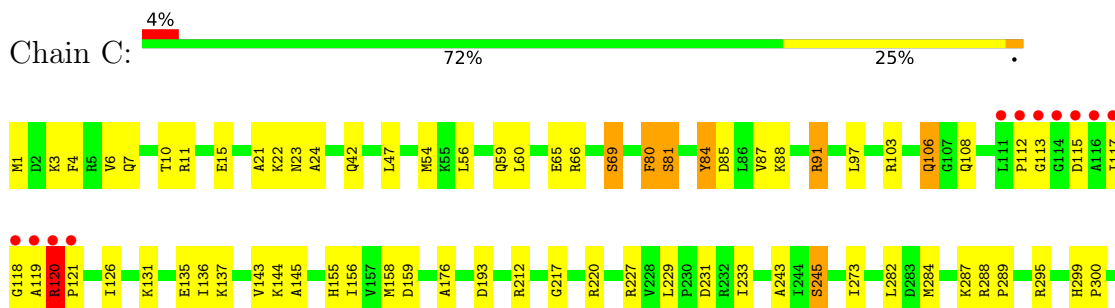
- Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase

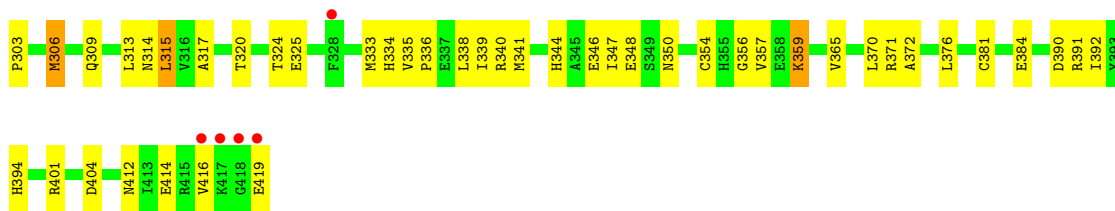


- Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase

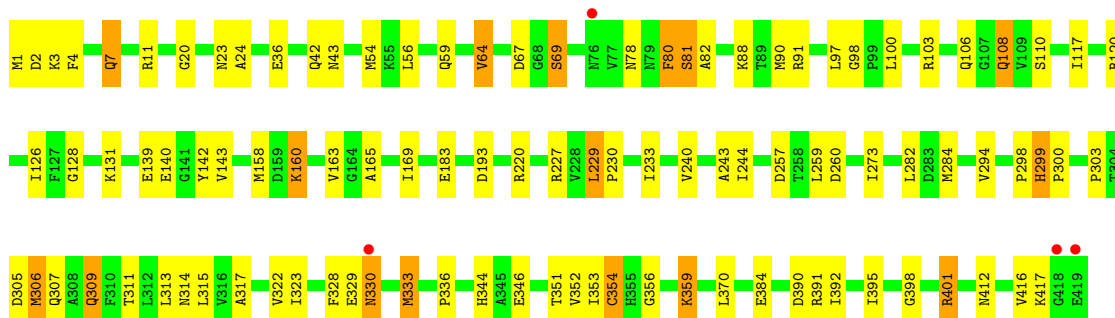
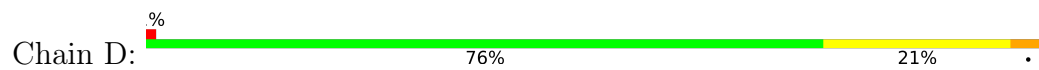


- Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase





● Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.11Å 101.42Å 213.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.92 – 2.30 19.92 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (19.92-2.30) 99.6 (19.92-2.30)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.90 (at 2.30Å)	Xtrriage
Refinement program	CNS 1.3	Depositor
R, $R_{free}$	0.198 , 0.246 0.198 , 0.245	Depositor DCC
$R_{free}$ test set	1180 reflections (1.50%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.4	Xtrriage
Anisotropy	0.028	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 39.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	13403	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% 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: UPG, EDO, ACT, IAS

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	0.68	4/3180 (0.1%)	1.25	22/4308 (0.5%)
1	B	0.67	3/3180 (0.1%)	1.28	29/4308 (0.7%)
1	C	0.71	6/3181 (0.2%)	1.25	24/4308 (0.6%)
1	D	0.74	10/3180 (0.3%)	1.28	28/4308 (0.6%)
All	All	0.70	23/12721 (0.2%)	1.26	103/17232 (0.6%)

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	306	MET	SD-CE	-8.39	1.58	1.79
1	D	299	HIS	CD2-NE2	-7.09	1.30	1.37
1	C	306	MET	SD-CE	-6.91	1.62	1.79
1	D	299	HIS	CG-ND1	-6.78	1.30	1.38
1	A	309	GLN	CD-OE1	6.58	1.36	1.23
1	D	330	ASN	CG-OD1	6.32	1.35	1.23
1	D	298	PRO	C-O	-6.21	1.16	1.23
1	B	309	GLN	CD-OE1	5.90	1.34	1.23
1	D	59	GLN	CD-OE1	5.87	1.34	1.23
1	B	78	ASN	CG-OD1	5.86	1.34	1.23
1	C	309	GLN	CD-OE1	5.86	1.34	1.23
1	B	59	GLN	CD-OE1	5.79	1.34	1.23
1	A	59	GLN	CD-OE1	5.60	1.34	1.23
1	C	59	GLN	CD-OE1	5.59	1.34	1.23
1	C	106	GLN	CD-OE1	5.58	1.34	1.23
1	D	309	GLN	CD-OE1	5.47	1.33	1.23
1	C	155	HIS	ND1-CE1	5.47	1.38	1.32
1	A	344	HIS	ND1-CE1	5.42	1.38	1.32
1	D	344	HIS	ND1-CE1	5.36	1.38	1.32
1	C	344	HIS	ND1-CE1	5.33	1.37	1.32
1	D	7	GLN	CD-OE1	5.22	1.33	1.23
1	D	108	GLN	CD-OE1	5.20	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	307	GLN	CD-OE1	5.04	1.33	1.23

