



Full wwPDB X-ray Structure Validation Report ⓘ

May 7, 2026 – 08:13 AM EDT

PDB ID : 7ZKW / pdb_00007zkw
Title : Crystal structure of cystinosin from Arabidopsis thaliana in complex with Cystine and sybody
Authors : Parker, J.L.; Loebel, M.; Newstead, S.
Deposited on : 2022-04-13
Resolution : 3.37 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

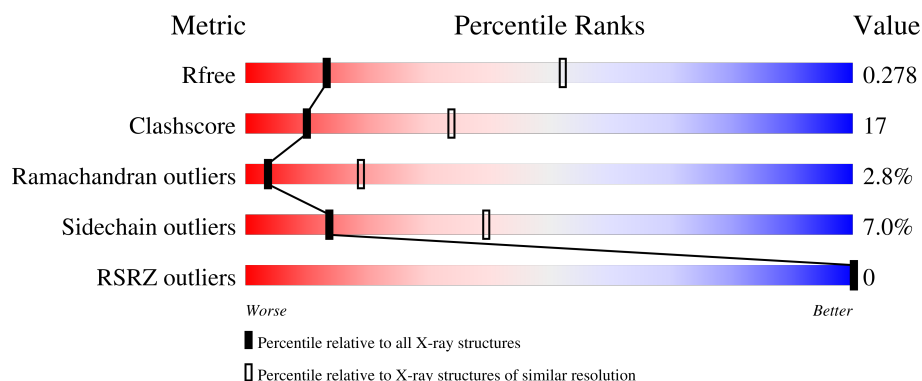
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.37 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	1047 (3.42-3.34)
Clashscore	190562	1067 (3.42-3.34)
Ramachandran outliers	187476	1056 (3.42-3.34)
Sidechain outliers	187428	1056 (3.42-3.34)
RSRZ outliers	180081	1047 (3.42-3.34)

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	 57% 26% 5% 12%
1	B	277	 55% 26% 6% 12%
2	C	121	 67% 25% 6% 2%
2	D	121	 67% 30% 3% 2%

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
3	IYY	B	301	-	-	X	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 11744 atoms, of which 5818 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 Cystinosin homolog.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	243	Total	C	H	N	O	S	116	0	0
			3978	1330	1991	310	335	12			
1	B	243	Total	C	H	N	O	S	116	0	0
			3978	1330	1991	310	335	12			

There are 14 discrepancies between the modelled and reference sequences:

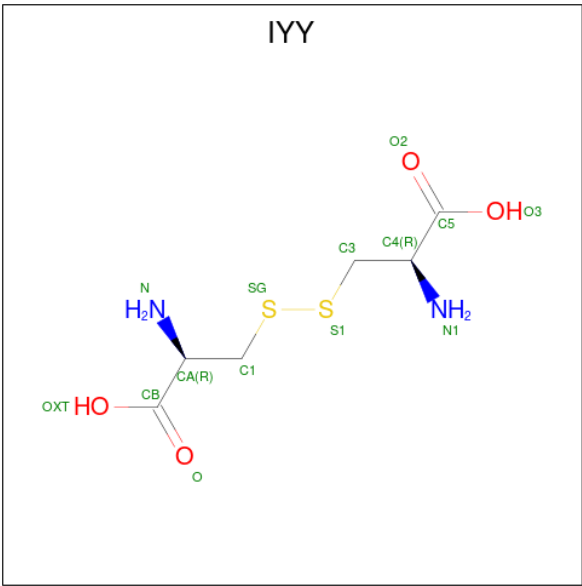
Chain	Residue	Modelled	Actual	Comment	Reference
A	271	GLY	-	expression tag	UNP P57758
A	272	GLU	-	expression tag	UNP P57758
A	273	ASN	-	expression tag	UNP P57758
A	274	LEU	-	expression tag	UNP P57758
A	275	TYR	-	expression tag	UNP P57758
A	276	PHE	-	expression tag	UNP P57758
A	277	GLN	-	expression tag	UNP P57758
B	271	GLY	-	expression tag	UNP P57758
B	272	GLU	-	expression tag	UNP P57758
B	273	ASN	-	expression tag	UNP P57758
B	274	LEU	-	expression tag	UNP P57758
B	275	TYR	-	expression tag	UNP P57758
B	276	PHE	-	expression tag	UNP P57758
B	277	GLN	-	expression tag	UNP P57758

- Molecule 2 is a protein called sybody.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	121	Total	C	H	N	O	S	71	0	0
			1868	604	906	170	184	4			
2	D	121	Total	C	H	N	O	S	71	0	0
			1868	604	906	170	184	4			

- Molecule 3 is L-cystine (CCD ID: IYY) (formula: C₆H₁₂N₂O₄S₂) (labeled as "Ligand of

Interest" by depositor).

