



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:36 AM UTC

PDB ID : 1U0M / pdb_00001u0m
Title : Crystal Structure of 1,3,6,8-Tetrahydroxynaphthalene Synthase (THNS) from *Streptomyces coelicolor* A3(2): a Bacterial Type III Polyketide Synthase (PKS) Provides Insights into Enzymatic Control of Reactive Polyketide Intermediates
Authors : Austin, M.B.; Izumikawa, M.; Bowman, M.E.; Udworthy, D.W.; Ferrer, J.L.; Moore, B.S.; Noel, J.P.
Deposited on : 2004-07-13
Resolution : 2.22 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)

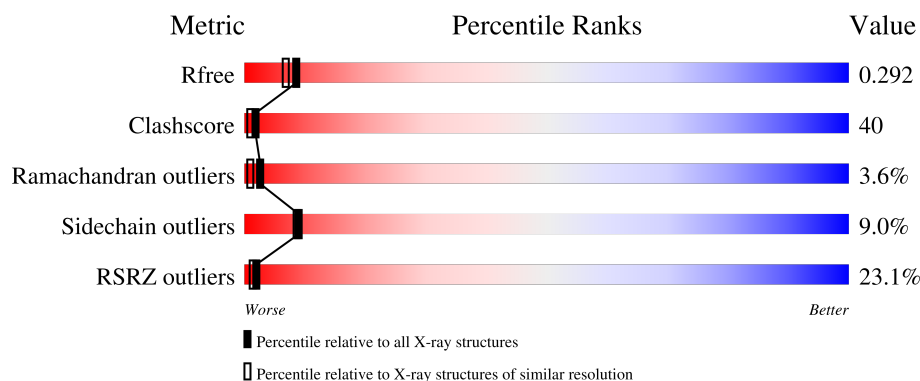
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.22 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	7682 (2.24-2.20)
Clashscore	190562	8402 (2.24-2.20)
Ramachandran outliers	187476	8303 (2.24-2.20)
Sidechain outliers	187428	8304 (2.24-2.20)
RSRZ outliers	180081	7683 (2.24-2.20)

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	382	
1	B	382	

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5504 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.

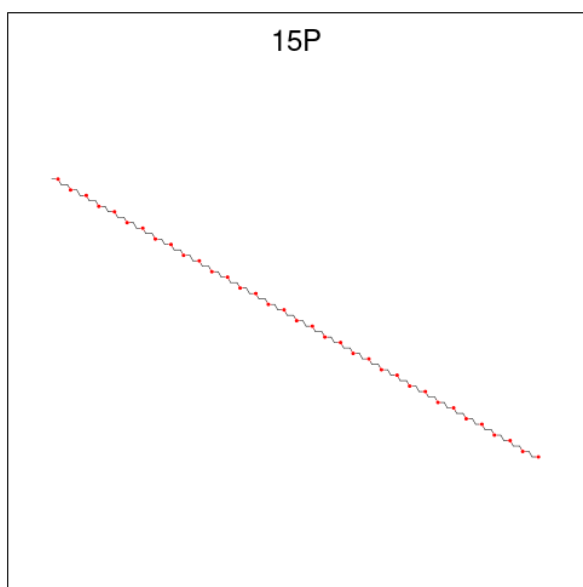
- Molecule 1 is a protein called putative polyketide synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	348	Total	C	N	O	S	0	0	0
			2653	1676	459	502	16			
1	B	348	Total	C	N	O	S	0	0	0
			2653	1676	459	502	16			

There are 16 discrepancies between the modelled and reference sequences:

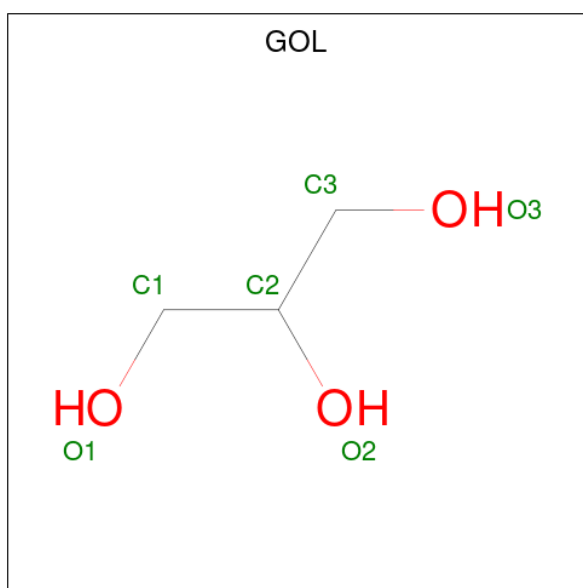
Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	GLY	-	cloning artifact	UNP Q9FCA7
A	-6	SER	-	cloning artifact	UNP Q9FCA7
A	-5	HIS	-	cloning artifact	UNP Q9FCA7
A	-4	GLY	-	cloning artifact	UNP Q9FCA7
A	-3	GLY	-	cloning artifact	UNP Q9FCA7
A	-2	SER	-	cloning artifact	UNP Q9FCA7
A	-1	GLY	-	cloning artifact	UNP Q9FCA7
A	0	PHE	-	cloning artifact	UNP Q9FCA7
B	-7	GLY	-	cloning artifact	UNP Q9FCA7
B	-6	SER	-	cloning artifact	UNP Q9FCA7
B	-5	HIS	-	cloning artifact	UNP Q9FCA7
B	-4	GLY	-	cloning artifact	UNP Q9FCA7
B	-3	GLY	-	cloning artifact	UNP Q9FCA7
B	-2	SER	-	cloning artifact	UNP Q9FCA7
B	-1	GLY	-	cloning artifact	UNP Q9FCA7
B	0	PHE	-	cloning artifact	UNP Q9FCA7

- Molecule 2 is POLYETHYLENE GLYCOL (N=34) (CCD ID: 15P) (formula: C₆₉H₁₄₀O₃₅).



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

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

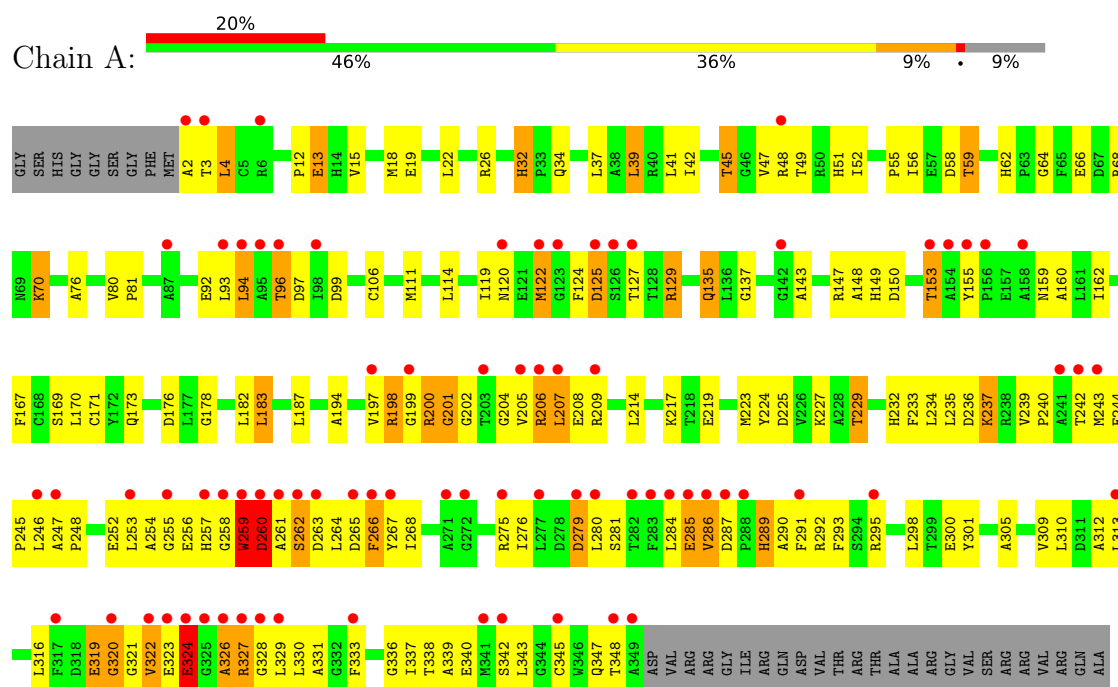
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	70	Total 70	O 70	0	0
4	B	78	Total 78	O 78	0	0