All (103) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	122	VAL	N-CA-C	-11.14	101.82	112.29
1	B	120	ARG	N-CA-C	10.09	124.23	110.31
1	B	65	GLU	N-CA-C	9.15	123.42	109.23
1	B	86	LEU	N-CA-C	8.97	124.28	113.16
1	A	76	ASN	N-CA-C	8.61	124.01	111.87
1	A	307	GLN	N-CA-C	8.58	120.25	111.07
1	D	69	SER	N-CA-C	8.46	123.26	110.14
1	B	143	VAL	N-CA-C	-8.45	95.42	107.75
1	D	307	GLN	N-CA-C	7.71	120.43	111.02
1	B	97	LEU	N-CA-C	7.55	119.20	110.97
1	C	81	SER	N-CA-C	7.50	121.43	108.76
1	B	90	MET	N-CA-C	7.47	122.84	107.37
1	B	123	ASP	N-CA-C	7.46	120.28	111.71
1	A	24	ALA	N-CA-C	-7.45	104.32	113.41
1	B	307	GLN	N-CA-C	7.40	120.00	111.11
1	C	84	TYR	N-CA-C	7.34	120.21	111.33
1	B	257	ASP	N-CA-C	7.25	121.22	112.38
1	D	90	MET	N-CA-C	7.09	121.13	107.44
1	D	78	ASN	N-CA-C	7.04	122.16	113.50
1	D	273	ILE	N-CA-C	6.98	118.65	108.53
1	C	365	VAL	N-CA-C	6.97	118.98	108.80
1	D	82	ALA	CA-C-N	6.96	126.87	119.85
1	D	82	ALA	C-N-CA	6.96	126.87	119.85
1	C	97	LEU	N-CA-C	6.93	118.52	110.97
1	C	6	VAL	N-CA-C	6.83	118.43	108.53
1	D	330	ASN	N-CA-C	6.82	120.79	111.17
1	B	23	ASN	N-CA-C	6.72	121.08	113.01
1	A	344	HIS	CB-CG-CD2	-6.55	122.68	131.20
1	C	344	HIS	CB-CG-CD2	-6.55	122.68	131.20
1	D	81	SER	N-CA-C	6.50	120.18	108.48
1	A	273	ILE	N-CA-C	6.44	117.75	108.48
1	D	64	VAL	N-CA-C	6.41	117.35	108.12
1	D	344	HIS	CB-CG-CD2	-6.41	122.87	131.20
1	C	23	ASN	N-CA-C	6.34	120.12	112.38
1	A	328	PHE	N-CA-C	6.34	120.40	110.32
1	B	259	LEU	N-CA-C	6.33	120.31	112.59
1	A	97	LEU	N-CA-C	6.33	118.74	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	106	GLN	N-CA-C	6.29	117.97	108.46
1	D	24	ALA	N-CA-C	-6.21	105.72	113.55
1	C	155	HIS	CB-CG-CD2	-6.21	123.13	131.20
1	C	143	VAL	N-CA-C	-6.17	98.74	107.75
1	D	163	VAL	N-CA-C	-6.15	104.52	110.42
1	D	23	ASN	N-CA-C	6.15	120.39	113.01
1	D	417	LYS	N-CA-C	6.13	119.92	110.42
1	B	88	LYS	N-CA-C	6.13	118.74	111.33
1	A	90	MET	N-CA-C	6.07	121.38	107.48
1	D	333	MET	N-CA-C	5.97	119.39	111.75
1	D	88	LYS	N-CA-C	5.97	119.39	111.75
1	C	69	SER	N-CA-C	5.91	118.83	110.14
1	D	103	ARG	N-CA-C	5.88	118.92	111.69
1	D	311	THR	N-CA-C	-5.86	104.80	111.07
1	C	80	PHE	N-CA-C	5.84	119.97	112.26
1	D	257	ASP	N-CA-C	5.78	119.80	112.87
1	B	120	ARG	CB-CA-C	5.76	116.69	108.68
1	C	15	GLU	N-CA-C	5.75	118.59	109.50
1	A	257	ASP	N-CA-C	5.72	119.74	112.87
1	C	359	LYS	N-CA-C	5.68	117.91	108.99
1	A	390	ASP	N-CA-C	5.67	118.92	110.52
1	B	311	THR	N-CA-C	-5.65	105.21	111.36
1	B	397	ARG	N-CA-C	5.65	118.20	111.71
1	A	344	HIS	CB-CG-ND1	5.64	131.16	122.70
1	A	35	ALA	N-CA-C	5.61	117.83	109.59
1	B	24	ALA	N-CA-C	-5.59	106.51	113.55
1	B	64	VAL	N-CA-C	5.58	116.15	108.12
1	B	247	GLY	N-CA-C	5.58	120.78	112.41
1	C	344	HIS	CB-CG-ND1	5.56	131.04	122.70
1	B	82	ALA	CA-C-N	5.56	125.53	120.03
1	B	82	ALA	C-N-CA	5.56	125.53	120.03
1	A	232	ARG	N-CA-C	5.55	117.33	111.28
1	C	273	ILE	N-CA-C	5.55	116.58	108.53
1	C	287	LYS	N-CA-C	5.55	118.33	110.50
1	D	344	HIS	CB-CG-ND1	5.55	131.02	122.70
1	A	23	ASN	N-CA-C	5.49	119.60	113.01
1	C	155	HIS	CB-CG-ND1	5.48	130.92	122.70
1	A	358	GLU	N-CA-C	5.47	117.05	111.14
1	C	156	ILE	N-CA-C	5.44	115.78	108.17
1	D	229	LEU	N-CA-C	5.44	117.89	110.01
1	A	104	PHE	N-CA-C	5.37	120.11	113.50
1	B	15	GLU	N-CA-C	5.36	117.97	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	76	ASN	N-CA-C	5.34	120.03	111.81
1	C	60	LEU	N-CA-C	-5.30	106.98	113.50
1	D	97	LEU	N-CA-C	5.28	117.46	111.02
1	D	328	PHE	N-CA-C	5.28	118.72	110.32
1	A	2	ASP	N-CA-C	5.26	117.08	110.24
1	D	80	PHE	N-CA-C	5.26	118.55	112.97
1	B	288	ARG	CB-CA-C	5.24	116.97	109.11
1	A	414	GLU	N-CA-C	5.21	116.92	108.26
1	B	417	LYS	N-CA-C	5.21	117.92	109.79
1	B	273	ILE	N-CA-C	5.21	116.08	108.53
1	B	69	SER	N-CA-C	5.20	117.76	109.81
1	A	162	SER	N-CA-C	5.19	116.85	108.34
1	C	120	ARG	N-CA-C	5.18	121.25	109.81
1	C	24	ALA	N-CA-C	-5.17	106.66	113.12
1	C	315	LEU	N-CA-C	5.16	119.05	112.34
1	C	414	GLU	N-CA-C	5.13	117.76	108.69
1	A	156	ILE	N-CA-C	5.12	115.23	107.80
1	B	156	ILE	N-CA-C	5.11	115.46	107.99
1	B	217	GLY	N-CA-C	5.08	117.30	111.36
1	A	351	THR	N-CA-C	5.06	117.37	109.52
1	A	417	LYS	N-CA-C	5.05	117.05	110.53
1	C	245	SER	N-CA-C	5.05	120.17	112.54
1	D	303	PRO	N-CA-C	5.03	118.39	110.80
1	D	354	CYS	N-CA-C	5.01	117.41	109.24

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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	3144	0	3215	76	0
1	B	3144	0	3215	65	0
1	C	3145	0	3215	80	0
1	D	3144	0	3215	72	0
2	A	4	0	6	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	8	0	12	0	0
2	C	8	0	12	3	0
2	D	24	0	36	4	0
3	A	4	0	3	1	0
3	D	4	0	3	0	0
4	A	36	0	22	1	0
4	D	36	0	22	0	0
5	A	180	0	0	4	0
5	B	168	0	0	3	0
5	C	171	0	0	6	0
5	D	183	0	0	2	0
All	All	13403	0	12976	284	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 11.