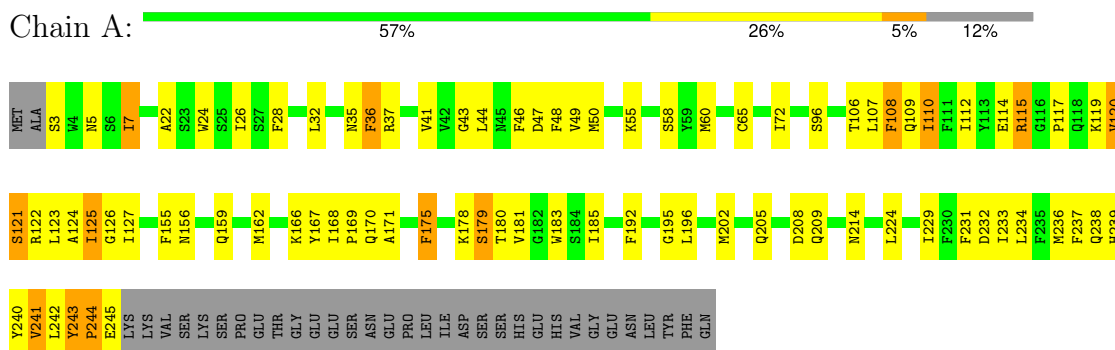


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	S	1	0
			26	6	12	2	4	2		
3	B	1	Total	C	H	N	O	S	1	0
			26	6	12	2	4	2		

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: Cystinosin homolog

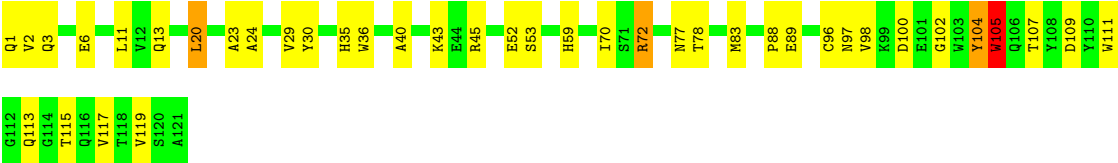


Chain D:

67%

30%

..



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	283.37Å 64.06Å 55.44Å 90.00° 99.95° 90.00°	Depositor
Resolution (Å)	69.78 – 3.37 69.78 – 3.45	Depositor EDS
% Data completeness (in resolution range)	92.8 (69.78-3.37) 92.8 (69.78-3.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.11 (at 3.49Å)	Xtriage
Refinement program	REFMAC 5.8.0350	Depositor
R, R_{free}	0.249 , 0.280 0.249 , 0.278	Depositor DCC
R_{free} test set	637 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	74.6	Xtriage
Anisotropy	0.246	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 0.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.31$, $\langle L^2 \rangle = 0.15$	Xtriage
Estimated twinning fraction	0.307 for -h-2*1,-k,l	Xtriage
Reported twinning fraction	0.676 for H, K, L 0.324 for -H-4/2L, -K, L	Depositor
Outliers	3 of 13058 reflections (0.023%)	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	11744	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.35% 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: IYY

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	0.89	0/2049	1.44	10/2789 (0.4%)
1	B	0.92	1/2049 (0.0%)	1.45	11/2789 (0.4%)
2	C	0.88	0/987	1.54	13/1340 (1.0%)
2	D	0.86	2/987 (0.2%)	1.49	9/1340 (0.7%)
All	All	0.90	3/6072 (0.0%)	1.47	43/8258 (0.5%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	35	HIS	CE1-NE2	6.06	1.38	1.32
1	B	23	SER	C-O	5.35	1.30	1.24
2	D	59	HIS	CE1-NE2	5.08	1.37	1.32

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	74	ASN	CA-CB-CG	-13.16	99.44	112.60
2	D	72	ARG	NE-CZ-NH2	-10.25	109.97	119.20
1	B	56	HIS	CA-CB-CG	-9.93	103.87	113.80
2	D	89	GLU	CB-CG-CD	9.84	129.33	112.60
2	C	72	ARG	NE-CZ-NH1	9.77	131.27	121.50
2	D	72	ARG	NE-CZ-NH1	9.33	130.83	121.50
2	D	72	ARG	CD-NE-CZ	9.21	137.30	124.40
2	C	72	ARG	NE-CZ-NH2	-8.93	111.17	119.20
2	C	104	TYR	CA-C-O	-8.86	109.26	119.98
2	C	72	ARG	CD-NE-CZ	8.64	136.50	124.40
2	C	104	TYR	CB-CA-C	8.53	123.94	111.65
1	A	237	PHE	CA-CB-CG	7.76	121.56	113.80
2	D	104	TYR	CA-C-O	-7.34	110.01	120.51
2	D	45	ARG	NE-CZ-NH1	-7.29	114.21	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	31	ARG	CB-CG-CD	7.16	127.77	111.30
1	A	175	PHE	CA-CB-CG	7.13	120.94	113.80
1	B	175	PHE	CA-CB-CG	6.94	120.74	113.80
2	C	44	GLU	CB-CG-CD	6.86	124.26	112.60
2	D	13	GLN	CB-CG-CD	-6.50	101.56	112.60
1	B	122	ARG	N-CA-C	-6.07	100.56	109.18
2	D	45	ARG	NE-CZ-NH2	6.05	124.65	119.20
1	B	38	ARG	CB-CA-C	-5.89	99.03	110.75
2	C	57	GLU	CB-CG-CD	5.85	122.55	112.60
2	C	2	VAL	N-CA-CB	5.80	118.56	110.56
2	D	104	TYR	CB-CA-C	5.79	121.94	110.42
1	A	241	VAL	CA-C-N	5.67	129.33	120.82
1	A	241	VAL	C-N-CA	5.67	129.33	120.82
1	B	44	LEU	N-CA-CB	-5.55	100.87	109.69
1	B	38	ARG	CG-CD-NE	-5.54	99.82	112.00
1	B	180	THR	CA-CB-OG1	-5.52	101.33	109.60
1	A	115	ARG	CA-C-O	5.51	128.38	120.51
2	C	112	GLY	CA-C-O	-5.50	116.29	121.90
1	A	115	ARG	O-C-N	5.37	129.73	122.59
2	C	31	ARG	CD-NE-CZ	5.25	131.75	124.40
1	B	82	ASP	CA-CB-CG	-5.19	107.41	112.60
1	B	82	ASP	N-CA-CB	-5.17	102.51	110.16
1	B	209	GLN	CB-CA-C	-5.17	100.14	110.42
1	A	171	ALA	O-C-N	5.14	127.57	122.12
1	A	110	ILE	CA-C-O	-5.10	115.44	120.85
1	B	108	PHE	N-CA-C	-5.10	105.63	111.14
1	A	36	PHE	CA-CB-CG	-5.02	108.78	113.80
2	C	1	GLN	CB-CG-CD	5.01	121.11	112.60
1	A	108	PHE	N-CA-C	-5.00	105.74	111.14