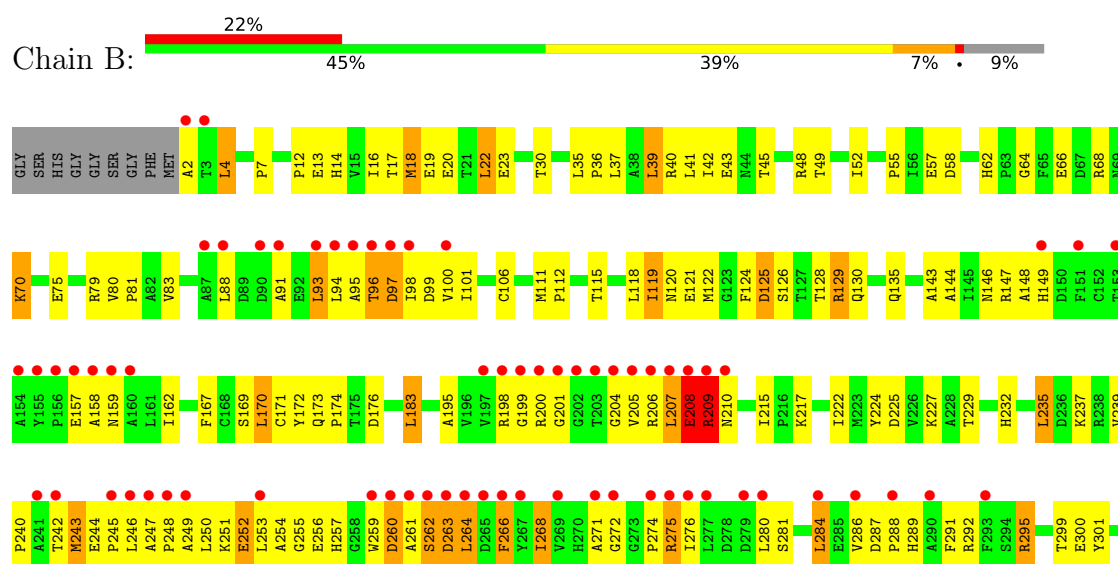
3 Residue-property plots [i](#)

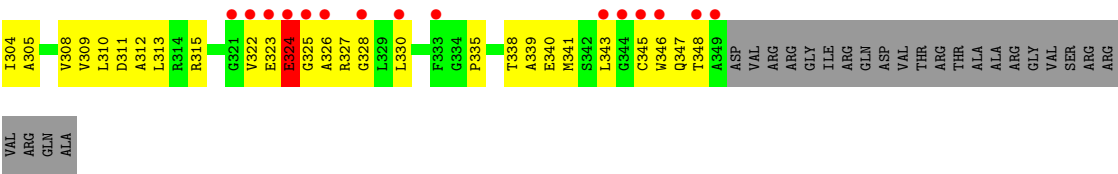
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: putative polyketide synthase



- Molecule 1: putative polyketide synthase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	76.68Å 69.69Å 81.14Å 90.00° 95.42° 90.00°	Depositor
Resolution (Å)	40.39 – 2.22 40.39 – 2.22	Depositor EDS
% Data completeness (in resolution range)	87.9 (40.39-2.22) 88.0 (40.39-2.22)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.98 (at 2.22Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.253 , 0.292 0.253 , 0.292	Depositor DCC
R_{free} test set	1854 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	34.1	Xtriage
Anisotropy	0.874	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 51.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5504	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.51% 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: 15P, GOL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.50	0/2710	1.01	17/3688 (0.5%)
1	B	0.46	0/2710	0.99	12/3688 (0.3%)
All	All	0.48	0/5420	1.00	29/7376 (0.4%)

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	284	LEU	N-CA-C	-8.48	102.93	113.28
1	A	319	GLU	N-CA-C	-7.72	103.31	112.89
1	A	326	ALA	N-CA-C	-7.21	100.34	110.50
1	B	225	ASP	N-CA-C	-6.95	97.91	109.24
1	B	308	VAL	N-CA-C	6.94	117.08	110.42
1	A	225	ASP	N-CA-C	-6.85	97.57	108.73
1	A	259	TRP	N-CA-C	-6.60	103.75	112.34
1	A	305	ALA	CB-CA-C	-6.00	109.64	116.54
1	A	155	TYR	CA-C-N	5.96	127.29	119.84
1	A	155	TYR	C-N-CA	5.96	127.29	119.84
1	A	32	HIS	CA-C-N	5.93	125.80	119.28
1	A	32	HIS	C-N-CA	5.93	125.80	119.28
1	B	70	LYS	N-CA-C	-5.91	104.84	111.28
1	B	96	THR	N-CA-C	5.87	120.43	113.16
1	A	262	SER	N-CA-C	-5.68	105.17	111.71
1	B	305	ALA	CB-CA-C	-5.68	110.01	116.54
1	A	135	GLN	N-CA-C	5.58	119.62	112.26
1	A	260	ASP	N-CA-C	5.51	122.54	110.80
1	A	279	ASP	N-CA-C	-5.45	106.13	112.89
1	B	97	ASP	N-CA-C	-5.45	106.41	113.16
1	B	215	ILE	CA-C-N	5.37	125.29	119.76
1	B	215	ILE	C-N-CA	5.37	125.29	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	208	GLU	N-CA-C	5.30	122.09	110.80
1	A	223	MET	N-CA-C	5.22	115.94	108.74
1	A	13	GLU	N-CA-C	5.20	119.34	112.89
1	A	187	LEU	N-CA-C	5.18	119.81	112.93
1	B	148	ALA	N-CA-C	-5.12	105.78	111.36
1	B	91	ALA	N-CA-C	-5.11	106.88	113.01
1	A	96	THR	N-CA-C	5.09	119.36	113.20

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	2653	0	2601	235	0
1	B	2653	0	2601	205	0
2	A	19	0	24	1	0
2	B	19	0	24	1	0
3	A	6	0	8	2	0
3	B	6	0	8	3	0
4	A	70	0	0	2	0
4	B	78	0	0	3	0
All	All	5504	0	5266	424	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 40.