All (284) 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:139:GLU:HB3	1:A:142:TYR:CZ	1.63	1.34
1:A:139:GLU:HB3	1:A:142:TYR:CE2	1.70	1.24
1:B:59:GLN:OE1	1:B:86:LEU:HD21	1.37	1.20
1:A:139:GLU:CB	1:A:142:TYR:CZ	2.40	1.05
1:D:233:ILE:HG23	1:D:306:MET:HE3	1.42	1.00
1:A:139:GLU:O	1:A:140:GLU:HB3	1.62	0.96
1:A:139:GLU:HB2	1:A:142:TYR:OH	1.63	0.96
1:A:142:TYR:HD2	5:A:687:HOH:O	1.47	0.96
1:D:42:GLN:HA	1:D:69:SER:HB3	1.48	0.95
1:A:139:GLU:CB	1:A:142:TYR:OH	2.13	0.95
1:D:108:GLN:HG2	2:D:506:EDO:H22	1.51	0.92
1:B:42:GLN:HA	1:B:69:SER:HB3	1.50	0.92
1:B:54:MET:HE1	1:B:66:ARG:HB3	1.52	0.91
1:D:401:ARG:HG3	1:D:401:ARG:HH11	1.36	0.90
1:B:15:GLU:HG2	1:B:250:VAL:HB	1.53	0.88
1:B:59:GLN:OE1	1:B:86:LEU:CD2	2.24	0.84
1:B:359:LYS:HZ2	1:B:384:GLU:HB2	1.46	0.80
1:B:359:LYS:NZ	1:B:384:GLU:HB2	1.97	0.80
1:D:233:ILE:HG23	1:D:306:MET:CE	2.13	0.78
1:D:54:MET:HE3	1:D:64:VAL:HG12	1.64	0.77
1:C:233:ILE:HG23	1:C:306:MET:CE	2.15	0.77
1:A:91:ARG:HG3	1:A:91:ARG:HH11	1.51	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:MET:HE3	1:B:70:VAL:HG13	1.68	0.75
1:B:5:ARG:NH2	1:B:414:GLU:OE2	2.20	0.74
1:A:193:ASP:CG	1:A:229:LEU:HD22	2.14	0.72
1:B:158:MET:HE1	1:B:169:ILE:HD12	1.72	0.71
1:D:306:MET:HE2	1:D:306:MET:HA	1.73	0.70
1:A:88:LYS:HG3	1:A:89:THR:H	1.54	0.70
1:D:1:MET:HE3	1:D:391:ARG:NH1	2.07	0.70
1:D:401:ARG:HG3	1:D:401:ARG:NH1	2.08	0.69
1:D:158:MET:HE1	1:D:165:ALA:HB3	1.74	0.69
1:A:193:ASP:CB	1:A:229:LEU:HD22	2.23	0.69
1:C:233:ILE:HG23	1:C:306:MET:HE2	1.75	0.67
1:A:336:PRO:HG2	1:B:333:MET:HE2	1.77	0.67
1:C:334:HIS:HB3	1:C:372:ALA:HB1	1.76	0.67
1:C:317:ALA:O	1:C:356:GLY:HA3	1.95	0.67
1:A:56:LEU:C	1:A:56:LEU:HD23	2.20	0.66
1:C:42:GLN:HA	1:C:69:SER:HB3	1.78	0.66
1:D:98:GLY:HA3	5:D:668:HOH:O	1.94	0.66
1:C:233:ILE:HA	1:C:306:MET:HE3	1.78	0.66
1:C:113:GLY:C	1:C:115:ASP:H	2.02	0.66
1:A:137:LYS:HE2	1:C:137:LYS:HD3	1.77	0.65
1:B:121:PRO:HB3	1:B:123:ASP:OD2	1.96	0.65
1:C:335:VAL:HB	1:C:336:PRO:HD3	1.78	0.65
1:A:176:ALA:O	1:A:217:GLY:HA3	1.96	0.64
1:A:193:ASP:OD2	1:A:229:LEU:HD22	1.97	0.64
1:B:324:THR:HG23	1:B:351:THR:HG22	1.80	0.63
1:B:418:GLY:O	1:B:419:GLU:C	2.41	0.63
1:B:403:GLU:HG3	5:B:746:HOH:O	1.99	0.62
1:A:139:GLU:CB	1:A:142:TYR:CE2	2.64	0.62
1:D:323:ILE:HB	1:D:352:VAL:HG12	1.80	0.62
1:C:120:ARG:HG2	1:C:120:ARG:HH11	1.65	0.61
1:B:150:ARG:HH12	1:B:219:GLU:HA	1.65	0.61
1:B:334:HIS:HB3	1:B:372:ALA:HB1	1.83	0.61
1:C:313:LEU:C	1:C:313:LEU:HD23	2.26	0.61
1:A:135:GLU:HG2	1:A:146:SER:O	2.01	0.60
1:A:36:GLU:OE1	1:A:220:ARG:HD2	2.01	0.60
1:C:3:LYS:HG3	1:C:416:VAL:CG2	2.31	0.60
1:D:370:LEU:CD1	1:D:395:ILE:HA	2.32	0.60
1:A:336:PRO:HG2	1:B:333:MET:CE	2.31	0.60
1:A:160:LYS:HB2	1:A:160:LYS:NZ	2.17	0.60
1:A:86:LEU:C	1:A:88:LYS:H	2.10	0.59
1:A:15:GLU:HG2	1:A:250:VAL:HB	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:36:GLU:HB2	1:D:220:ARG:CZ	2.32	0.59
1:B:401:ARG:HH21	1:B:404:ASP:HB3	1.66	0.58
1:A:232:ARG:HB2	1:A:259:LEU:HD21	1.86	0.58
1:B:323:ILE:HB	1:B:352:VAL:CG1	2.34	0.58
1:B:64:VAL:HG22	1:B:72:ILE:CD1	2.34	0.58
1:B:401:ARG:HE	1:B:404:ASP:HB2	1.69	0.58
1:C:113:GLY:C	1:C:115:ASP:N	2.61	0.58
1:C:336:PRO:O	1:C:340:ARG:HG3	2.05	0.57
1:D:3:LYS:HE3	1:D:390:ASP:OD1	2.04	0.57
1:D:315:LEU:HD23	1:D:354:CYS:HB3	1.85	0.57
1:B:335:VAL:HB	1:B:336:PRO:HD3	1.87	0.57
1:C:10:THR:HG22	1:C:381:CYS:O	2.05	0.56
1:A:91:ARG:HG3	1:A:91:ARG:NH1	2.20	0.56
1:D:322:VAL:HG13	1:D:353:ILE:HD13	1.86	0.56
1:A:252:ARG:NH2	2:A:501:EDO:H12	2.21	0.56
1:B:315:LEU:HD23	1:B:354:CYS:HB3	1.87	0.56
1:D:2:ASP:HB3	1:D:392:ILE:HD11	1.87	0.56
1:B:361:SER:HB2	5:B:759:HOH:O	2.05	0.55
1:C:117:ILE:HD11	1:D:346:GLU:HG2	1.88	0.55
1:C:320:THR:HA	1:C:354:CYS:O	2.06	0.55
1:B:313:LEU:HD23	1:B:313:LEU:C	2.31	0.55
1:B:323:ILE:HB	1:B:352:VAL:HG13	1.89	0.54
1:B:83:PRO:HD2	1:B:86:LEU:HD11	1.89	0.54
1:C:193:ASP:CB	1:C:229:LEU:HD22	2.36	0.54
1:A:139:GLU:O	1:A:140:GLU:CB	2.42	0.54
1:C:193:ASP:CG	1:C:229:LEU:HD22	2.32	0.54
1:B:54:MET:HE1	1:B:66:ARG:CB	2.32	0.54
1:A:3:LYS:HG2	1:A:390:ASP:OD1	2.07	0.54
1:D:56:LEU:HD23	1:D:56:LEU:O	2.07	0.54
1:A:88:LYS:HG3	1:A:89:THR:N	2.23	0.53
1:B:64:VAL:HG22	1:B:72:ILE:HD13	1.89	0.53