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1987	1991	1986	74	2
1	B	1987	1991	1986	92	0
2	C	962	906	904	26	4
2	D	962	906	904	26	4
3	A	14	12	0	4	0
3	B	14	12	0	8	0
All	All	5926	5818	5780	202	6

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 17.

All (202) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:GLY:O	2:D:105:TRP:CE3	2.07	1.07
1:A:233:ILE:HA	1:A:236:MET:SD	2.08	0.94
1:B:241:VAL:O	1:B:242:LEU:C	2.14	0.89
1:B:47:ASP:OD2	1:B:120:VAL:HB	1.72	0.88
1:B:233:ILE:HA	1:B:236:MET:SD	2.14	0.88
1:B:47:ASP:CG	1:B:120:VAL:HB	1.99	0.87
1:B:224:LEU:HD11	3:B:301:IYY:OXT	1.82	0.80
2:C:99:LYS:NZ	2:C:109:ASP:OD1	2.14	0.79
1:B:32:LEU:HD21	1:B:106:THR:HG23	1.67	0.76
1:B:182:GLY:O	2:D:105:TRP:CD2	2.38	0.76
1:B:180:THR:CG2	1:B:239:HIS:ND1	2.50	0.75
1:B:241:VAL:O	1:B:242:LEU:O	2.06	0.74
1:A:183:TRP:HE1	1:A:185:ILE:HG13	1.52	0.74
1:B:44:LEU:HD21	1:B:110:ILE:HD11	1.68	0.74
2:D:36:TRP:HD1	2:D:70:ILE:HD12	1.53	0.74
1:B:237:PHE:O	1:B:238:GLN:C	2.31	0.73
1:A:119:LYS:O	1:A:120:VAL:O	2.06	0.72
2:D:97:ASN:OD1	2:D:98:VAL:N	2.23	0.72
2:C:36:TRP:HD1	2:C:70:ILE:HD12	1.53	0.72
3:B:301:IYY:O2	3:B:301:IYY:S1	2.48	0.71
1:A:117:PRO:HB3	2:C:59:HIS:ND1	2.05	0.71
1:B:192:PHE:HE1	1:B:229:ILE:HG23	1.55	0.71
2:D:23:ALA:HA	2:D:78:THR:HG22	1.73	0.70
1:B:119:LYS:C	1:B:121:SER:H	1.97	0.70
2:C:23:ALA:HA	2:C:78:THR:HG22	1.71	0.70
1:B:180:THR:HG21	1:B:239:HIS:ND1	2.06	0.70
1:B:179:SER:OG	1:B:181:VAL:HG23	1.91	0.69
1:A:117:PRO:CB	2:C:59:HIS:ND1	2.55	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:LEU:O	1:A:238:GLN:HG3	1.92	0.69
1:A:43:GLY:O	2:C:107:THR:HG21	1.93	0.69
1:B:47:ASP:OD1	1:B:120:VAL:HB	1.93	0.68
1:A:47:ASP:OD1	1:A:120:VAL:HG23	1.95	0.67
1:B:183:TRP:HE1	1:B:185:ILE:HG13	1.59	0.67
1:B:32:LEU:HD21	1:B:106:THR:CG2	2.25	0.66
1:B:38:ARG:O	1:B:39:ARG:C	2.38	0.66
1:B:55:LYS:NZ	3:B:301:IYY:O	2.28	0.66
1:B:42:VAL:HG22	1:B:116:GLY:HA2	1.77	0.66
2:C:72:ARG:HG2	2:C:74:ASN:OD1	1.95	0.65
1:B:114:GLU:C	1:B:116:GLY:H	2.03	0.65
1:B:208:ASP:OD1	1:B:209:GLN:NE2	2.30	0.64
2:C:88:PRO:HA	2:C:119:VAL:HB	1.79	0.64
1:A:28:PHE:O	1:A:32:LEU:HD13	1.97	0.64
1:B:23:SER:O	1:B:26:ILE:HG22	1.97	0.64
1:B:242:LEU:HD23	1:B:242:LEU:H	1.63	0.63
2:C:97:ASN:OD1	2:C:99:LYS:NZ	2.31	0.62
1:B:58:SER:HB3	1:B:155:PHE:O	1.99	0.62
2:C:102:GLY:H	2:C:107:THR:HG22	1.64	0.62
1:A:44:LEU:HD11	1:A:49:VAL:CG2	2.30	0.62
1:A:107:LEU:HA	1:A:110:ILE:HG12	1.81	0.62
1:B:192:PHE:CE1	1:B:229:ILE:HG23	2.34	0.62
2:D:102:GLY:H	2:D:107:THR:HG22	1.65	0.61
1:A:183:TRP:NE1	1:A:185:ILE:HG13	2.15	0.61
1:A:108:PHE:O	1:A:112:ILE:HG22	2.00	0.61
1:B:34:LEU:HD11	1:B:38:ARG:NH2	2.15	0.61
1:B:112:ILE:N	1:B:112:ILE:HD13	2.15	0.60
1:A:24:TRP:CD2	3:A:301:IYY:N	2.70	0.60
1:B:209:GLN:O	1:B:211:SER:N	2.34	0.60
1:A:110:ILE:O	1:A:114:GLU:HB2	2.01	0.60
1:B:114:GLU:C	1:B:116:GLY:N	2.59	0.59
2:C:20:LEU:HD23	2:C:83:MET:SD	2.42	0.59
1:B:38:ARG:O	1:B:40:SER:N	2.35	0.59
2:C:36:TRP:HD1	2:C:70:ILE:CD1	2.15	0.59
1:B:41:VAL:HG21	1:B:110:ILE:HA	1.84	0.59