All (424) 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:260:ASP:OD1	1:A:261:ALA:N	1.83	1.12
1:B:93:LEU:HD12	1:B:97:ASP:HB2	1.30	1.10
1:B:275:ARG:HH11	1:B:275:ARG:HB2	1.18	1.04
1:A:148:ALA:HB1	1:A:197:VAL:HG21	1.41	1.02
1:A:266:PHE:HB3	1:A:328:GLY:HA2	1.40	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:323:GLU:HB2	1:B:326:ALA:HB2	1.46	0.97
1:A:2:ALA:HA	1:A:199:GLY:HA2	1.44	0.97
1:B:88:LEU:HD22	1:B:93:LEU:HD21	1.44	0.97
1:A:2:ALA:N	1:A:207:LEU:HD23	1.82	0.95
1:B:244:GLU:HB3	1:B:245:PRO:HD3	1.49	0.94
1:A:120:ASN:HD21	1:B:217:LYS:H	0.97	0.94
1:A:322:VAL:O	1:A:324:GLU:N	1.99	0.94
1:A:52:ILE:HD12	1:A:59:THR:HG21	1.46	0.94
1:B:243:MET:HE1	1:B:246:LEU:HD23	1.49	0.92
1:A:2:ALA:O	1:A:207:LEU:HB3	1.70	0.90
1:A:37:LEU:O	1:A:41:LEU:HD13	1.69	0.90
1:A:243:MET:HE2	1:A:280:LEU:HD23	1.53	0.90
1:B:266:PHE:CD2	1:B:328:GLY:HA3	2.08	0.89
1:A:206:ARG:HD3	1:A:347:GLN:NE2	1.88	0.89
1:A:111:MET:HE1	1:B:106:CYS:HB2	1.56	0.88
1:A:254:ALA:O	1:A:260:ASP:HA	1.73	0.87
1:B:94:LEU:HG	1:B:96:THR:H	1.40	0.86
1:B:275:ARG:HB2	1:B:275:ARG:NH1	1.90	0.86
1:A:237:LYS:CD	1:A:237:LYS:H	1.87	0.86
1:B:243:MET:HE3	1:B:243:MET:HA	1.56	0.85
1:A:209:ARG:HB2	1:A:209:ARG:NH1	1.91	0.85
1:A:244:GLU:HB3	1:A:245:PRO:HD3	1.59	0.84
1:B:93:LEU:HD12	1:B:97:ASP:CB	2.07	0.83
1:A:167:PHE:HB3	1:A:170:LEU:HD23	1.58	0.83
1:A:18:MET:HE2	1:A:22:LEU:HD13	1.59	0.83
1:A:322:VAL:O	1:A:322:VAL:HG12	1.77	0.83
1:B:75:GLU:O	1:B:79:ARG:HG3	1.79	0.82
1:A:208:GLU:HB2	1:A:343:LEU:O	1.80	0.81
1:A:262:SER:O	1:A:264:LEU:HG	1.80	0.81
1:A:322:VAL:C	1:A:324:GLU:H	1.89	0.81
1:A:237:LYS:H	1:A:237:LYS:CE	1.93	0.81
1:B:93:LEU:CD1	1:B:97:ASP:HB2	2.10	0.81
1:A:66:GLU:HG2	1:A:70:LYS:HE2	1.63	0.81
1:B:119:ILE:HA	1:B:124:PHE:HB2	1.63	0.80
1:A:322:VAL:O	1:A:322:VAL:CG1	2.28	0.80
1:A:120:ASN:HD21	1:B:217:LYS:N	1.79	0.80
1:A:120:ASN:ND2	1:B:217:LYS:H	1.77	0.79
1:A:321:GLY:O	1:A:322:VAL:HB	1.82	0.79
1:A:237:LYS:H	1:A:237:LYS:HE3	1.48	0.79
1:A:206:ARG:NH1	1:A:208:GLU:OE1	2.15	0.79
1:B:266:PHE:HD2	1:B:328:GLY:HA3	1.48	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:ARG:CZ	1:A:202:GLY:HA2	2.13	0.78
1:A:266:PHE:CB	1:A:328:GLY:HA2	2.12	0.78
1:B:62:HIS:HD2	1:B:64:GLY:H	1.32	0.77
1:A:206:ARG:HB3	1:A:345:CYS:O	1.85	0.76
1:B:171:CYS:O	3:B:4000:GOL:H31	1.85	0.76
1:A:243:MET:CE	1:A:246:LEU:HD23	2.17	0.75
1:A:259:TRP:N	1:A:259:TRP:HE3	1.85	0.75
1:B:18:MET:HE1	1:B:42:ILE:HG22	1.68	0.75
1:A:275:ARG:HG2	1:A:276:ILE:H	1.52	0.75
1:A:2:ALA:N	1:A:207:LEU:CD2	2.51	0.74
1:A:206:ARG:N	1:A:345:CYS:O	2.19	0.74
1:A:18:MET:HE1	1:A:42:ILE:HG22	1.70	0.74
1:B:99:ASP:OD1	1:B:158:ALA:HA	1.86	0.74
1:B:243:MET:HE2	1:B:280:LEU:HD23	1.69	0.73
1:A:275:ARG:HG2	1:A:276:ILE:N	2.02	0.73
1:A:198:ARG:HD2	1:A:200:ARG:NH1	2.03	0.73
1:A:254:ALA:HA	1:A:343:LEU:HD11	1.69	0.73
1:A:209:ARG:HB2	1:A:209:ARG:HH11	1.51	0.73
1:A:247:ALA:HB3	1:A:248:PRO:HD3	1.71	0.72
1:A:208:GLU:HB3	1:A:257:HIS:NE2	2.04	0.72
1:A:237:LYS:H	1:A:237:LYS:HD3	1.53	0.71
1:B:2:ALA:HB3	1:B:207:LEU:HD23	1.71	0.71
1:B:37:LEU:O	1:B:41:LEU:HD13	1.91	0.71
1:B:260:ASP:C	1:B:262:SER:H	1.99	0.71
1:A:268:ILE:HB	1:A:330:LEU:HD23	1.73	0.70
1:B:268:ILE:HB	1:B:330:LEU:HD23	1.73	0.70
1:A:267:TYR:CE2	1:A:286:VAL:HG21	2.26	0.70
1:B:35:LEU:O	1:B:39:LEU:HD22	1.92	0.70
1:A:106:CYS:CB	1:B:111:MET:HE1	2.21	0.70
1:B:88:LEU:HD22	1:B:93:LEU:CD2	2.22	0.70
1:A:209:ARG:HH11	1:A:209:ARG:CB	2.05	0.69
1:B:246:LEU:HD12	1:B:249:ALA:HB3	1.75	0.69
1:B:48:ARG:HG2	1:B:299:THR:HG23	1.74	0.69
1:B:323:GLU:CD	1:B:323:GLU:H	2.00	0.69
1:A:143:ALA:HB2	1:A:340:GLU:HG3	1.75	0.68
1:A:171:CYS:O	3:A:2000:GOL:H31	1.93	0.68
1:A:62:HIS:HD2	1:A:64:GLY:H	1.42	0.68
1:A:200:ARG:HG2	1:A:201:GLY:N	2.07	0.68
1:B:280:LEU:HD12	1:B:291:PHE:CZ	2.27	0.68
1:A:45:THR:HG22	1:A:47:VAL:H	1.58	0.68
1:B:22:LEU:HD12	1:B:39:LEU:HD12	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:MET:HB3	1:B:124:PHE:HD2	1.58	0.68
1:A:66:GLU:CG	1:A:70:LYS:HE2	2.24	0.68
1:A:198:ARG:NE	1:A:202:GLY:HA2	2.09	0.68
1:A:18:MET:HE2	1:A:22:LEU:CD1	2.24	0.67
1:A:137:GLY:H	1:B:111:MET:HE2	1.60	0.67
1:B:311:ASP:O	1:B:315:ARG:HG2	1.95	0.67
1:B:93:LEU:HG	1:B:94:LEU:N	2.10	0.67
1:A:264:LEU:HB2	1:A:267:TYR:CE1	2.28	0.67
1:A:55:PRO:O	1:A:59:THR:HG22	1.94	0.67
1:A:111:MET:HE1	1:B:106:CYS:CB	2.24	0.67
1:A:13:GLU:H	1:A:13:GLU:CD	2.02	0.66
1:B:266:PHE:HD2	1:B:328:GLY:CA	2.08	0.66
1:A:217:LYS:H	1:B:120:ASN:ND2	1.94	0.66
1:B:125:ASP:OD2	1:B:125:ASP:N	2.26	0.66
1:B:266:PHE:CD2	1:B:328:GLY:CA	2.79	0.66
1:B:286:VAL:HG12	1:B:287:ASP:N	2.09	0.66
1:A:237:LYS:HE3	1:A:237:LYS:N	2.10	0.66
1:B:248:PRO:O	1:B:252:GLU:HB2	1.96	0.66
1:B:324:GLU:OE1	1:B:348:THR:N	2.29	0.66
