



Full wwPDB X-ray Structure Validation Report i

Feb 5, 2024 – 04:17 AM EST

PDB ID : 1U0M
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.; Udwary, 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 i 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](#) i) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)

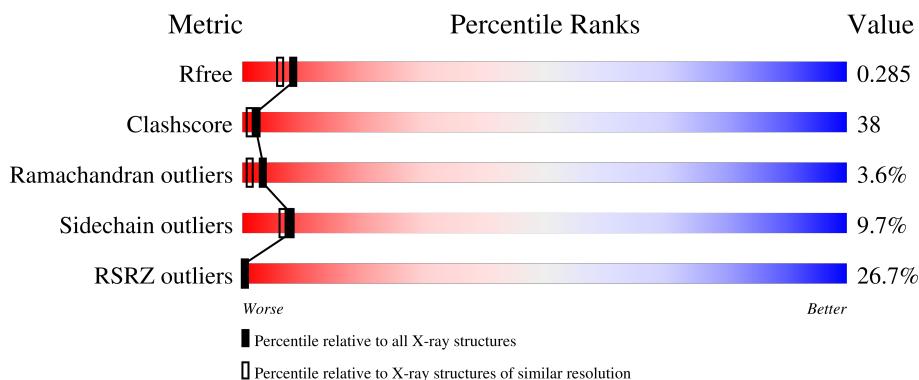
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

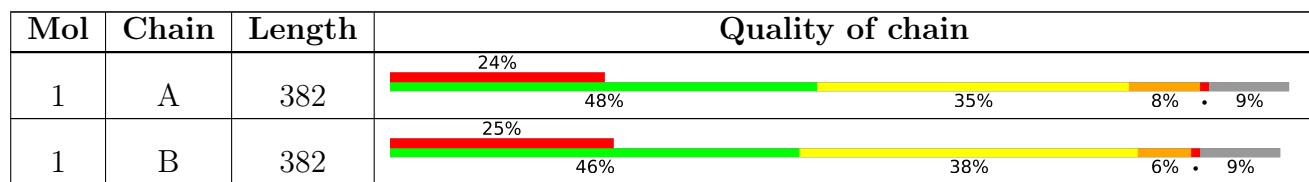
The reported resolution of this entry is 2.22 Å.

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}	130704	5912 (2.24-2.20)
Clashscore	141614	6646 (2.24-2.20)
Ramachandran outliers	138981	6543 (2.24-2.20)
Sidechain outliers	138945	6544 (2.24-2.20)
RSRZ outliers	127900	5797 (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.



Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

2 Entry composition (i)

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.

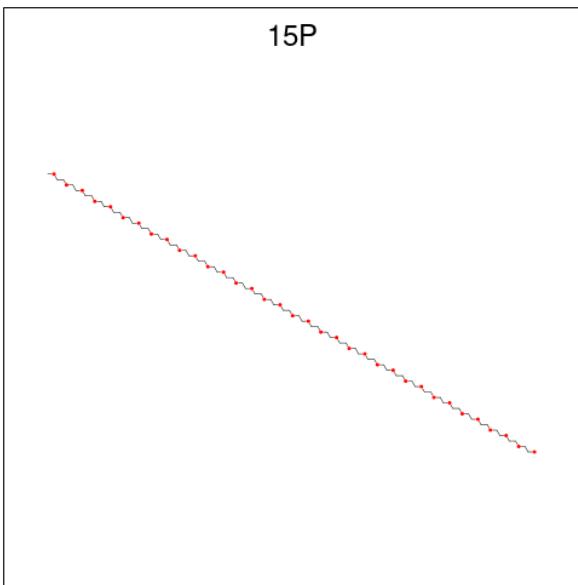
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	348	Total	C	N	O	S	0	0	0
			2653	1676	459	502	16			

Mol	Chain	Residues	Total	C	N	O	S	ZeroOcc	AltConf	Trace
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