1:A:46:PHE:HB2	1:A:120:VAL:HG22	1.82	0.59
2:C:74:ASN:OD1	2:C:74:ASN:N	2.30	0.58
1:A:58:SER:HB3	1:A:155:PHE:O	2.02	0.58
1:A:208:ASP:OD2	1:A:209:GLN:NE2	2.37	0.58
2:D:36:TRP:HD1	2:D:70:ILE:CD1	2.16	0.58
2:D:88:PRO:HA	2:D:119:VAL:HB	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:THR:HG21	1:A:239:HIS:HB2	1.86	0.57
1:A:108:PHE:CZ	1:A:112:ILE:HD12	2.39	0.57
1:B:168:ILE:HB	1:B:169:PRO:HD3	1.85	0.57
2:D:20:LEU:HD23	2:D:83:MET:SD	2.44	0.57
1:A:170:GLN:CD	2:C:105:TRP:CD1	2.82	0.57
1:A:41:VAL:HG21	1:A:110:ILE:HA	1.86	0.57
1:A:180:THR:HG23	1:A:183:TRP:HB2	1.88	0.56
1:A:180:THR:CG2	1:A:239:HIS:ND1	2.69	0.56
1:B:179:SER:OG	1:B:181:VAL:CG2	2.53	0.56
1:B:209:GLN:O	1:B:210:ASN:C	2.47	0.56
1:A:159:GLN:HE22	1:A:224:LEU:HB2	1.71	0.56
1:B:183:TRP:NE1	1:B:185:ILE:HG13	2.20	0.56
1:A:124:ALA:O	1:A:125:ILE:C	2.48	0.55
1:B:159:GLN:HE22	1:B:224:LEU:HB2	1.72	0.55
1:B:237:PHE:CZ	1:B:242:LEU:HD21	2.41	0.55
1:B:46:PHE:HB2	1:B:120:VAL:HG23	1.90	0.54
2:D:20:LEU:HD11	2:D:115:THR:HG23	1.90	0.54
1:B:43:GLY:O	2:D:107:THR:HG21	2.07	0.54
1:B:224:LEU:HD11	3:B:301:IYY:CB	2.38	0.54
1:A:35:ASN:ND2	1:A:41:VAL:HG12	2.22	0.54
1:B:13:TYR:CD1	1:B:201:GLN:HG2	2.42	0.54
1:B:119:LYS:C	1:B:121:SER:N	2.65	0.54
1:A:234:LEU:HG	1:A:238:GLN:HE21	1.73	0.54
1:A:60:MET:HG3	1:A:96:SER:HB3	1.90	0.54
1:B:61:ILE:O	1:B:65:CYS:SG	2.66	0.54
1:B:181:VAL:HG11	2:D:100:ASP:HB3	1.89	0.53
1:A:166:LYS:HE2	3:A:301:IYY:O	2.09	0.53
1:A:166:LYS:O	2:C:103:TRP:CD1	2.62	0.53
1:B:170:GLN:OE1	2:D:104:TYR:N	2.31	0.53
1:A:202:MET:HE2	1:A:214:ASN:HD22	1.74	0.52
2:D:109:ASP:OD2	2:D:111:TRP:CZ2	2.62	0.52
1:B:192:PHE:CE2	1:B:196:LEU:HD11	2.45	0.52
1:A:168:ILE:HB	1:A:169:PRO:HD3	1.92	0.52
1:A:180:THR:HG21	1:A:239:HIS:CB	2.39	0.52
1:B:119:LYS:O	1:B:121:SER:N	2.43	0.52
1:A:121:SER:O	1:A:125:ILE:HB	2.10	0.52
2:D:97:ASN:ND2	2:D:111:TRP:CZ3	2.75	0.52
1:A:36:PHE:O	1:A:37:ARG:C	2.53	0.52
1:B:183:TRP:HA	2:D:105:TRP:CZ3	2.45	0.51
1:B:24:TRP:NE1	1:B:194:GLY:HA3	2.26	0.51
1:A:175:PHE:HA	1:A:243:TYR:OH	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:ALA:O	1:A:26:ILE:HG22	2.11	0.51
1:A:114:GLU:HG2	1:A:115:ARG:H	1.76	0.51
1:A:244:PRO:O	1:A:245:GLU:HG3	2.10	0.50
1:B:41:VAL:CG2	1:B:114:GLU:HA	2.42	0.50
1:A:119:LYS:O	1:A:120:VAL:C	2.55	0.50
2:D:83:MET:HE2	2:D:117:VAL:HG11	1.93	0.50
1:A:170:GLN:CD	2:C:105:TRP:NE1	2.69	0.50
1:A:166:LYS:CE	3:A:301:IYY:O	2.59	0.50
1:A:180:THR:HG21	1:A:239:HIS:CG	2.46	0.50
2:D:40:ALA:HB3	2:D:43:LYS:HD2	1.93	0.50
1:B:237:PHE:CE2	1:B:242:LEU:HD21	2.47	0.50
2:C:83:MET:HE2	2:C:117:VAL:HG11	1.94	0.50
1:B:32:LEU:CD2	1:B:106:THR:HG22	2.42	0.50
1:A:122:ARG:O	1:A:123:LEU:C	2.55	0.49
1:A:46:PHE:HB2	1:A:120:VAL:CG2	2.43	0.49
1:A:156:ASN:O	1:A:159:GLN:HG3	2.12	0.49
1:B:32:LEU:CD2	1:B:106:THR:CG2	2.91	0.49
1:B:55:LYS:HG3	1:B:162:MET:HB2	1.94	0.49
1:B:170:GLN:CD	2:D:105:TRP:CD1	2.91	0.49
1:B:47:ASP:OD2	1:B:120:VAL:CB	2.54	0.48
1:B:156:ASN:O	1:B:159:GLN:HG3	2.12	0.48
1:A:114:GLU:HG2	1:A:115:ARG:N	2.28	0.48