1:A:150:ASP:O	1:A:153:THR:HG23	1.95	0.65
1:A:246:LEU:HD21	1:A:333:PHE:CZ	2.32	0.65
1:A:266:PHE:HB2	1:A:327:ARG:O	1.95	0.65
1:B:288:PRO:O	1:B:295:ARG:NH2	2.31	0.64
1:B:173:GLN:HB2	3:B:4000:GOL:H11	1.78	0.64
1:A:81:PRO:HB3	1:A:122:MET:HE1	1.80	0.64
1:A:259:TRP:N	1:A:259:TRP:CE3	2.65	0.64
1:A:264:LEU:HB2	1:A:267:TYR:HE1	1.62	0.64
1:A:148:ALA:CB	1:A:197:VAL:HG21	2.21	0.64
1:A:149:HIS:CE1	1:A:207:LEU:HD13	2.32	0.64
1:B:143:ALA:O	1:B:147:ARG:HG2	1.98	0.63
1:A:255:GLY:HA2	1:A:260:ASP:HB2	1.80	0.63
1:A:94:LEU:HD12	1:A:96:THR:HB	1.79	0.63
1:A:122:MET:HB3	1:A:124:PHE:CD2	2.33	0.63
1:A:286:VAL:HG12	1:A:287:ASP:N	2.13	0.63
1:A:92:GLU:C	1:A:93:LEU:HD22	2.22	0.63
1:A:42:ILE:O	1:A:45:THR:HB	1.99	0.63
1:B:255:GLY:N	1:B:260:ASP:HB2	2.14	0.63
1:B:143:ALA:HB2	1:B:340:GLU:HG3	1.81	0.63
1:A:254:ALA:C	1:A:260:ASP:HA	2.24	0.63
1:B:289:HIS:CE1	1:B:292:ARG:HD3	2.34	0.63
1:A:280:LEU:HD12	1:A:291:PHE:CZ	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:MET:HG2	1:B:124:PHE:CE2	2.34	0.62
1:B:206:ARG:CZ	1:B:207:LEU:HD11	2.29	0.62
1:B:41:LEU:HB3	1:B:183:LEU:HD11	1.81	0.62
1:A:93:LEU:CD2	1:A:200:ARG:HH12	2.12	0.62
1:A:45:THR:HG23	1:A:47:VAL:HG23	1.80	0.62
1:A:18:MET:HE3	1:A:18:MET:HA	1.82	0.62
1:A:93:LEU:HD21	1:A:200:ARG:HH12	1.65	0.62
1:A:265:ASP:HB2	1:A:326:ALA:HB1	1.81	0.61
1:B:259:TRP:CH2	1:B:345:CYS:SG	2.92	0.61
1:A:93:LEU:HD21	1:A:200:ARG:NH1	2.15	0.61
1:B:13:GLU:CD	1:B:13:GLU:H	2.08	0.61
1:A:236:ASP:O	1:A:239:VAL:HG23	2.00	0.61
1:A:255:GLY:C	1:A:257:HIS:H	2.09	0.61
1:A:262:SER:O	1:A:264:LEU:N	2.34	0.61
1:A:119:ILE:HA	1:A:124:PHE:HB2	1.83	0.61
1:A:309:VAL:HG23	1:A:310:LEU:HD13	1.81	0.61
1:A:159:ASN:ND2	1:A:198:ARG:HA	2.16	0.61
1:B:243:MET:HG3	1:B:280:LEU:HD23	1.82	0.61
1:B:35:LEU:HB3	1:B:36:PRO:HD3	1.82	0.61
1:A:267:TYR:CZ	1:A:286:VAL:HG21	2.36	0.60
1:B:17:THR:OG1	1:B:20:GLU:HG2	2.01	0.60
1:B:243:MET:HA	1:B:243:MET:CE	2.31	0.60
1:B:254:ALA:HB1	1:B:260:ASP:HA	1.84	0.60
1:A:207:LEU:O	1:A:207:LEU:HG	2.00	0.60
1:A:99:ASP:O	1:A:129:ARG:HG2	2.02	0.60
1:A:316:LEU:HD23	1:A:316:LEU:O	2.02	0.60
1:A:287:ASP:OD1	1:A:290:ALA:N	2.35	0.59
1:A:260:ASP:CG	1:A:261:ALA:N	2.60	0.59
1:A:275:ARG:HG2	1:A:276:ILE:HG13	1.84	0.59
1:A:106:CYS:HB2	1:B:111:MET:HE1	1.84	0.59
1:B:209:ARG:HB2	1:B:257:HIS:CD2	2.37	0.59
1:B:206:ARG:NH1	1:B:207:LEU:HD11	2.17	0.59
1:B:250:LEU:HD23	1:B:341:MET:SD	2.42	0.59
1:B:18:MET:HE2	1:B:22:LEU:CD2	2.32	0.59
1:B:45:THR:O	1:B:274:PRO:HG3	2.03	0.59
1:B:309:VAL:HG23	1:B:310:LEU:HD13	1.84	0.59
1:A:41:LEU:HD23	1:A:183:LEU:HD21	1.85	0.58
1:A:237:LYS:CD	1:A:237:LYS:N	2.63	0.58
1:B:167:PHE:HB3	1:B:170:LEU:HD22	1.85	0.58
1:B:235:LEU:CD2	1:B:239:VAL:HG11	2.33	0.58
1:B:206:ARG:O	1:B:207:LEU:O	2.21	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:ALA:HB3	1:A:197:VAL:CG2	2.33	0.57
1:A:26:ARG:HG3	1:A:39:LEU:HD21	1.87	0.57
1:B:66:GLU:O	1:B:70:LYS:HG2	2.04	0.57
1:A:217:LYS:H	1:B:120:ASN:HD21	1.51	0.57
1:B:243:MET:CE	1:B:246:LEU:HD23	2.29	0.57
1:B:122:MET:HG2	1:B:124:PHE:HE2	1.70	0.57
1:B:208:GLU:O	1:B:209:ARG:HB2	2.02	0.57
1:A:41:LEU:CD2	1:A:183:LEU:HD21	2.35	0.57
1:A:81:PRO:CB	1:A:122:MET:HE1	2.35	0.57
1:B:4:LEU:O	1:B:204:GLY:HA3	2.05	0.57
1:B:7:PRO:HB3	1:B:195:ALA:HB2	1.87	0.57
1:B:206:ARG:HB2	1:B:347:GLN:NE2	2.19	0.56
1:A:106:CYS:HB3	1:B:111:MET:HE1	1.87	0.56
1:A:280:LEU:HD13	1:A:280:LEU:O	2.06	0.56
1:A:45:THR:CG2	1:A:47:VAL:HG23	2.35	0.56
1:B:19:GLU:O	1:B:23:GLU:HG3	2.05	0.56
1:B:246:LEU:HD12	1:B:246:LEU:O	2.04	0.56
1:A:207:LEU:HD12	1:A:208:GLU:N	2.20	0.56
1:A:148:ALA:HB1	1:A:197:VAL:CG2	2.25	0.56
1:B:57:GLU:CD	1:B:57:GLU:H	2.14	0.56
1:A:2:ALA:CA	1:A:199:GLY:HA2	2.29	0.56
1:A:258:GLY:C	1:A:260:ASP:N	2.57	0.56
1:B:40:ARG:HD2	4:B:4057:HOH:O	2.05	0.56
1:A:229:THR:OG1	1:A:232:HIS:HE1	1.88	0.56
1:A:257:HIS:HE1	1:A:259:TRP:CE2	2.23	0.56
1:A:62:HIS:HE1	1:A:173:GLN:HE22	1.52	0.55
1:B:229:THR:OG1	1:B:232:HIS:HE1	1.88	0.55
1:A:243:MET:HE3	1:A:246:LEU:HD23	1.85	0.55
1:A:207:LEU:HD12	1:A:207:LEU:C	2.32	0.55
1:A:227:LYS:HD2	1:A:232:HIS:CE1	2.41	0.55
1:B:146:ASN:OD1	1:B:210:ASN:HB2	2.06	0.55
1:A:149:HIS:NE2	1:A:207:LEU:HD13	2.22	0.55
1:A:197:VAL:HG23	1:A:197:VAL:O	2.06	0.55
1:A:268:ILE:HD11	1:A:316:LEU:HD12	1.88	0.55
1:B:22:LEU:CD1	1:B:39:LEU:HD12	2.36	0.55
1:A:137:GLY:H	1:B:111:MET:CE	2.20	0.55
1:A:237:LYS:HD3	1:A:237:LYS:N	2.19	0.55
1:B:229:THR:OG1	1:B:232:HIS:CE1	2.59	0.55
1:B:323:GLU:O	1:B:325:GLY:N	2.40	0.55
1:A:48:ARG:HE	1:A:49:THR:HG23	1.72	0.55
1:B:93:LEU:C	1:B:93:LEU:HD23	2.31	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:207:LEU:CD1	1:B:208:GLU:H	2.19	0.54
1:B:18:MET:SD	1:B:43:GLU:HA	2.47	0.54
1:B:167:PHE:CB	1:B:170:LEU:HD22	2.37	0.54