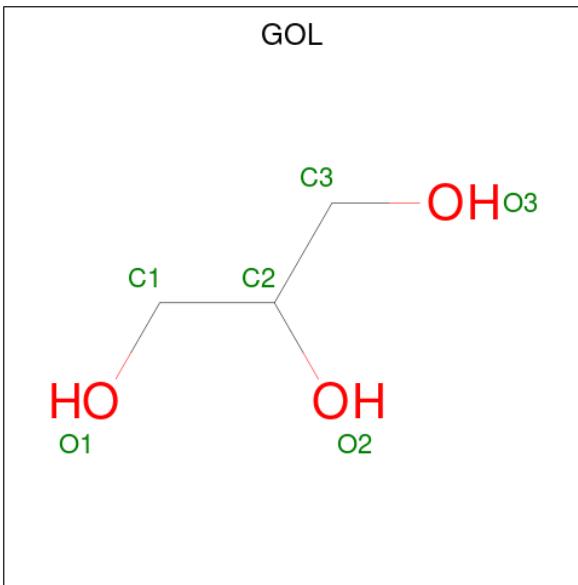
- Molecule 2 is POLYETHYLENE GLYCOL (N=34) (three-letter code: 15P) (formula: C₆₉H₁₄₀O₃₅).



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

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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

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

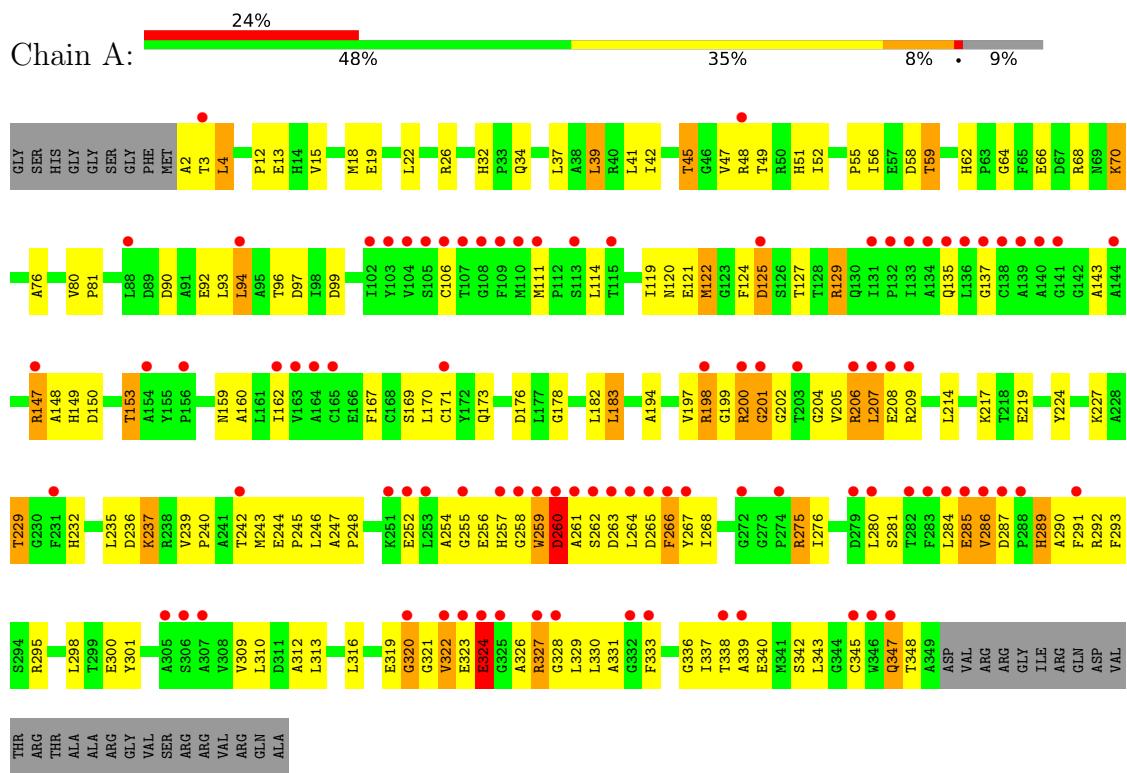
- Molecule 4 is water.