1:A:192:PHE:O	1:A:196:LEU:HD13	2.14	0.48
1:B:44:LEU:CD2	1:B:110:ILE:HD11	2.40	0.48
1:A:109:GLN:HA	1:A:112:ILE:CG2	2.44	0.47
1:A:109:GLN:HA	1:A:112:ILE:HG22	1.96	0.47
1:A:117:PRO:HG3	2:C:33:ARG:HD3	1.96	0.47
1:B:122:ARG:O	1:B:124:ALA:N	2.47	0.47
1:A:32:LEU:HD11	1:A:106:THR:CG2	2.44	0.47
1:B:208:ASP:O	1:B:210:ASN:N	2.47	0.47
1:B:24:TRP:CD2	3:B:301:IYY:N	2.83	0.47
1:B:224:LEU:CD1	3:B:301:IYY:OXT	2.60	0.47
1:B:41:VAL:HG22	1:B:114:GLU:HA	1.97	0.47
2:C:105:TRP:CD1	2:C:105:TRP:H	2.33	0.47
1:B:56:HIS:HE1	3:B:301:IYY:SG	2.38	0.46
1:A:48:PHE:CZ	2:C:104:TYR:HB2	2.50	0.46
1:A:234:LEU:O	1:A:238:GLN:N	2.38	0.46
1:B:111:PHE:C	1:B:112:ILE:HD13	2.41	0.46
2:D:104:TYR:O	2:D:105:TRP:O	2.32	0.46
1:B:232:ASP:HB3	1:B:236:MET:HE3	1.96	0.46
1:A:180:THR:HG21	1:A:239:HIS:ND1	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:LYS:HG3	1:A:162:MET:HB2	1.97	0.46
1:B:237:PHE:O	1:B:238:GLN:O	2.32	0.46
2:D:29:VAL:HG23	2:D:72:ARG:HD2	1.98	0.46
1:A:47:ASP:OD2	1:A:120:VAL:HB	2.16	0.46
1:A:243:TYR:C	1:A:244:PRO:O	2.59	0.46
1:A:192:PHE:O	1:A:196:LEU:CD1	2.64	0.45
1:B:181:VAL:HG11	2:D:100:ASP:CB	2.46	0.45
1:B:21:PHE:O	1:B:22:ALA:C	2.59	0.45
1:B:60:MET:HG3	1:B:96:SER:HB3	1.98	0.45
1:A:47:ASP:OD1	1:A:120:VAL:CG2	2.62	0.45
1:B:24:TRP:CD1	1:B:194:GLY:HA3	2.52	0.45
1:B:50:MET:HE2	1:B:50:MET:HB2	1.68	0.45
1:B:123:LEU:HD23	1:B:123:LEU:C	2.41	0.45
2:D:6:GLU:HB3	2:D:115:THR:HG22	1.98	0.45
1:A:232:ASP:HB3	1:A:236:MET:HE3	1.99	0.44
1:B:128:VAL:HG13	1:B:132:TRP:CD1	2.52	0.44
1:B:156:ASN:CG	1:B:220:GLY:HA3	2.43	0.44
1:A:65:CYS:HB3	1:A:72:ILE:CD1	2.48	0.43
1:A:170:GLN:CD	2:C:105:TRP:HE1	2.26	0.43
1:B:167:TYR:HB3	1:B:231:PHE:CG	2.53	0.43
1:B:112:ILE:N	1:B:112:ILE:CD1	2.82	0.43
1:B:238:GLN:HA	1:B:242:LEU:HG	2.01	0.43
1:B:46:PHE:CE2	1:B:118:GLN:HB2	2.53	0.43
1:B:65:CYS:HB3	1:B:72:ILE:CD1	2.49	0.42
2:C:73:ASP:HB2	2:C:80:TYR:HE2	1.83	0.42
1:A:183:TRP:CE2	1:A:239:HIS:CD2	3.06	0.42
1:A:112:ILE:HD13	1:A:112:ILE:HG21	1.79	0.42
1:A:178:LYS:O	1:A:179:SER:O	2.38	0.42
1:B:185:ILE:HD12	1:B:185:ILE:H	1.85	0.42
2:D:97:ASN:OD1	2:D:97:ASN:C	2.61	0.42
2:D:24:ALA:HB3	2:D:77:ASN:OD1	2.20	0.42
1:A:124:ALA:O	1:A:127:ILE:N	2.53	0.42
1:B:140:PHE:O	1:B:144:PRO:HD3	2.20	0.42
1:A:239:HIS:CD2	1:A:240:TYR:CE1	3.09	0.41
1:A:117:PRO:CA	2:C:59:HIS:ND1	2.83	0.41
1:B:183:TRP:CE2	1:B:239:HIS:CD2	3.08	0.41
2:D:6:GLU:HB3	2:D:115:THR:CG2	2.50	0.41
1:B:114:GLU:O	1:B:116:GLY:N	2.54	0.41
1:A:125:ILE:HG22	1:A:126:GLY:N	2.34	0.41
1:A:167:TYR:HB3	1:A:231:PHE:CG	2.56	0.41
1:B:178:LYS:O	1:B:179:SER:O	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:MET:HE2	1:A:60:MET:HB3	1.99	0.41
2:C:52:GLU:OE1	2:C:57:GLU:HB3	2.20	0.41
3:A:301:IYY:O2	3:A:301:IYY:S1	2.79	0.41
2:C:67:ARG:HD3	2:C:87:LYS:NZ	2.35	0.41
1:B:41:VAL:HG22	1:B:114:GLU:CA	2.50	0.41
1:B:92:ASP:OD2	1:B:221:LYS:HD2	2.21	0.41
2:C:67:ARG:HD3	2:C:87:LYS:HZ1	1.86	0.41
1:A:195:GLY:C	1:A:229:ILE:HD11	2.46	0.40
1:B:24:TRP:CE3	3:B:301:IYY:N	2.89	0.40
1:B:47:ASP:OD1	1:B:120:VAL:C	2.64	0.40