1:B:280:LEU:HD13	1:B:280:LEU:O	2.08	0.54
1:A:266:PHE:CE1	1:A:316:LEU:HD11	2.42	0.54
1:B:247:ALA:N	1:B:248:PRO:HD2	2.22	0.54
1:A:96:THR:O	1:A:96:THR:HG22	2.08	0.53
1:B:286:VAL:CG1	1:B:287:ASP:N	2.71	0.53
1:B:253:LEU:HD13	1:B:343:LEU:HD11	1.90	0.53
1:A:125:ASP:C	1:A:127:THR:H	2.17	0.52
1:A:265:ASP:CB	1:A:326:ALA:HB1	2.38	0.52
1:A:4:LEU:HD13	1:A:313:LEU:HD11	1.92	0.52
1:A:32:HIS:CE1	1:A:34:GLN:HB2	2.44	0.52
1:B:205:VAL:HG21	1:B:266:PHE:HZ	1.74	0.52
1:A:162:ILE:O	1:A:194:ALA:HA	2.10	0.52
1:B:243:MET:HE3	1:B:246:LEU:HB3	1.91	0.52
1:A:48:ARG:NE	1:A:49:THR:HG23	2.23	0.52
1:A:293:PHE:CE1	1:A:316:LEU:HA	2.45	0.52
1:B:18:MET:HG3	1:B:22:LEU:HD23	1.92	0.52
1:B:97:ASP:O	1:B:159:ASN:HB2	2.09	0.52
1:A:321:GLY:O	1:A:322:VAL:CB	2.57	0.52
1:B:115:THR:O	1:B:119:ILE:HG12	2.09	0.52
1:A:170:LEU:HD22	1:A:170:LEU:N	2.24	0.52
1:A:319:GLU:O	1:A:320:GLY:C	2.53	0.52
1:B:100:VAL:HG23	1:B:129:ARG:HB2	1.91	0.52
1:B:338:THR:HG22	1:B:339:ALA:N	2.25	0.52
1:A:97:ASP:O	1:A:159:ASN:HB2	2.10	0.51
1:B:115:THR:OG1	1:B:130:GLN:NE2	2.43	0.51
1:A:284:LEU:C	1:A:285:GLU:HG3	2.35	0.51
1:B:144:ALA:HB1	1:B:162:ILE:HG23	1.92	0.51
1:A:3:THR:HG23	1:A:205:VAL:O	2.10	0.51
1:B:18:MET:HA	1:B:18:MET:HE3	1.92	0.51
1:A:149:HIS:O	1:A:153:THR:HG22	2.11	0.51
1:A:255:GLY:O	1:A:257:HIS:N	2.44	0.51
1:A:275:ARG:H	1:A:275:ARG:HD2	1.76	0.51
1:B:207:LEU:HD12	1:B:208:GLU:N	2.24	0.51
1:A:41:LEU:HB3	1:A:183:LEU:HD11	1.92	0.51
1:B:93:LEU:HG	1:B:94:LEU:O	2.11	0.51
1:B:260:ASP:O	1:B:262:SER:N	2.43	0.51
1:B:239:VAL:HG23	1:B:240:PRO:HD3	1.93	0.51
1:B:260:ASP:C	1:B:262:SER:N	2.68	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:254:ALA:HB3	1:B:260:ASP:HB2	1.93	0.50
1:A:208:GLU:OE2	1:A:257:HIS:NE2	2.44	0.50
1:A:281:SER:HB3	1:A:291:PHE:HE1	1.75	0.50
1:A:111:MET:HE2	1:B:135:GLN:HA	1.94	0.50
1:B:18:MET:CE	1:B:42:ILE:HG22	2.40	0.50
1:A:289:HIS:CE1	1:A:292:ARG:HD3	2.46	0.50
1:B:281:SER:O	1:B:286:VAL:O	2.29	0.50
1:A:12:PRO:HG2	1:A:51:HIS:HB3	1.93	0.50
1:B:251:LYS:HA	1:B:260:ASP:OD1	2.12	0.50
1:B:323:GLU:CD	1:B:323:GLU:N	2.68	0.50
1:B:255:GLY:C	1:B:257:HIS:H	2.19	0.50
1:B:263:ASP:CG	1:B:263:ASP:O	2.54	0.50
1:A:309:VAL:HG23	1:A:310:LEU:CD1	2.41	0.49
1:B:300:GLU:HG2	1:B:301:TYR:CD2	2.47	0.49
1:B:122:MET:HB3	1:B:124:PHE:CD2	2.43	0.49
1:A:280:LEU:HD12	1:A:291:PHE:CE2	2.46	0.49
1:B:207:LEU:CD1	1:B:208:GLU:N	2.75	0.49
1:B:2:ALA:HA	1:B:198:ARG:O	2.11	0.49
1:A:48:ARG:HG3	1:A:49:THR:N	2.27	0.49
1:A:235:LEU:CD1	1:A:239:VAL:HG21	2.42	0.49
1:A:94:LEU:CD1	1:A:96:THR:HB	2.42	0.49
1:A:229:THR:OG1	1:A:232:HIS:CE1	2.66	0.49
1:B:266:PHE:CE2	1:B:328:GLY:HA3	2.46	0.49
1:B:18:MET:HE2	1:B:22:LEU:HD22	1.94	0.49
1:B:41:LEU:CB	1:B:183:LEU:HD21	2.42	0.49
1:A:18:MET:HE1	1:A:42:ILE:CG2	2.40	0.49
1:A:56:ILE:HA	1:A:59:THR:HG23	1.95	0.49
1:B:254:ALA:CB	1:B:260:ASP:HA	2.42	0.49
1:B:300:GLU:HG2	1:B:301:TYR:CE2	2.48	0.49
1:A:129:ARG:HG3	1:A:129:ARG:HH11	1.77	0.49
1:A:169:SER:HA	2:A:1000:15P:H132	1.95	0.49
1:B:264:LEU:HD12	1:B:327:ARG:CB	2.43	0.49
1:A:135:GLN:HA	1:B:111:MET:HE3	1.95	0.48
1:B:2:ALA:HA	1:B:199:GLY:HA2	1.95	0.48
1:B:80:VAL:HB	1:B:81:PRO:HD3	1.96	0.48
1:A:209:ARG:NH1	1:A:257:HIS:CD2	2.82	0.48
1:A:257:HIS:CE1	1:A:259:TRP:CE2	3.01	0.48
1:B:146:ASN:O	1:B:149:HIS:HB3	2.14	0.48
1:B:239:VAL:N	1:B:240:PRO:HD2	2.28	0.48
1:A:239:VAL:N	1:A:240:PRO:HD2	2.29	0.48
1:A:255:GLY:HA2	1:A:260:ASP:CB	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:ASP:OD2	1:B:288:PRO:HD2	2.14	0.48
1:B:255:GLY:C	1:B:257:HIS:N	2.71	0.48
1:A:198:ARG:HB2	1:A:200:ARG:HD3	1.94	0.48
1:A:206:ARG:HG2	1:A:345:CYS:HB2	1.96	0.48
1:A:243:MET:HE1	1:A:246:LEU:HD23	1.95	0.48
1:A:268:ILE:HG23	1:A:312:ALA:HB3	1.94	0.48
1:B:30:THR:HG22	4:B:4028:HOH:O	2.12	0.48
1:A:198:ARG:NE	1:A:202:GLY:CA	2.77	0.48
1:B:206:ARG:HG3	1:B:206:ARG:HH11	1.79	0.47
1:A:81:PRO:HB2	4:A:2059:HOH:O	2.14	0.47
1:A:137:GLY:N	1:B:111:MET:HE2	2.26	0.47
1:A:258:GLY:C	1:A:260:ASP:H	2.18	0.47
1:A:80:VAL:HB	1:A:81:PRO:HD3	1.97	0.47
1:A:275:ARG:HG3	1:A:275:ARG:HH11	1.79	0.47
1:A:284:LEU:O	1:A:285:GLU:HB2	2.14	0.47
1:B:227:LYS:HD2	1:B:232:HIS:CE1	2.49	0.47
1:B:260:ASP:CG	1:B:261:ALA:N	2.70	0.47
1:A:94:LEU:HD12	1:A:96:THR:CB	2.44	0.47
1:A:176:ASP:OD2	1:A:232:HIS:HD2	1.97	0.47
1:B:96:THR:HG22	1:B:96:THR:O	2.14	0.47
1:A:235:LEU:HD12	1:A:239:VAL:HG21	1.96	0.47
1:A:284:LEU:O	1:A:285:GLU:CB	2.61	0.47
1:A:338:THR:HG22	1:A:339:ALA:N	2.28	0.47
1:B:49:THR:HG23	1:B:300:GLU:O	2.15	0.47
1:A:173:GLN:HB2	3:A:2000:GOL:H11	1.97	0.47
1:A:214:LEU:HD22	1:A:337:ILE:O	2.14	0.47
1:A:242:THR:O	1:A:245:PRO:HD2	2.14	0.47
1:A:286:VAL:HG12	1:A:287:ASP:H	1.78	0.47
1:B:79:ARG:O	1:B:83:VAL:HG23	2.14	0.47
1:B:98:ILE:HB	1:B:124:PHE:HE1	1.80	0.47