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

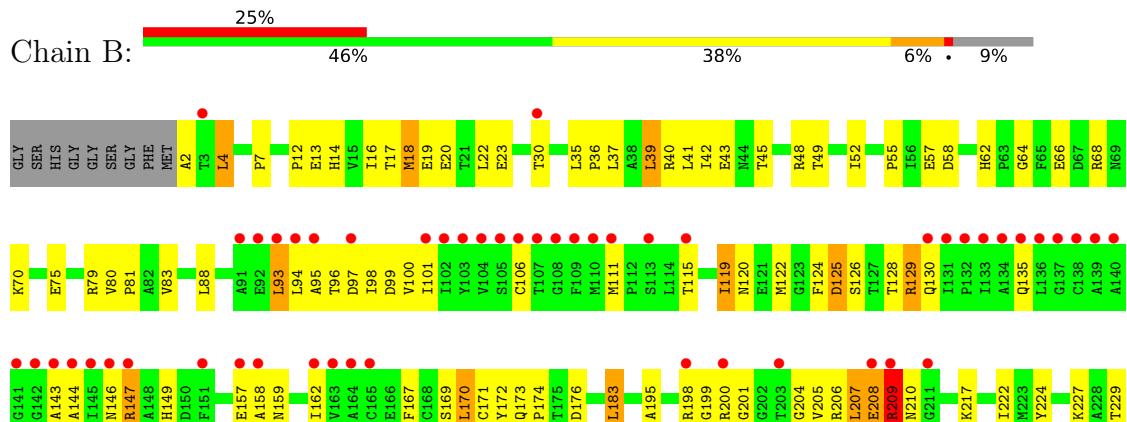
3 Residue-property plots

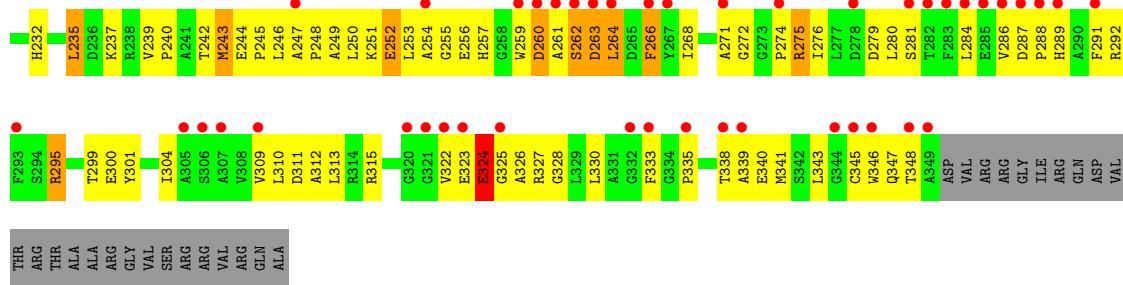
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



- Molecule 1: putative polyketide synthase





4 Data and refinement statistics i

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
$< I/\sigma(I) >$ ¹	5.98 (at 2.22Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R , R_{free}	0.253 , 0.292 0.243 , 0.285	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)	0.35 , 52.6	EDS
L-test for twinning ²	$< L > = 0.50$, $< L^2 > = 0.33$	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 $< |L| >$, $< L^2 >$ 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: GOL, 15P

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.38	0/2710	0.66	0/3688
1	B	0.36	0/2710	0.65	0/3688
All	All	0.37	0/5420	0.65	0/7376

There are no bond length outliers.

There are no bond angle outliers.

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	2653	0	2601	221	0
1	B	2653	0	2601	198	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	407	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 38.