1:D:36:GLU:HB2	1:D:220:ARG:NH2	2.24	0.53
1:B:417:LYS:O	1:B:419:GLU:HG2	2.08	0.53
1:C:348:GLU:OE2	1:D:120:ARG:HD2	2.08	0.53
1:B:84:TYR:CE2	1:B:88:LYS:HD3	2.44	0.53
1:B:139:GLU:HG3	1:B:140:GLU:HG2	1.91	0.53
1:D:243:ALA:HA	1:D:284:MET:CG	2.39	0.53
1:B:299:HIS:CG	1:B:300:PRO:HA	2.44	0.53
1:D:11:ARG:HB3	5:D:741:HOH:O	2.10	0.52
1:B:401:ARG:HH21	1:B:404:ASP:CB	2.22	0.52
1:C:176:ALA:O	1:C:217:GLY:HA3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:LEU:C	1:A:313:LEU:HD23	2.34	0.52
1:C:315:LEU:HD23	1:C:354:CYS:HB3	1.91	0.52
1:C:333:MET:HE2	1:D:336:PRO:HG2	1.92	0.52
1:B:118:GLY:O	1:B:119:ALA:HB2	2.09	0.52
1:C:22:LYS:HD3	1:C:47:LEU:CD1	2.40	0.52
1:A:56:LEU:HD23	1:A:56:LEU:O	2.09	0.52
1:D:306:MET:CE	1:D:309:GLN:NE2	2.73	0.52
1:B:3:LYS:HG2	1:B:390:ASP:HA	1.92	0.51
1:B:288:ARG:HG3	1:B:289:PRO:HD2	1.92	0.51
3:A:502:ACT:H3	4:A:503:UPG:O1B	2.11	0.51
1:D:54:MET:HE3	1:D:64:VAL:CG1	2.36	0.51
1:C:419:GLU:OXT	1:C:419:GLU:HG2	2.10	0.51
1:A:293:THR:OG1	1:D:183:GLU:HG2	2.10	0.50
1:D:126:ILE:HG12	1:D:143:VAL:HG21	1.93	0.50
1:A:160:LYS:HB2	1:A:160:LYS:HZ2	1.75	0.50
1:A:401:ARG:HH11	1:A:404:ASP:HB2	1.76	0.50
1:B:78:ASN:OD1	1:B:78:ASN:O	2.30	0.50
1:D:193:ASP:CG	1:D:229:LEU:HD22	2.36	0.50
1:D:305:ASP:O	1:D:306:MET:HE2	2.12	0.50
1:C:282:LEU:C	1:C:282:LEU:HD23	2.37	0.50
1:D:193:ASP:CB	1:D:229:LEU:HD22	2.41	0.50
1:C:416:VAL:HG23	1:C:416:VAL:O	2.12	0.50
1:D:230:PRO:HD3	2:D:501:EDO:H12	1.94	0.49
1:C:56:LEU:C	1:C:56:LEU:HD23	2.37	0.49
1:C:303:PRO:HG2	1:C:306:MET:HB2	1.94	0.49
1:D:299:HIS:CG	1:D:300:PRO:HA	2.48	0.49
1:C:339:ILE:C	1:C:341:MET:H	2.18	0.49
1:D:359:LYS:HD2	1:D:384:GLU:HB2	1.95	0.49
1:C:113:GLY:HA3	5:C:765:HOH:O	2.13	0.49
1:C:401:ARG:HG3	1:C:401:ARG:HH11	1.77	0.49
1:C:91:ARG:HB2	1:C:119:ALA:HB2	1.95	0.49
1:A:24:ALA:HB2	1:A:229:LEU:HD21	1.95	0.48
1:A:323:ILE:HB	1:A:352:VAL:HG12	1.95	0.48
1:D:110:SER:HB2	2:D:506:EDO:O1	2.13	0.48
1:D:139:GLU:HB2	1:D:142:TYR:CE2	2.48	0.48
1:A:297:ALA:HB1	1:A:298:PRO:CD	2.44	0.48
1:C:314:ASN:HB3	1:C:354:CYS:HB2	1.95	0.48
1:B:320:THR:HA	1:B:354:CYS:O	2.14	0.48
5:C:665:HOH:O	1:D:330:ASN:HB2	2.11	0.48
1:A:315:LEU:HD21	1:A:345:ALA:HB2	1.95	0.48
1:C:357:VAL:HG22	5:C:626:HOH:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:359:LYS:HD3	1:C:384:GLU:HB2	1.96	0.48
1:A:117:ILE:O	1:A:117:ILE:HG22	2.12	0.48
1:A:243:ALA:HA	1:A:284:MET:HG3	1.95	0.47
1:B:56:LEU:HD23	1:B:56:LEU:C	2.39	0.47
1:A:86:LEU:C	1:A:88:LYS:N	2.72	0.47
1:A:193:ASP:OD2	1:A:229:LEU:CD2	2.61	0.47
1:A:401:ARG:NH1	1:A:401:ARG:HG3	2.29	0.47
1:A:282:LEU:C	1:A:282:LEU:HD23	2.40	0.47
1:C:21:ALA:HB2	1:C:231:ASP:HA	1.96	0.47
1:A:401:ARG:NH1	1:A:404:ASP:HB2	2.29	0.47
1:C:288:ARG:HG3	1:C:289:PRO:HD2	1.96	0.47
1:D:306:MET:HE1	1:D:309:GLN:NE2	2.29	0.47
1:C:22:LYS:HD3	1:C:47:LEU:HD13	1.97	0.47
1:C:54:MET:HE1	1:C:66:ARG:HG2	1.97	0.47
1:D:20:GLY:HA3	1:D:43:ASN:O	2.15	0.47
1:C:3:LYS:HG3	1:C:416:VAL:HG23	1.96	0.47
1:C:84:TYR:HE1	1:C:112:PRO:HA	1.78	0.47
1:D:80:PHE:HD1	1:D:100:LEU:HD22	1.79	0.47
1:D:56:LEU:HD23	1:D:56:LEU:C	2.40	0.46
1:A:85:ASP:HB3	5:A:770:HOH:O	2.15	0.46
1:A:243:ALA:HA	1:A:284:MET:CG	2.44	0.46
1:B:419:GLU:OE1	1:B:419:GLU:HA	2.15	0.46
1:C:233:ILE:HG21	1:C:371:ARG:CZ	2.46	0.46
1:C:227:ARG:HD3	5:C:738:HOH:O	2.15	0.46
1:A:299:HIS:CG	1:A:300:PRO:HA	2.51	0.46
1:A:244:ILE:HD12	1:A:382:ILE:HD13	1.96	0.46
1:C:126:ILE:HG23	1:C:136:ILE:HG21	1.98	0.46
1:C:346:GLU:CD	1:D:117:ILE:HG23	2.40	0.46
1:B:244:ILE:HD12	1:B:382:ILE:HD13	1.97	0.46
1:D:401:ARG:NH1	1:D:401:ARG:CG	2.76	0.46
1:B:359:LYS:HZ1	1:B:384:GLU:HB2	1.79	0.46
1:D:4:PHE:CD1	1:D:392:ILE:HG21	2.51	0.46
1:C:401:ARG:HH11	1:C:404:ASP:HB2	1.80	0.46
1:D:128:GLY:HA3	1:D:169:ILE:HD11	1.98	0.46
1:A:87:VAL:HA	1:A:93:SER:OG	2.15	0.45
1:B:289:PRO:HG2	1:B:317:ALA:HA	1.98	0.45
1:B:364:GLN:HG2	1:B:388:VAL:HB	1.99	0.45
1:D:227:ARG:HE	2:D:501:EDO:C2	2.29	0.45
1:C:212:ARG:HH11	2:C:501:EDO:C2	2.29	0.45
1:A:7:GLN:HB2	1:A:412:ASN:CG	2.42	0.45
1:D:282:LEU:HD23	1:D:282:LEU:C	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:GLU:O	1:A:139:GLU:HG3	2.15	0.45
1:A:252:ARG:HH22	2:A:501:EDO:H12	1.80	0.45