All (6) 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)
2:C:11:LEU:HB2	2:D:30:TYR:HE2[4_546]	1.11	0.49
2:C:11:LEU:N	2:D:30:TYR:OH[4_546]	1.98	0.22
1:A:5:ASN:O	1:A:7:ILE:H[2_555]	1.46	0.14
2:C:30:TYR:CE2	2:D:11:LEU:HD21[4_547]	1.50	0.10
2:C:30:TYR:CD2	2:D:11:LEU:CD2[4_547]	2.17	0.03
1:A:5:ASN:O	1:A:7:ILE:N[2_555]	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	241/277 (87%)	215 (89%)	21 (9%)	5 (2%)	5	24
1	B	241/277 (87%)	212 (88%)	18 (8%)	11 (5%)	2	12
2	C	119/121 (98%)	110 (92%)	7 (6%)	2 (2%)	7	27
2	D	119/121 (98%)	112 (94%)	5 (4%)	2 (2%)	7	27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	720/796 (90%)	649 (90%)	51 (7%)	20 (3%)	4	19

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	120	VAL
1	A	121	SER
1	B	39	ARG
1	B	120	VAL
1	B	179	SER
1	B	242	LEU
1	B	244	PRO
2	C	53	SER
2	D	53	SER
2	D	105	TRP
1	A	179	SER
1	B	115	ARG
1	B	123	LEU
1	B	210	ASN
1	A	244	PRO
1	B	208	ASP
1	B	22	ALA
1	B	114	GLU
2	C	105	TRP
1	A	241	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	218/249 (88%)	210 (96%)	8 (4%)	30	55
1	B	218/249 (88%)	203 (93%)	15 (7%)	14	40
2	C	98/98 (100%)	85 (87%)	13 (13%)	4	16
2	D	98/98 (100%)	90 (92%)	8 (8%)	10	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	632/694 (91%)	588 (93%)	44 (7%)	14	39

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	SER
1	A	7	ILE
1	A	50	MET
1	A	125	ILE
1	A	181	VAL
1	A	205	GLN
1	A	242	LEU
1	A	243	TYR
1	B	3	SER
1	B	7	ILE
1	B	15	ILE
1	B	25	SER
1	B	50	MET
1	B	56	HIS
1	B	60	MET
1	B	112	ILE
1	B	120	VAL
1	B	178	LYS
1	B	189	LEU
1	B	190	LEU
1	B	241	VAL
1	B	242	LEU
1	B	245	GLU
2	C	2	VAL
2	C	19	ARG
2	C	20	LEU
2	C	52	GLU
2	C	57	GLU
2	C	87	LYS
2	C	89	GLU
2	C	96	CYS
2	C	99	LYS
2	C	104	TYR
2	C	105	TRP
2	C	113	GLN
2	C	115	THR
2	D	1	GLN