1:B:253:LEU:HD13	1:B:253:LEU:O	2.15	0.47
1:B:261:ALA:O	1:B:262:SER:HB3	2.14	0.47
1:A:295:ARG:HB2	1:A:295:ARG:NH1	2.30	0.47
1:A:59:THR:HB	4:A:2016:HOH:O	2.15	0.46
1:B:12:PRO:HB2	1:B:52:ILE:O	2.15	0.46
1:A:209:ARG:NH1	1:A:257:HIS:HD2	2.14	0.46
1:A:242:THR:C	1:A:245:PRO:HD2	2.41	0.46
1:A:329:LEU:HD23	1:A:343:LEU:HD23	1.96	0.46
1:A:129:ARG:HG3	1:A:129:ARG:NH1	2.31	0.46
1:A:284:LEU:HD23	1:A:286:VAL:HG23	1.97	0.46
1:A:254:ALA:O	1:A:260:ASP:CA	2.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:271:ALA:HB1	1:B:276:ILE:CG2	2.46	0.46
1:B:149:HIS:CD2	1:B:210:ASN:HD22	2.34	0.45
1:A:62:HIS:CE1	1:A:173:GLN:HE22	2.33	0.45
1:B:157:GLU:HG3	1:B:200:ARG:HH21	1.81	0.45
1:B:280:LEU:HD12	1:B:291:PHE:HZ	1.77	0.45
1:B:286:VAL:HG12	1:B:287:ASP:H	1.80	0.45
1:B:206:ARG:HB2	1:B:347:GLN:HE21	1.81	0.45
1:A:281:SER:HB3	1:A:291:PHE:CE1	2.51	0.45
1:B:119:ILE:HD12	1:B:128:THR:HB	1.98	0.45
1:B:222:ILE:O	1:B:335:PRO:HB3	2.17	0.45
1:A:209:ARG:HH11	1:A:257:HIS:HD2	1.64	0.45
1:A:316:LEU:HD23	1:A:316:LEU:C	2.42	0.45
1:B:206:ARG:NH2	1:B:207:LEU:HD11	2.32	0.45
1:B:286:VAL:CG1	1:B:287:ASP:H	2.30	0.45
1:B:322:VAL:HG11	1:B:346:TRP:CD2	2.51	0.45
1:A:217:LYS:HA	1:A:217:LYS:HD3	1.81	0.44
1:B:41:LEU:HD23	1:B:183:LEU:HD21	2.00	0.44
1:B:149:HIS:CG	1:B:210:ASN:HD22	2.35	0.44
1:B:262:SER:OG	1:B:284:LEU:O	2.35	0.44
1:B:239:VAL:HG23	1:B:240:PRO:CD	2.48	0.44
1:B:309:VAL:HG23	1:B:310:LEU:CD1	2.45	0.44
1:A:4:LEU:HD13	1:A:313:LEU:CD1	2.48	0.44
1:A:55:PRO:HD2	1:A:58:ASP:OD2	2.18	0.44
1:A:125:ASP:OD1	1:A:125:ASP:N	2.41	0.44
1:A:243:MET:HG2	1:A:279:ASP:C	2.42	0.44
1:B:75:GLU:OE1	1:B:79:ARG:HD2	2.17	0.44
1:B:313:LEU:HD23	1:B:313:LEU:HA	1.90	0.43
1:A:243:MET:HE3	1:A:243:MET:HA	1.99	0.43
1:A:4:LEU:O	1:A:204:GLY:HA3	2.18	0.43
1:A:125:ASP:C	1:A:127:THR:N	2.76	0.43
1:A:94:LEU:HG	1:A:97:ASP:OD2	2.18	0.43
1:A:76:ALA:O	1:A:80:VAL:HG23	2.19	0.43
1:B:4:LEU:HD13	1:B:313:LEU:CD1	2.49	0.43
1:B:111:MET:HA	1:B:112:PRO:C	2.43	0.43
1:B:176:ASP:OD2	1:B:232:HIS:HD2	2.01	0.43
1:B:237:LYS:HE3	4:B:4076:HOH:O	2.18	0.43
1:A:206:ARG:NH1	1:A:206:ARG:HG2	2.34	0.43
1:A:309:VAL:HG23	1:A:310:LEU:N	2.34	0.43
1:B:4:LEU:HD13	1:B:313:LEU:HD11	1.99	0.43
1:B:312:ALA:O	1:B:315:ARG:HB2	2.18	0.43
1:A:208:GLU:HB3	1:A:257:HIS:CD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:VAL:HG23	1:A:310:LEU:H	1.84	0.43
1:B:41:LEU:CD2	1:B:183:LEU:HD21	2.48	0.43
1:B:222:ILE:HB	1:B:335:PRO:HA	2.01	0.43
1:B:264:LEU:HD13	1:B:264:LEU:HA	1.85	0.42
1:A:147:ARG:HD3	1:A:147:ARG:HA	1.73	0.42
1:A:198:ARG:NH2	1:A:201:GLY:O	2.50	0.42
1:A:219:GLU:HA	1:A:336:GLY:O	2.19	0.42
1:A:92:GLU:O	1:A:93:LEU:HD22	2.18	0.42
1:B:169:SER:HA	2:B:3000:15P:H121	2.01	0.42
1:B:253:LEU:HD13	1:B:253:LEU:C	2.44	0.42
1:A:32:HIS:HE1	1:A:34:GLN:HB2	1.81	0.42
1:A:253:LEU:C	1:A:253:LEU:HD13	2.44	0.42
1:B:100:VAL:HG22	1:B:101:ILE:N	2.33	0.42
1:B:172:TYR:CE2	1:B:174:PRO:HG3	2.55	0.42
1:B:16:ILE:HG13	1:B:20:GLU:HG3	2.00	0.42
1:A:331:ALA:HA	1:A:340:GLU:O	2.20	0.42
1:B:246:LEU:O	1:B:249:ALA:HB3	2.20	0.42
1:A:15:VAL:HG22	1:A:51:HIS:CD2	2.55	0.42
1:B:254:ALA:HB3	1:B:260:ASP:CB	2.50	0.42
1:B:147:ARG:HA	1:B:147:ARG:HD3	1.74	0.41
1:B:149:HIS:NE2	1:B:207:LEU:HB2	2.34	0.41
1:B:118:LEU:O	1:B:119:ILE:C	2.63	0.41
1:B:173:GLN:CG	3:B:4000:GOL:H32	2.50	0.41
1:B:240:PRO:O	1:B:243:MET:HB2	2.20	0.41
1:A:47:VAL:HG22	1:A:298:LEU:O	2.19	0.41
1:A:178:GLY:O	1:A:182:LEU:HD13	2.20	0.41
1:B:235:LEU:HD22	1:B:239:VAL:HG21	2.01	0.41
1:A:330:LEU:O	1:A:342:SER:N	2.53	0.41
1:B:14:HIS:HB2	1:B:52:ILE:HG13	2.02	0.41
1:B:62:HIS:HD2	1:B:64:GLY:N	2.09	0.41
1:B:208:GLU:O	1:B:209:ARG:CB	2.67	0.41
1:B:268:ILE:HD12	1:B:313:LEU:HA	2.02	0.41
1:B:55:PRO:HD2	1:B:58:ASP:OD2	2.19	0.41
1:A:233:PHE:C	1:A:234:LEU:HD12	2.46	0.41
1:A:300:GLU:HG2	1:A:301:TYR:CD2	2.56	0.41
1:B:239:VAL:HA	1:B:242:THR:HG23	2.02	0.41
1:B:268:ILE:O	1:B:268:ILE:HG22	2.21	0.41
1:A:143:ALA:CB	1:A:340:GLU:HG3	2.46	0.40
1:A:205:VAL:HG22	1:A:266:PHE:HE2	1.85	0.40
1:A:206:ARG:HG2	1:A:206:ARG:HH11	1.85	0.40
1:A:275:ARG:HG3	1:A:275:ARG:NH1	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:209:ARG:HD2	1:B:257:HIS:HB2	2.04	0.40
1:A:169:SER:OG	1:A:170:LEU:HD22	2.21	0.40
1:B:205:VAL:HG21	1:B:266:PHE:CZ	2.56	0.40
1:B:207:LEU:HD13	1:B:208:GLU:H	1.85	0.40
1:A:12:PRO:O	1:A:51:HIS:CD2	2.74	0.40
1:A:81:PRO:HB3	1:A:122:MET:CE	2.49	0.40
1:A:255:GLY:C	1:A:257:HIS:N	2.75	0.40
1:B:119:ILE:CD1	1:B:128:THR:HB	2.51	0.40
1:A:111:MET:CE	1:B:135:GLN:HA	2.50	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	346/382 (91%)	311 (90%)	23 (7%)	12 (4%)	3	1
1	B	346/382 (91%)	306 (88%)	27 (8%)	13 (4%)	2	1
All	All	692/764 (91%)	617 (89%)	50 (7%)	25 (4%)	2	1