All (407) 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
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: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: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: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: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: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: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:111:MET:HE2	1:B:135:GLN:HA	1.64	0.79
1:A:206:ARG:NH1	1:A:208:GLU:OE1	2.15	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:266:PHE:HD2	1:B:328:GLY:HA3	1.48	0.78
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:B:243:MET:HE3	1:B:246:LEU:HD23	1.67	0.77
1:A:206:ARG:HB3	1:A:345:CYS:O	1.85	0.76
1:A:322:VAL:C	1:A:324:GLU:H	1.89	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: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:B:99:ASP:OD1	1:B:158:ALA:HA	1.86	0.74
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:243:MET:HE3	1:A:246:LEU:HD23	1.71	0.72
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: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: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: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
1:B:122:MET:HB3	1:B:124:PHE:HD2	1.58	0.68
1:B:286:VAL:HG12	1:B:287:ASP:N	2.09	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:A:237:LYS:HE3	1:A:237:LYS:N	2.10	0.66
1:B:18:MET:HA	1:B:18:MET:HE3	1.76	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:B:260:ASP:C	1:B:262:SER:H	1.99	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:B:323:GLU:CD	1:B:323:GLU:H	2.00	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:B:18:MET:HE2	1:B:42:ILE:HG22	1.78	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: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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:MET:CE	1:B:246:LEU:HD23	2.29	0.62
1:A:13:GLU:H	1:A:13:GLU:CD	2.02	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:A:236:ASP:O	1:A:239:VAL:HG23	2.00	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:CE	1:B:243:MET:HA	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:275:ARG:HG2	1:A:276:ILE:HG13	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: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:258:GLY:C	1:A:260:ASP:N	2.57	0.58
1:A:92:GLU:C	1:A:93:LEU:HD22	2.22	0.58
1:A:254:ALA:C	1:A:260:ASP:HA	2.24	0.58
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
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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:LEU:CD2	1:A:183:LEU:HD21	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:13:GLU:CD	1:B:13:GLU:H	2.08	0.56
1:B:206:ARG:HB2	1:B:347:GLN:NE2	2.19	0.56
1:A:255:GLY:C	1:A:257:HIS:H	2.09	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:A:2:ALA:CA	1:A:199:GLY:HA2	2.29	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:B:243:MET:HE1	1:B:333:PHE:CE1	2.41	0.55
1:A:18:MET:HE1	1:A:42:ILE:HG22	1.87	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:A:260:ASP:CG	1:A:261:ALA:N	2.60	0.55
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:243:MET:HA	1:B:243:MET:HE2	1.89	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:A:137:GLY:H	1:B:111:MET:HE1	1.72	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:B:338:THR:HG22	1:B:339:ALA:N	2.25	0.52
1:A:170:LEU:HD22	1:A:170:LEU:N	2.24	0.52
1:B:100:VAL:HG23	1:B:129:ARG:HB2	1.91	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:B:57:GLU:H	1:B:57:GLU:CD	2.14	0.51
1:A:81:PRO:HB3	1:A:122:MET:HE2	1.93	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: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:93:LEU:C	1:B:93:LEU:HD23	2.31	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:A:207:LEU:HD12	1:A:207:LEU:C	2.32	0.50
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: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:18:MET:CE	1:B:42:ILE:HG22	2.40	0.50
1:A:309:VAL:HG23	1:A:310:LEU:CD1	2.41	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:41:LEU:CB	1:B:183:LEU:HD21	2.42	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:18:MET:HE2	1:A:18:MET:O	2.13	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
1:B:287:ASP:OD2	1:B:288:PRO:HD2	2.14	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: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:125:ASP:C	1:A:127:THR:H	2.17	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: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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:319:GLU:O	1:A:320:GLY:C	2.53	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:243:MET:CE	1:A:280:LEU:HD23	2.45	0.46
1:A:106:CYS:CB	1:B:111:MET:HE1	2.45	0.46
1:A:209:ARG:NH1	1:A:257:HIS:HD2	2.14	0.46
1:A:329:LEU:HD23	1:A:343:LEU:HD23	1.96	0.46
1:A:284:LEU:C	1:A:285:GLU:HG3	2.35	0.46
1:B:18:MET:HE3	1:B:18:MET:CA	2.43	0.46
1:B:260:ASP:C	1:B:262:SER:N	2.68	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
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:B:255:GLY:C	1:B:257:HIS:H	2.19	0.45
1:B:263:ASP:CG	1:B:263:ASP:O	2.54	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:B:323:GLU:CD	1:B:323:GLU:N	2.68	0.45
1:A:209:ARG:HH11	1:A:257:HIS:HD2	1.64	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:93:LEU:CG	1:B:94:LEU:N	2.79	0.44
1:A:18:MET:HE1	1:A:22:LEU:CD1	2.47	0.44
1:A:125:ASP:OD1	1:A:125:ASP:N	2.41	0.44
1:B:75:GLU:OE1	1:B:79:ARG:HD2	2.17	0.44
1:A:135:GLN:C	1:B:111:MET:HE2	2.38	0.43
1:B:313:LEU:HD23	1:B:313:LEU:HA	1.90	0.43
1:A:4:LEU:O	1:A:204:GLY:HA3	2.18	0.43
1:A:258:GLY:C	1:A:260:ASP:H	2.18	0.43
1:B:255:GLY:C	1:B:257:HIS:N	2.71	0.43
1:A:111:MET:CE	1:B:106:CYS:HB2	2.48	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: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:B:243:MET:CE	1:B:280:LEU:HD23	2.49	0.43
1:A:81:PRO:HB3	1:A:122:MET:CE	2.49	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:260:ASP:CG	1:B:261:ALA:N	2.70	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:32:HIS:HE1	1:A:34:GLN:HB2	1.81	0.42
1:A:243:MET:HE2	1:A:280:LEU:HD23	2.01	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:173:GLN:CG	3:B:4000:GOL:HG32	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:242:THR:C	1:A:245:PRO:HD2	2.41	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: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:A:106:CYS:HB3	1:B:111:MET:HE1	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
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:B:119:ILE:CD1	1:B:128:THR:HB	2.51	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%)	3 1
All	All	692/764 (91%)	617 (89%)	50 (7%)	25 (4%)	3 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
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 [\(i\)](#)