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Mol	Chain	Res	Type
2	D	2	VAL
2	D	3	GLN
2	D	20	LEU
2	D	52	GLU
2	D	96	CYS
2	D	105	TRP
2	D	113	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	ASN
1	A	214	ASN
1	B	31	GLN
1	B	35	ASN
1	B	118	GLN
1	B	214	ASN
2	D	116	GLN

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 ⓘ

2 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
3	IYY	A	301	-	11,13,13	0.43	0	8,16,16	1.17	1 (12%)
3	IYY	B	301	-	11,13,13	0.65	0	8,16,16	1.04	1 (12%)

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	IYY	A	301	-	-	10/15/15/15	-
3	IYY	B	301	-	-	10/15/15/15	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	301	IYY	C1-SG-S1	-2.56	97.25	103.86
3	B	301	IYY	C1-SG-S1	-2.12	98.38	103.86

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	301	IYY	C1-CA-CB-O
3	B	301	IYY	C1-CA-CB-OXT
3	B	301	IYY	C3-C4-C5-O2
3	A	301	IYY	N-CA-CB-OXT
3	A	301	IYY	N1-C4-C5-O3
3	A	301	IYY	C1-CA-CB-O
3	A	301	IYY	C1-CA-CB-OXT
3	A	301	IYY	C3-C4-C5-O3
3	A	301	IYY	C3-C4-C5-O2
3	B	301	IYY	C3-C4-C5-O3
3	B	301	IYY	C4-C3-S1-SG
3	B	301	IYY	N1-C4-C5-O2
3	A	301	IYY	C4-C3-S1-SG

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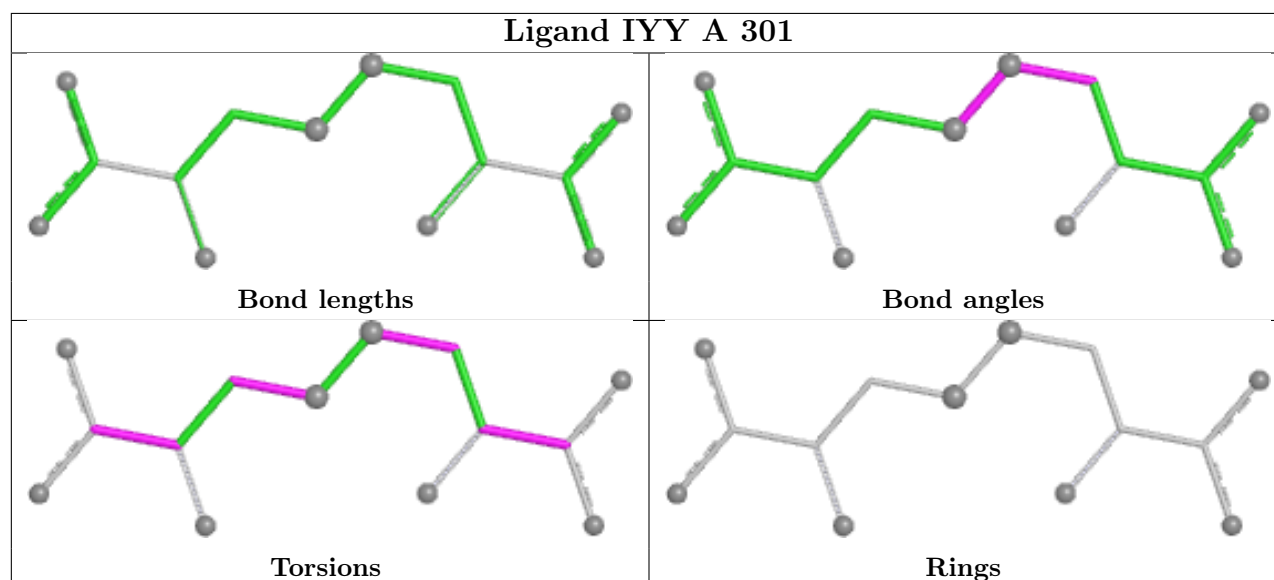
Mol	Chain	Res	Type	Atoms
3	B	301	IYY	N1-C4-C5-O3
3	B	301	IYY	CA-C1-SG-S1
3	B	301	IYY	N-CA-CB-OXT
3	A	301	IYY	CA-C1-SG-S1
3	A	301	IYY	N-CA-CB-O
3	A	301	IYY	N1-C4-C5-O2
3	B	301	IYY	N-CA-CB-O