1:B:83:PRO:HD2	1:B:86:LEU:CD1	2.46	0.45
1:C:334:HIS:O	1:C:338:LEU:HG	2.17	0.45
1:D:142:TYR:CD1	1:D:142:TYR:C	2.94	0.45
1:B:359:LYS:NZ	1:B:384:GLU:OE1	2.50	0.45
1:A:193:ASP:HB2	1:A:229:LEU:HD22	1.97	0.45
1:D:7:GLN:HB2	1:D:412:ASN:CG	2.42	0.45
1:D:323:ILE:HB	1:D:352:VAL:CG1	2.45	0.45
1:C:3:LYS:HB3	1:C:390:ASP:HA	1.99	0.45
1:C:212:ARG:NH1	2:C:501:EDO:H21	2.32	0.45
1:D:370:LEU:HD12	1:D:395:ILE:HA	1.98	0.45
1:A:111:LEU:O	1:A:141:GLY:HA2	2.17	0.44
1:D:313:LEU:C	1:D:313:LEU:HD23	2.42	0.44
1:B:143:VAL:HG13	1:B:143:VAL:O	2.18	0.44
1:B:416:VAL:HG23	1:B:416:VAL:O	2.17	0.44
1:B:419:GLU:OE1	1:B:419:GLU:CA	2.60	0.44
1:C:325:GLU:O	1:C:350:ASN:ND2	2.51	0.44
1:A:137:LYS:HB2	1:A:137:LYS:HE3	1.69	0.44
1:A:158:MET:HE3	5:A:601:HOH:O	2.17	0.44
1:B:176:ALA:O	1:B:217:GLY:HA3	2.18	0.44
1:D:370:LEU:HD21	1:D:398:GLY:HA3	1.99	0.44
1:A:315:LEU:HD22	1:A:343:ALA:HB1	2.00	0.44
1:C:339:ILE:C	1:C:341:MET:N	2.75	0.44
1:C:85:ASP:O	1:C:88:LYS:HG2	2.18	0.44
1:B:15:GLU:CG	1:B:250:VAL:HB	2.37	0.44
1:C:347:ILE:CD1	1:D:333:MET:HE1	2.48	0.44
1:D:314:ASN:HB3	1:D:354:CYS:HB2	1.99	0.44
1:C:212:ARG:HH11	2:C:501:EDO:H21	1.83	0.43
1:C:295:ARG:HG2	1:C:324:THR:HB	2.00	0.43
1:A:24:ALA:CB	1:A:229:LEU:CD2	2.96	0.43
1:B:24:ALA:C	1:B:27:PRO:HD2	2.43	0.43
1:C:1:MET:HE3	1:C:391:ARG:HH12	1.83	0.43
1:B:41:ILE:O	1:B:69:SER:HB2	2.19	0.43
1:C:120:ARG:HG2	1:C:120:ARG:NH1	2.31	0.43
1:C:135:GLU:OE1	1:C:137:LYS:HE2	2.19	0.43
1:D:91:ARG:HG3	1:D:91:ARG:HH11	1.83	0.43
1:A:118:GLY:C	1:A:120:ARG:H	2.25	0.43
1:D:3:LYS:HG3	1:D:416:VAL:HG23	2.01	0.43
1:C:193:ASP:HB2	1:C:229:LEU:HD22	2.00	0.43
1:C:370:LEU:HD13	1:C:394:HIS:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:160:LYS:HB2	1:D:160:LYS:NZ	2.34	0.43
1:B:54:MET:CE	1:B:66:ARG:HB3	2.36	0.42
1:C:65:GLU:HB2	5:C:632:HOH:O	2.18	0.42
1:A:9:PRO:HD3	1:A:384:GLU:HA	2.01	0.42
1:B:2:ASP:OD2	1:B:415:ARG:HD3	2.19	0.42
1:B:42:GLN:HA	1:B:69:SER:CB	2.37	0.42
1:C:419:GLU:OXT	1:C:419:GLU:CG	2.68	0.42
1:A:56:LEU:HA	1:A:86:LEU:HD13	2.01	0.42
1:A:114:GLY:HA3	1:C:131:LYS:NZ	2.34	0.42
1:B:54:MET:HE3	1:B:70:VAL:CG1	2.43	0.42
1:C:338:LEU:HD21	1:C:376:LEU:HD23	2.01	0.42
1:D:160:LYS:NZ	1:D:160:LYS:CB	2.82	0.42
1:D:306:MET:HE2	1:D:309:GLN:NE2	2.33	0.42
1:D:317:ALA:O	1:D:356:GLY:HA3	2.19	0.42
1:D:233:ILE:CG2	1:D:306:MET:HE3	2.32	0.42
1:A:34:LEU:HD21	1:A:99:PRO:HA	2.01	0.42
1:A:317:ALA:O	1:A:356:GLY:HA3	2.20	0.42
1:B:317:ALA:O	1:B:356:GLY:HA3	2.19	0.42
1:A:370:LEU:HD12	1:A:395:ILE:HA	2.02	0.42
1:A:322:VAL:HG13	1:A:353:ILE:HD13	2.01	0.42
1:C:7:GLN:HB2	1:C:412:ASN:HB3	2.02	0.42
1:C:81:SER:HB2	1:C:108:GLN:CG	2.50	0.42
1:C:144:LYS:HG2	1:C:145:ALA:N	2.35	0.42
1:D:131:LYS:HE3	1:D:131:LYS:HB3	1.83	0.42
1:A:4:PHE:HD2	1:A:4:PHE:HA	1.80	0.41
1:A:232:ARG:HB2	1:A:259:LEU:CD2	2.50	0.41
1:B:405:LYS:HD2	5:B:735:HOH:O	2.18	0.41
1:C:120:ARG:N	1:C:121:PRO:HD2	2.35	0.41
1:D:294:VAL:HB	1:D:323:ILE:HD13	2.02	0.41
1:C:4:PHE:CD2	1:C:392:ILE:HD13	2.55	0.41
1:A:119:ALA:O	1:A:121:PRO:HD3	2.21	0.41
1:A:264:ALA:O	1:A:268:GLU:HG3	2.20	0.41
1:B:401:ARG:NH2	1:B:404:ASP:OD1	2.53	0.41
1:D:243:ALA:HA	1:D:284:MET:HG3	2.01	0.41
1:A:252:ARG:HD2	5:A:699:HOH:O	2.20	0.41
1:C:233:ILE:CG2	1:C:306:MET:CE	2.93	0.41
1:A:54:MET:HE3	1:A:64:VAL:HG12	2.01	0.41
1:B:188:GLU:HA	1:B:189:PRO:HD3	1.95	0.41
1:C:80:PHE:CD2	1:C:106:GLN:NE2	2.89	0.41
1:C:220:ARG:NH1	5:C:689:HOH:O	2.53	0.41
1:D:54:MET:CE	1:D:64:VAL:HG12	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:81:SER:HB3	1:D:108:GLN:HB3	2.03	0.41
1:C:401:ARG:HD2	1:C:404:ASP:OD1	2.20	0.41
1:C:22:LYS:HD3	1:C:47:LEU:HD12	2.03	0.40
1:D:139:GLU:O	1:D:140:GLU:C	2.63	0.40
1:A:288:ARG:CG	1:A:289:PRO:HD2	2.51	0.40
1:B:243:ALA:HA	1:B:284:MET:CG	2.52	0.40
1:C:11:ARG:NE	1:C:245:SER:O	2.55	0.40
1:C:401:ARG:HG3	1:C:401:ARG:NH1	2.36	0.40
1:A:42:GLN:HB3	1:A:69:SER:OG	2.22	0.40
1:A:314:ASN:HB3	1:A:354:CYS:HB2	2.03	0.40
1:C:299:HIS:CG	1:C:300:PRO:HA	2.57	0.40
1:D:259:LEU:O	1:D:260:ASP:C	2.64	0.40
1:B:288:ARG:CG	1:B:289:PRO:HD2	2.52	0.40
1:C:243:ALA:HA	1:C:284:MET:CG	2.52	0.40
1:D:67:IAS:CG	1:D:69:SER:N	2.79	0.40
1:D:240:VAL:O	1:D:244:ILE:HG12	2.21	0.40