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	260	ASP
1	A	263	ASP
1	A	320	GLY
1	A	322	VAL
1	A	323	GLU
1	A	327	ARG
1	B	207	LEU
1	B	260	ASP
1	A	256	GLU

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Mol	Chain	Res	Type
1	A	285	GLU
1	A	289	HIS
1	A	324	GLU
1	B	324	GLU
1	B	95	ALA
1	B	126	SER
1	B	209	ARG
1	B	263	ASP
1	B	262	SER
1	A	286	VAL
1	B	208	GLU
1	B	272	GLY
1	B	201	GLY
1	A	201	GLY
1	B	119	ILE
1	B	304	ILE

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	277/304 (91%)	250 (90%)	27 (10%)	8	7
1	B	277/304 (91%)	254 (92%)	23 (8%)	10	10
All	All	554/608 (91%)	504 (91%)	50 (9%)	9	8

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	19	GLU
1	A	39	LEU
1	A	45	THR
1	A	59	THR
1	A	68	ARG
1	A	70	LYS

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Mol	Chain	Res	Type
1	A	94	LEU
1	A	114	LEU
1	A	122	MET
1	A	125	ASP
1	A	129	ARG
1	A	153	THR
1	A	183	LEU
1	A	198	ARG
1	A	200	ARG
1	A	206	ARG
1	A	207	LEU
1	A	224	TYR
1	A	229	THR
1	A	237	LYS
1	A	252	GLU
1	A	259	TRP
1	A	260	ASP
1	A	266	PHE
1	A	324	GLU
1	A	348	THR
1	B	4	LEU
1	B	18	MET
1	B	22	LEU
1	B	39	LEU
1	B	68	ARG
1	B	93	LEU
1	B	121	GLU
1	B	125	ASP
1	B	129	ARG
1	B	170	LEU
1	B	183	LEU
1	B	209	ARG
1	B	224	TYR
1	B	235	LEU
1	B	243	MET
1	B	252	GLU
1	B	256	GLU
1	B	264	LEU
1	B	266	PHE
1	B	268	ILE
1	B	275	ARG
1	B	295	ARG

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Mol	Chain	Res	Type
1	B	324	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	44	ASN
1	A	51	HIS
1	A	62	HIS
1	A	120	ASN
1	A	159	ASN
1	A	173	GLN
1	A	185	ASN
1	A	232	HIS
1	A	289	HIS
1	A	347	GLN
1	B	14	HIS
1	B	51	HIS
1	B	54	GLN
1	B	62	HIS
1	B	85	GLN
1	B	120	ASN
1	B	210	ASN
1	B	232	HIS
1	B	347	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

4 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	GOL	A	2000	-	5,5,5	0.24	0	5,5,5	0.90	0
3	GOL	B	4000	-	5,5,5	0.44	0	5,5,5	0.73	0
2	15P	B	3000	-	18,18,103	0.82	0	17,17,102	0.75	0
2	15P	A	1000	-	18,18,103	0.84	0	17,17,102	0.76	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	2000	-	-	2/4/4/4	-
3	GOL	B	4000	-	-	2/4/4/4	-
2	15P	B	3000	-	-	8/16/16/101	-
2	15P	A	1000	-	-	8/16/16/101	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1000	15P	O8-C17-C18-O9
2	B	3000	15P	O5-C10-C9-O4
2	A	1000	15P	O3-C7-C8-O4
2	B	3000	15P	O8-C17-C18-O9
3	A	2000	GOL	O1-C1-C2-C3
3	B	4000	GOL	O1-C1-C2-C3
2	B	3000	15P	O7-C15-C16-O8

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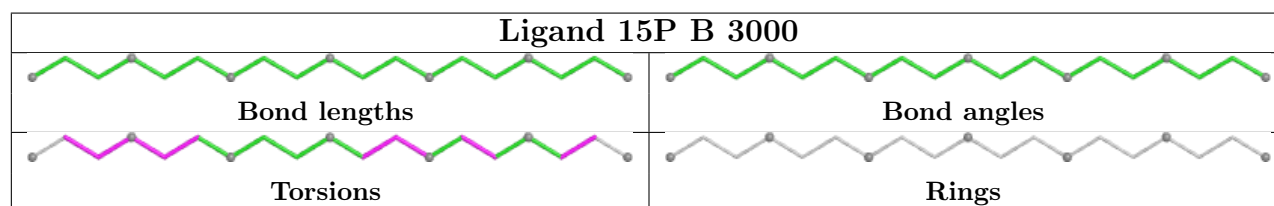
Mol	Chain	Res	Type	Atoms
2	A	1000	15P	O5-C11-C12-O6
3	B	4000	GOL	O1-C1-C2-O2
3	A	2000	GOL	O1-C1-C2-O2
2	A	1000	15P	C11-C12-O6-C13
2	A	1000	15P	C12-C11-O5-C10
2	B	3000	15P	O3-C7-C8-O4
2	B	3000	15P	C12-C11-O5-C10
2	A	1000	15P	C9-C10-O5-C11
2	A	1000	15P	O5-C10-C9-O4
2	A	1000	15P	C7-C8-O4-C9
2	B	3000	15P	C18-C17-O8-C16
2	B	3000	15P	O5-C11-C12-O6
2	B	3000	15P	C15-C16-O8-C17

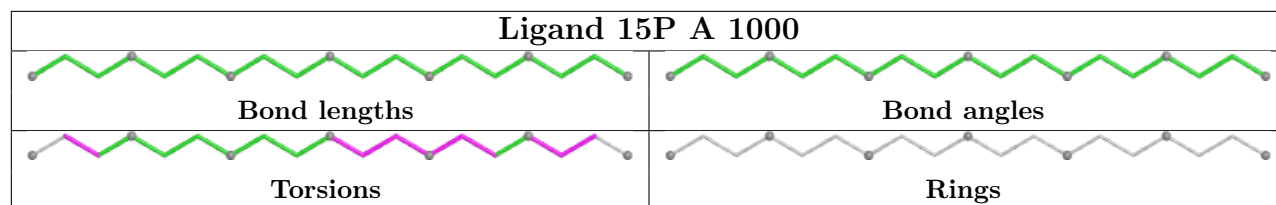
There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2000	GOL	2	0
3	B	4000	GOL	3	0
2	B	3000	15P	1	0
2	A	1000	15P	1	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	348/382 (91%)	1.18	78 (22%) 2 1	26, 49, 89, 99	0
1	B	348/382 (91%)	1.16	83 (23%) 2 1	25, 51, 86, 96	0
All	All	696/764 (91%)	1.17	161 (23%) 2 1	25, 50, 88, 99	0