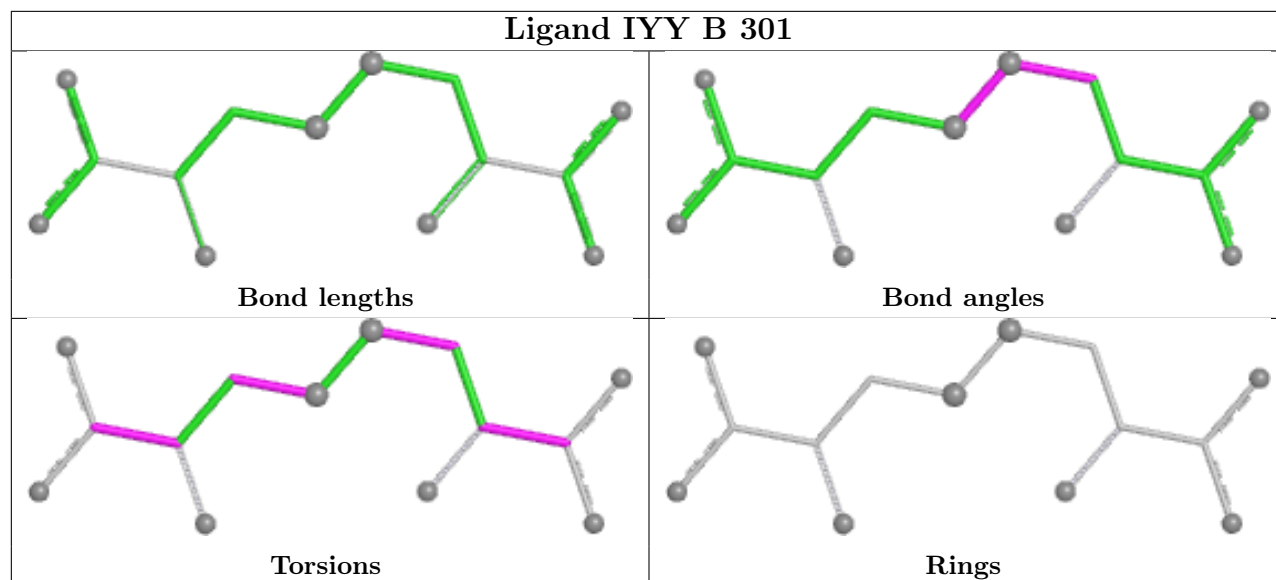
There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	301	IYY	4	0
3	B	301	IYY	8	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	243/277 (87%)	-1.17	0 100 100	58, 71, 78, 81	1 (0%)
1	B	243/277 (87%)	-1.18	0 100 100	58, 70, 77, 80	2 (0%)
2	C	121/121 (100%)	-1.31	0 100 100	53, 65, 70, 72	0
2	D	121/121 (100%)	-1.27	0 100 100	54, 64, 70, 72	0
All	All	728/796 (91%)	-1.21	0 100 100	53, 69, 77, 81	3 (0%)

There are no RSRZ outliers to report.

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.

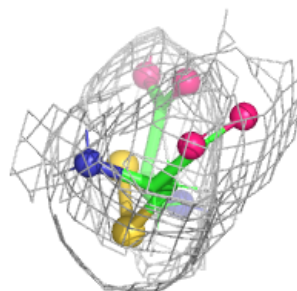
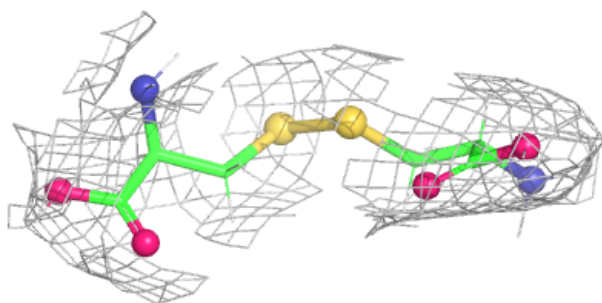
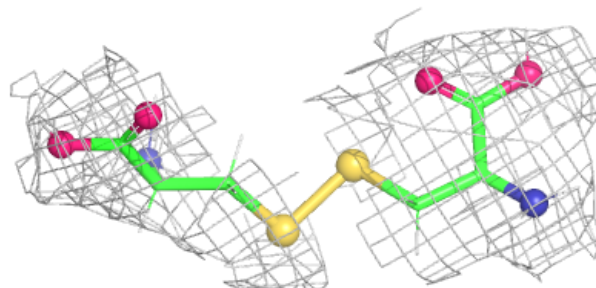
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	IYY	A	301	14/14	1.00	0.02	32,58,61,62	1
3	IYY	B	301	14/14	1.00	0.02	32,61,62,62	1

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.

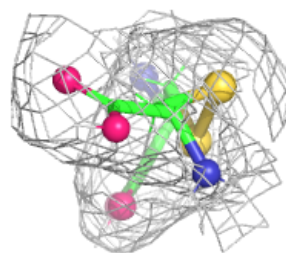
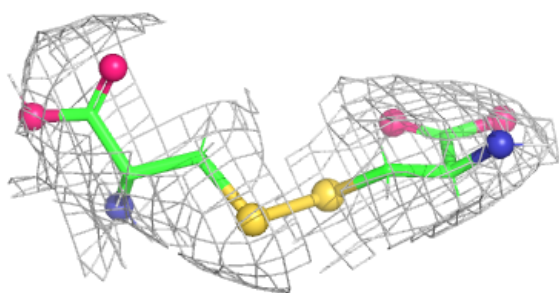
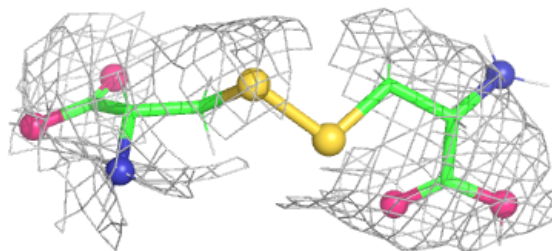
Electron density around IYY A 301:

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



Electron density around IYY B 301:

$2mF_o-DF_c$ (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.