There are no symmetry-related clashes.

## 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	415/419 (99%)	395 (95%)	17 (4%)	3 (1%)	18	23
1	B	415/419 (99%)	404 (97%)	9 (2%)	2 (0%)	24	31
1	C	415/419 (99%)	388 (94%)	25 (6%)	2 (0%)	24	31
1	D	415/419 (99%)	403 (97%)	12 (3%)	0	100	100
All	All	1660/1676 (99%)	1590 (96%)	63 (4%)	7 (0%)	30	38

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	120	ARG
1	A	140	GLU
1	B	119	ALA
1	A	88	LYS
1	A	118	GLY
1	B	117	ILE
1	C	118	GLY

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	329/329 (100%)	322 (98%)	7 (2%)	47	66
1	B	329/329 (100%)	328 (100%)	1 (0%)	86	93
1	C	329/329 (100%)	324 (98%)	5 (2%)	57	75
1	D	329/329 (100%)	324 (98%)	5 (2%)	57	75
All	All	1316/1316 (100%)	1298 (99%)	18 (1%)	59	76

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	87	VAL
1	A	106	GLN
1	A	135	GLU
1	A	139	GLU
1	A	160	LYS
1	A	336	PRO
1	A	397	ARG
1	B	39	VAL
1	C	87	VAL
1	C	91	ARG
1	C	103	ARG
1	C	158	MET
1	C	159	ASP
1	D	160	LYS
1	D	329	GLU

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Mol	Chain	Res	Type
1	D	351	THR
1	D	359	LYS
1	D	401	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	B	78	ASN
1	B	330	ASN
1	B	364	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

4 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	$\# Z  > 2$
1	IAS	B	67	1	6,7,8	1.10	0	3,8,10	0.95	0
1	IAS	C	67	1	6,7,8	1.10	0	3,8,10	1.05	0
1	IAS	A	67	1	6,7,8	0.92	0	3,8,10	1.06	0
1	IAS	D	67	1	6,7,8	1.03	0	3,8,10	0.88	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
1	IAS	B	67	1	-	1/7/7/8	-
1	IAS	C	67	1	-	0/7/7/8	-
1	IAS	A	67	1	-	2/7/7/8	-
1	IAS	D	67	1	-	2/7/7/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	D	67	IAS	O-C-CA-CB
1	A	67	IAS	O-C-CA-CB
1	A	67	IAS	OXT-C-CA-CB
1	D	67	IAS	OXT-C-CA-CB
1	B	67	IAS	OXT-C-CA-CB

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	67	IAS	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

15 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
2	EDO	C	501	-	3,3,3	0.49	0	2,2,2	0.35	0
3	ACT	A	502	-	3,3,3	1.07	0	3,3,3	0.82	0
2	EDO	D	501	-	3,3,3	0.61	0	2,2,2	0.31	0
4	UPG	D	508	-	37,38,38	1.42	5 (13%)	55,58,58	1.89	10 (18%)
2	EDO	D	503	-	3,3,3	0.48	0	2,2,2	0.35	0
2	EDO	D	505	-	3,3,3	0.60	0	2,2,2	0.25	0
4	UPG	A	503	-	37,38,38	1.23	3 (8%)	55,58,58	1.87	9 (16%)
2	EDO	C	502	-	3,3,3	0.43	0	2,2,2	0.38	0
2	EDO	B	501	-	3,3,3	0.55	0	2,2,2	0.34	0
2	EDO	D	502	-	3,3,3	0.53	0	2,2,2	0.31	0
2	EDO	A	501	-	3,3,3	0.49	0	2,2,2	0.32	0
3	ACT	D	507	-	3,3,3	1.07	0	3,3,3	0.84	0
2	EDO	D	506	-	3,3,3	0.42	0	2,2,2	0.34	0
2	EDO	B	502	-	3,3,3	0.50	0	2,2,2	0.33	0
2	EDO	D	504	-	3,3,3	0.48	0	2,2,2	0.34	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
2	EDO	C	501	-	-	1/1/1/1	-
2	EDO	D	501	-	-	1/1/1/1	-
4	UPG	D	508	-	-	1/23/59/59	0/3/3/3
2	EDO	D	503	-	-	0/1/1/1	-
2	EDO	D	505	-	-	0/1/1/1	-
4	UPG	A	503	-	-	2/23/59/59	0/3/3/3
2	EDO	C	502	-	-	1/1/1/1	-
2	EDO	B	501	-	-	1/1/1/1	-
2	EDO	D	502	-	-	1/1/1/1	-
2	EDO	A	501	-	-	1/1/1/1	-
2	EDO	D	506	-	-	1/1/1/1	-
2	EDO	B	502	-	-	1/1/1/1	-
2	EDO	D	504	-	-	0/1/1/1	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	508	UPG	PB-O3A	4.34	1.64	1.59
4	D	508	UPG	PA-O3A	3.90	1.63	1.59
4	A	503	UPG	PA-O3A	3.21	1.63	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	503	UPG	PB-O3A	2.58	1.62	1.59
4	D	508	UPG	O4C-C1C	2.23	1.47	1.42
4	A	503	UPG	O5'-C1'	2.19	1.47	1.41
4	D	508	UPG	O5'-C1'	2.11	1.47	1.41
4	D	508	UPG	C5C-C4C	2.08	1.57	1.51

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	503	UPG	O5C-PA-O1A	-6.93	81.49	108.94
4	D	508	UPG	O5C-PA-O1A	-6.85	81.80	108.94
4	A	503	UPG	O2A-PA-O5C	-4.70	86.28	107.57
4	A	503	UPG	C4-N3-C2	-4.63	120.87	126.61
4	D	508	UPG	O2A-PA-O5C	-4.28	88.19	107.57
4	D	508	UPG	C4-N3-C2	-4.26	121.32	126.61
4	A	503	UPG	C5-C4-N3	3.91	120.27	114.80
4	D	508	UPG	N3-C2-N1	3.85	119.90	114.89
4	D	508	UPG	O2A-PA-O3A	3.84	117.64	107.27
4	D	508	UPG	C5-C4-N3	3.72	120.01	114.80
4	A	503	UPG	N3-C2-N1	3.72	119.73	114.89
4	A	503	UPG	O2A-PA-O3A	3.51	116.76	107.27
4	A	503	UPG	O4-C4-C5	-3.11	119.80	125.16
4	D	508	UPG	O4-C4-C5	-2.94	120.10	125.16
4	A	503	UPG	PB-O3B-C1'	-2.79	109.87	121.21
4	D	508	UPG	O3A-PA-O1A	2.49	118.18	110.70
4	A	503	UPG	O2A-PA-O1A	2.47	123.93	112.44
4	D	508	UPG	PB-O3B-C1'	-2.31	111.81	121.21
4	D	508	UPG	C3C-C2C-C1C	2.28	105.78	101.46

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	503	UPG	O4C-C4C-C5C-O5C
4	A	503	UPG	C3C-C4C-C5C-O5C
2	B	502	EDO	O1-C1-C2-O2
2	D	502	EDO	O1-C1-C2-O2
2	C	502	EDO	O1-C1-C2-O2
2	C	501	EDO	O1-C1-C2-O2
2	A	501	EDO	O1-C1-C2-O2
2	D	506	EDO	O1-C1-C2-O2
2	B	501	EDO	O1-C1-C2-O2