All (161) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	266	PHE	6.6
1	A	349	ALA	5.7
1	A	260	ASP	5.7
1	A	207	LEU	5.2
1	B	93	LEU	5.2
1	B	203	THR	5.1
1	B	260	ASP	5.1
1	A	259	TRP	5.1
1	A	265	ASP	4.8
1	B	94	LEU	4.5
1	A	262	SER	4.5
1	A	203	THR	4.5
1	B	267	TYR	4.4
1	A	261	ALA	4.3
1	A	287	ASP	4.3
1	B	262	SER	4.3
1	B	266	PHE	4.3
1	B	253	LEU	4.2
1	A	3	THR	4.2
1	A	125	ASP	4.1
1	A	327	ARG	4.1
1	A	2	ALA	4.1
1	A	267	TYR	4.1
1	B	91	ALA	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	3	THR	4.0
1	A	328	GLY	4.0
1	A	284	LEU	3.8
1	A	322	VAL	3.8
1	B	346	TRP	3.8
1	A	263	ASP	3.7
1	A	155	TYR	3.7
1	B	349	ALA	3.7
1	B	153	THR	3.6
1	A	253	LEU	3.6
1	B	95	ALA	3.6
1	A	324	GLU	3.6
1	B	247	ALA	3.5
1	B	276	ILE	3.5
1	B	97	ASP	3.4
1	B	158	ALA	3.4
1	B	209	ARG	3.4
1	B	199	GLY	3.4
1	A	326	ALA	3.4
1	B	201	GLY	3.4
1	A	197	VAL	3.3
1	A	271	ALA	3.3
1	B	272	GLY	3.3
1	A	291	PHE	3.3
1	A	6	ARG	3.3
1	B	198	ARG	3.3
1	A	255	GLY	3.2
1	B	263	ASP	3.2
1	A	323	GLU	3.2
1	B	202	GLY	3.2
1	B	208	GLU	3.2
1	A	156	PRO	3.2
1	A	280	LEU	3.2
1	B	246	LEU	3.2
1	B	264	LEU	3.2
1	B	2	ALA	3.1
1	B	261	ALA	3.1
1	B	156	PRO	3.1
1	B	275	ARG	3.1
1	B	157	GLU	3.0
1	A	286	VAL	3.0
1	A	257	HIS	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	204	GLY	3.0
1	B	96	THR	3.0
1	A	199	GLY	3.0
1	B	288	PRO	3.0
1	A	313	LEU	2.9
1	B	290	ALA	2.9
1	B	207	LEU	2.9
1	B	205	VAL	2.9
1	B	348	THR	2.8
1	A	275	ARG	2.8
1	B	155	TYR	2.8
1	A	206	ARG	2.8
1	B	322	VAL	2.8
1	A	98	ILE	2.7
1	A	283	PHE	2.7
1	A	333	PHE	2.7
1	B	151	PHE	2.7
1	A	348	THR	2.7
1	A	329	LEU	2.7
1	B	286	VAL	2.7
1	A	154	ALA	2.6
1	B	98	ILE	2.6
1	A	94	LEU	2.6
1	B	88	LEU	2.6
1	B	277	LEU	2.6
1	B	265	ASP	2.6
1	A	48	ARG	2.6
1	A	242	THR	2.6
1	A	272	GLY	2.6
1	B	328	GLY	2.6
1	B	344	GLY	2.6
1	B	160	ALA	2.6
1	A	246	LEU	2.6
1	A	247	ALA	2.6
1	B	206	ARG	2.5
1	A	345	CYS	2.5
1	B	154	ALA	2.5
1	B	241	ALA	2.5
1	B	90	ASP	2.5
1	B	321	GLY	2.5
1	A	126	SER	2.5
1	B	197	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	242	THR	2.5
1	A	209	ARG	2.5
1	B	200	ARG	2.5
1	A	205	VAL	2.5
1	A	277	LEU	2.5
1	B	345	CYS	2.4
1	A	93	LEU	2.4
1	A	288	PRO	2.4
1	A	123	GLY	2.4
1	B	284	LEU	2.4
1	A	279	ASP	2.4
1	B	159	ASN	2.4
1	B	210	ASN	2.4
1	A	258	GLY	2.4
1	B	343	LEU	2.4
1	B	324	GLU	2.4
1	A	325	GLY	2.3
1	B	87	ALA	2.3
1	A	282	THR	2.3
1	B	269	VAL	2.3
1	A	295	ARG	2.3
1	A	95	ALA	2.3
1	A	120	ASN	2.3
1	B	271	ALA	2.3
1	B	293	PHE	2.3
1	B	330	LEU	2.3
1	B	279	ASP	2.3
1	B	325	GLY	2.3
1	A	243	MET	2.2
1	B	249	ALA	2.2
1	B	100	VAL	2.2
1	B	333	PHE	2.2
1	B	248	PRO	2.2
1	A	285	GLU	2.2
1	A	320	GLY	2.2
1	B	323	GLU	2.2
1	A	127	THR	2.2
1	B	245	PRO	2.2
1	A	96	THR	2.2
1	A	341	MET	2.1
1	A	153	THR	2.1
1	A	122	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	342	SER	2.1
1	B	326	ALA	2.1
1	B	259	TRP	2.1
1	B	274	PRO	2.1
1	A	142	GLY	2.1
1	A	317	PHE	2.1
1	A	87	ALA	2.0
1	A	158	ALA	2.0
1	A	241	ALA	2.0
1	B	149	HIS	2.0
1	B	280	LEU	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](#)

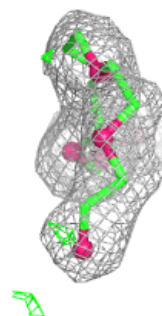
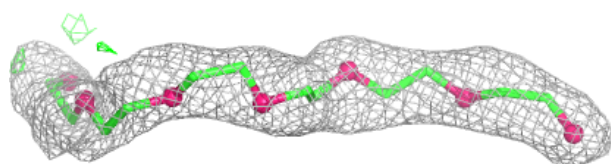
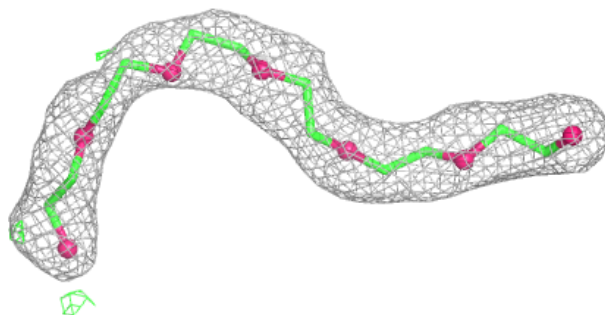
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	15P	A	1000	19/104	0.91	0.13	43,47,57,58	0
2	15P	B	3000	19/104	0.91	0.12	38,47,53,54	0
3	GOL	A	2000	6/6	0.93	0.13	35,44,47,49	0
3	GOL	B	4000	6/6	0.95	0.12	26,38,43,43	0

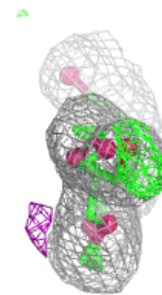
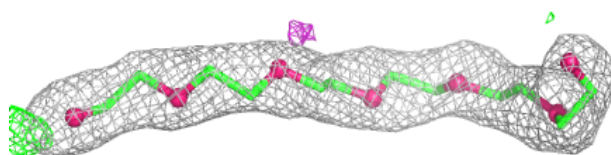
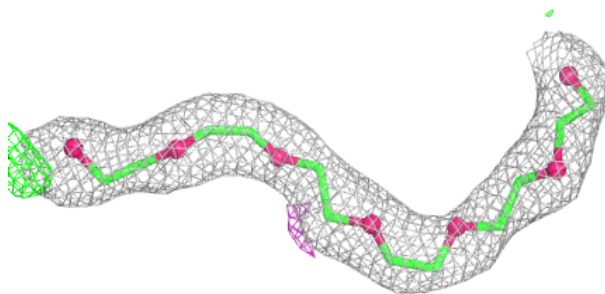
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 15P A 1000:

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

**Electron density around 15P B 3000:**

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



6.5 Other polymers ⓘ

There are no such residues in this entry.