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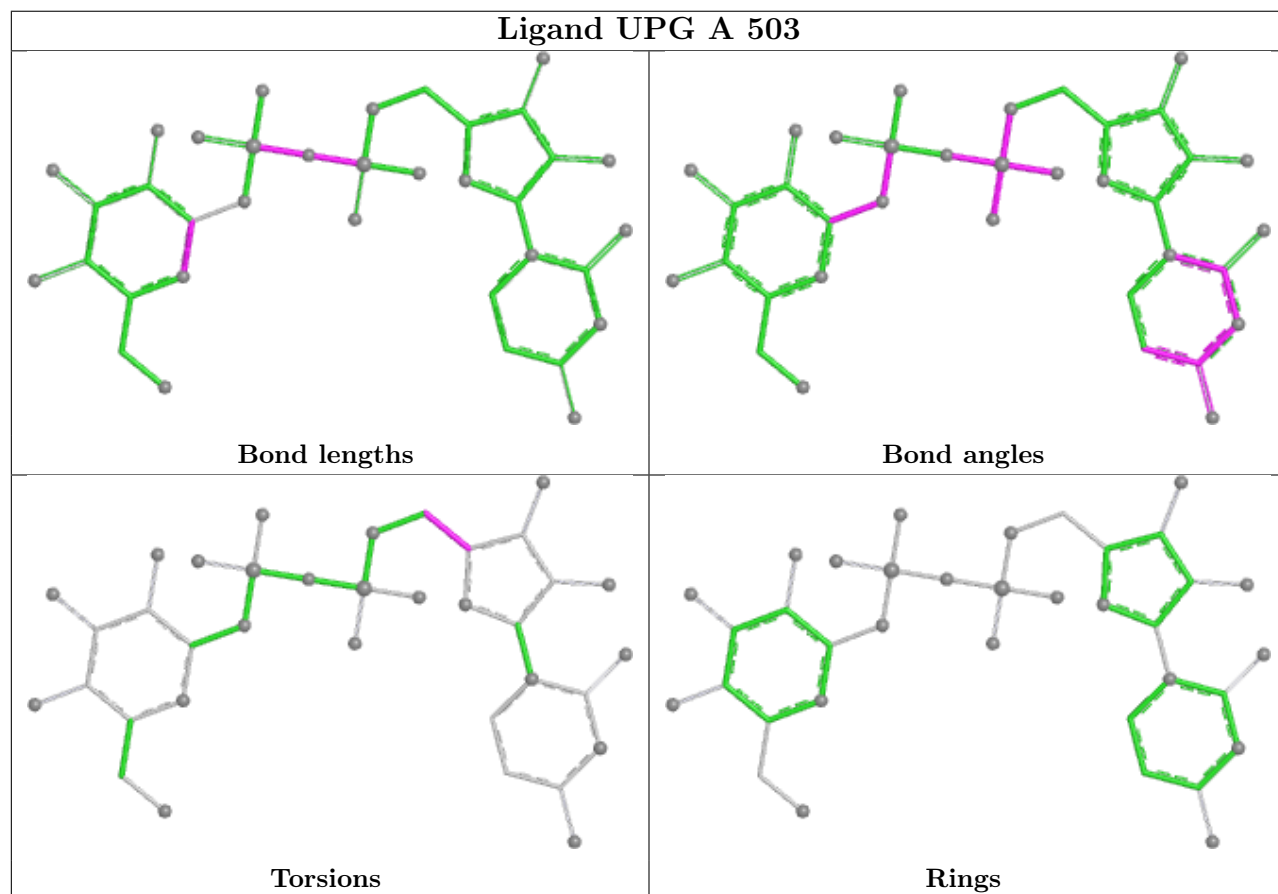
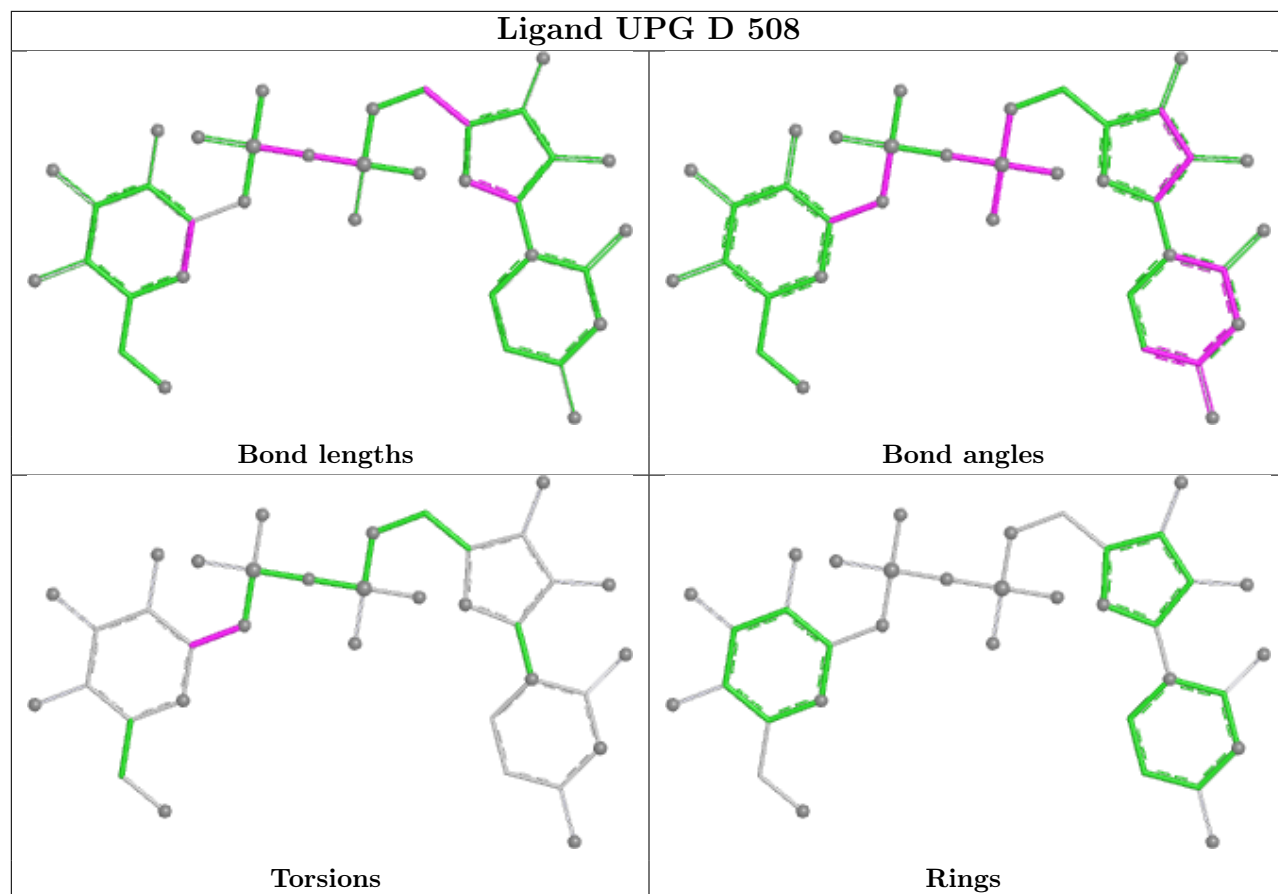
Mol	Chain	Res	Type	Atoms
2	D	501	EDO	O1-C1-C2-O2
4	D	508	UPG	C2'-C1'-O3B-PB

There are no ring outliers.

6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	501	EDO	3	0
3	A	502	ACT	1	0
2	D	501	EDO	2	0
4	A	503	UPG	1	0
2	A	501	EDO	2	0
2	D	506	EDO	2	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	418/419 (99%)	-0.20	17 (4%) 41 43	14, 25, 50, 87	0
1	B	418/419 (99%)	-0.29	12 (2%) 53 56	14, 25, 44, 87	0
1	C	418/419 (99%)	-0.10	16 (3%) 44 46	13, 26, 52, 91	0
1	D	418/419 (99%)	-0.38	4 (0%) 79 80	14, 25, 42, 61	0
All	All	1672/1676 (99%)	-0.24	49 (2%) 53 56	13, 25, 48, 91	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	117	ILE	6.7
1	A	116	ALA	6.4
1	A	117	ILE	5.7
1	B	117	ILE	5.1
1	C	114	GLY	5.0
1	B	118	GLY	4.5
1	C	116	ALA	4.3
1	B	116	ALA	4.2
1	A	118	GLY	4.0
1	B	120	ARG	3.7
1	C	120	ARG	3.7
1	A	418	GLY	3.6
1	C	115	ASP	3.5
1	B	119	ALA	3.5
1	C	119	ALA	3.3
1	B	115	ASP	3.3
1	B	113	GLY	3.3
1	C	418	GLY	3.2
1	A	88	LYS	3.1
1	C	419	GLU	3.1
1	C	416	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	89	THR	2.9
1	A	115	ASP	2.9
1	C	113	GLY	2.7
1	A	84	TYR	2.7
1	A	141	GLY	2.7
1	C	118	GLY	2.7
1	D	330	ASN	2.6
1	A	329	GLU	2.6
1	B	121	PRO	2.6
1	C	417	LYS	2.6
1	C	112	PRO	2.5
1	C	121	PRO	2.5
1	B	417	LYS	2.4
1	D	76	ASN	2.4
1	D	419	GLU	2.4
1	A	86	LEU	2.4
1	A	114	GLY	2.3
1	A	87	VAL	2.3
1	A	85	ASP	2.2
1	B	59	GLN	2.2
1	A	119	ALA	2.2
1	A	113	GLY	2.2
1	B	114	GLY	2.2
1	C	328	PHE	2.1
1	B	418	GLY	2.1
1	D	418	GLY	2.1
1	A	120	ARG	2.0
1	C	111	LEU	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
1	IAS	B	67	8/9	0.84	0.11	37,37,38,40	0
1	IAS	A	67	8/9	0.89	0.08	33,35,36,38	0
1	IAS	D	67	8/9	0.89	0.07	34,36,38,39	0
1	IAS	C	67	8/9	0.93	0.08	19,23,26,27	0

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.4 Ligands [i](#)

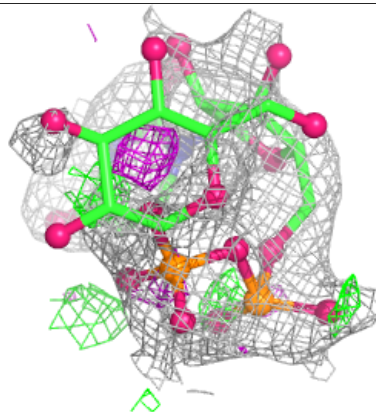
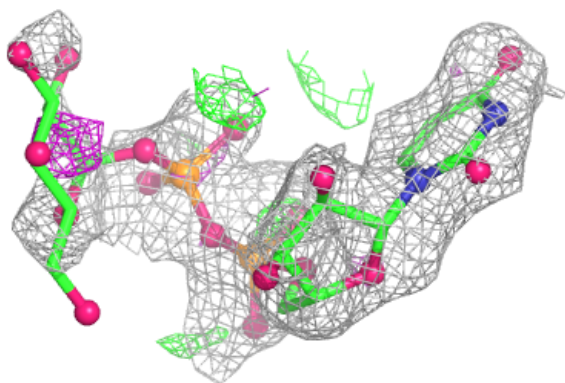
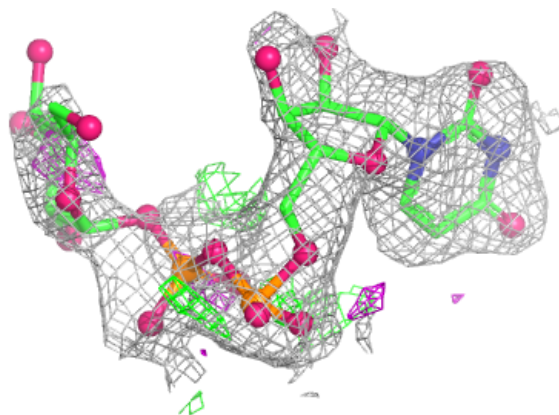
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

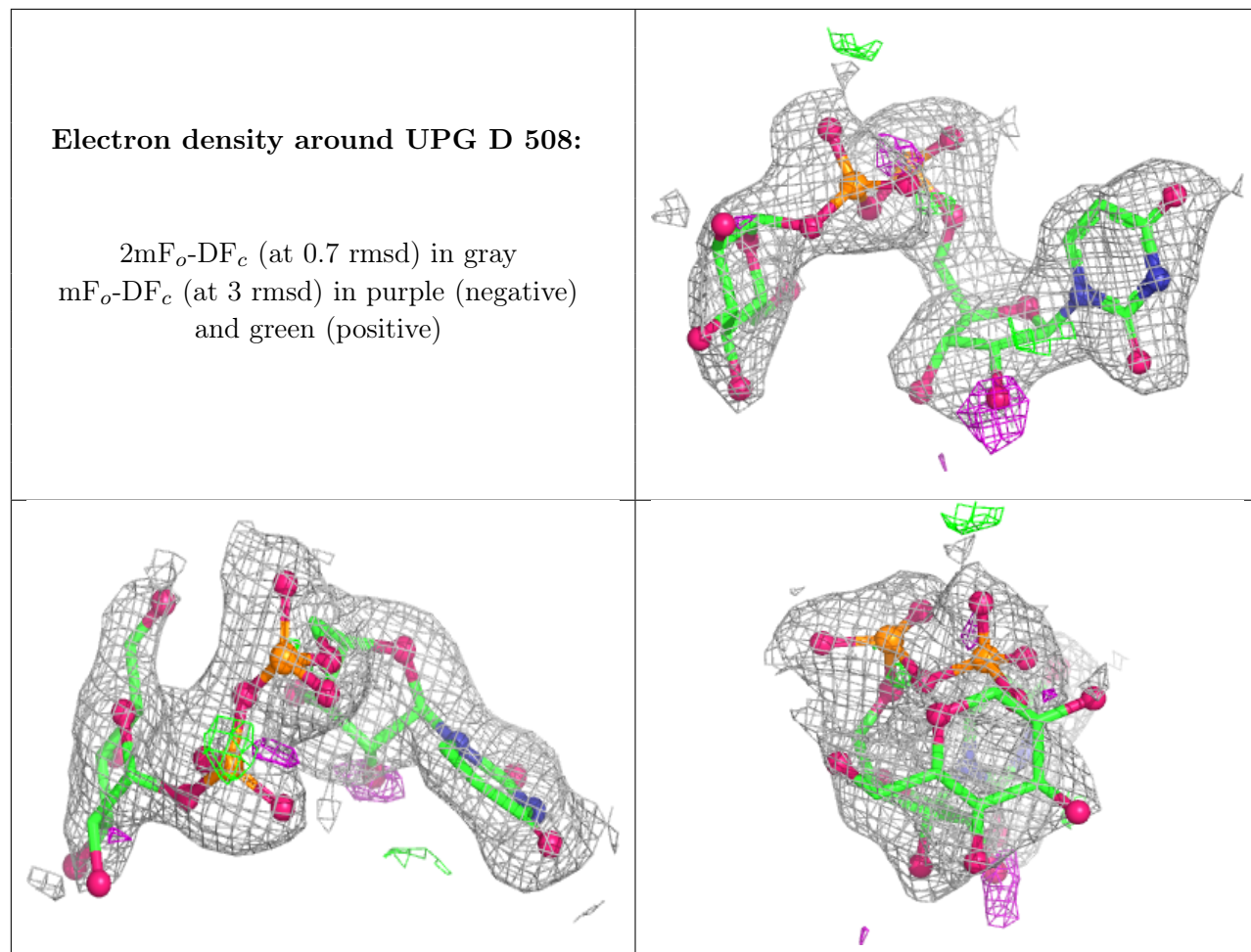
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	EDO	B	501	4/4	0.68	0.23	55,55,56,56	0
3	ACT	D	507	4/4	0.68	0.16	51,52,52,53	0
2	EDO	D	505	4/4	0.69	0.17	51,51,51,52	0
2	EDO	B	502	4/4	0.74	0.15	56,56,56,56	0
4	UPG	A	503	36/36	0.76	0.16	69,79,91,91	0
3	ACT	A	502	4/4	0.77	0.13	41,41,42,43	0
2	EDO	D	504	4/4	0.78	0.16	55,57,57,57	0
2	EDO	A	501	4/4	0.80	0.14	54,54,55,56	0
2	EDO	D	501	4/4	0.80	0.14	45,45,46,47	0
2	EDO	D	506	4/4	0.80	0.21	60,61,61,62	0
2	EDO	C	502	4/4	0.81	0.11	45,46,47,47	0
2	EDO	D	502	4/4	0.82	0.16	51,53,54,54	0
4	UPG	D	508	36/36	0.91	0.10	33,42,61,62	0
2	EDO	C	501	4/4	0.92	0.12	26,29,31,31	0
2	EDO	D	503	4/4	0.95	0.06	34,35,37,37	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 UPG A 503:**

$2mF_o-DF_c$  (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.