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	277/304 (91%)	245 (88%)	32 (12%)	5 4
1	B	277/304 (91%)	255 (92%)	22 (8%)	12 11
All	All	554/608 (91%)	500 (90%)	54 (10%)	8 6

All (54) 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
1	A	90	ASP
1	A	94	LEU
1	A	114	LEU
1	A	121	GLU
1	A	122	MET
1	A	125	ASP
1	A	129	ARG
1	A	147	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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	266	PHE
1	A	275	ARG
1	A	324	GLU
1	A	347	GLN
1	A	348	THR
1	B	4	LEU
1	B	18	MET
1	B	39	LEU
1	B	68	ARG
1	B	93	LEU
1	B	125	ASP
1	B	129	ARG
1	B	147	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	275	ARG
1	B	279	ASP
1	B	295	ARG
1	B	324	GLU

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

Mol	Chain	Res	Type
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	232	HIS
1	A	289	HIS
1	A	347	GLN
1	B	14	HIS
1	B	51	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	62	HIS
1	B	85	GLN
1	B	120	ASN
1	B	210	ASN
1	B	232	HIS
1	B	289	HIS
1	B	347	GLN

5.3.3 RNA [\(i\)](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [\(i\)](#)

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	0.23	0	5,5,5	0.84	0
3	GOL	B	4000	-	5,5,5	0.42	0	5,5,5	0.68	0
2	15P	A	1000	-	18,18,103	0.84	0	17,17,102	0.77	0
2	15P	B	3000	-	18,18,103	0.82	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	A	1000	-	-	8/16/16/101	-
2	15P	B	3000	-	-	7/16/16/101	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (19) 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
2	A	1000	15P	O5-C11-C12-O6
3	B	4000	GOL	O1-C1-C2-O2
2	B	3000	15P	O3-C7-C8-O4
2	A	1000	15P	C12-C11-O5-C10
2	A	1000	15P	C11-C12-O6-C13
2	B	3000	15P	C12-C11-O5-C10
3	A	2000	GOL	O1-C1-C2-O2
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	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:

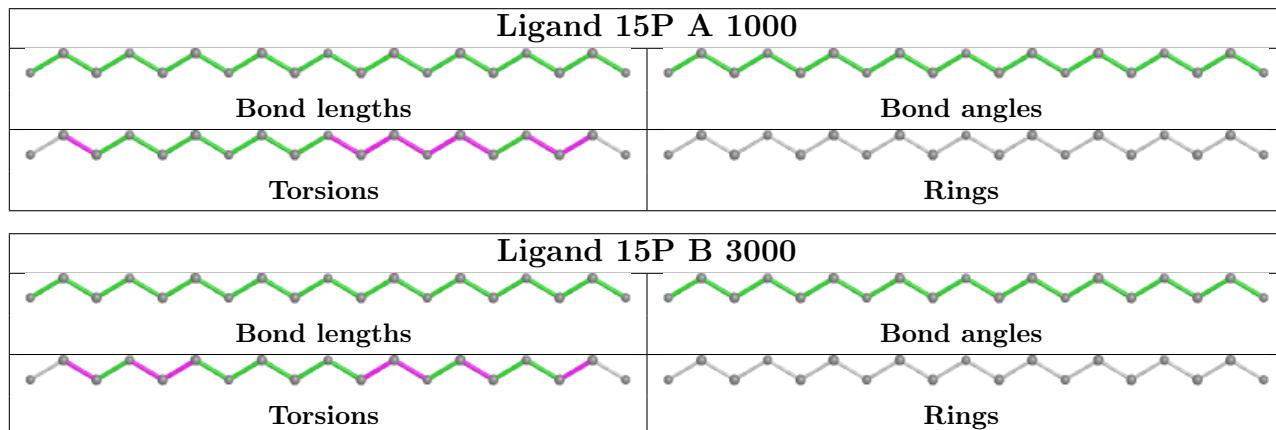
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2000	GOL	2	0
3	B	4000	GOL	3	0
2	A	1000	15P	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	3000	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 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	348/382 (91%)	1.37	91 (26%) 0 0	26, 49, 89, 99	0
1	B	348/382 (91%)	1.34	95 (27%) 0 0	25, 51, 86, 96	0
All	All	696/764 (91%)	1.36	186 (26%) 0 0	25, 50, 88, 99	0

All (186) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	286	VAL	7.2
1	A	260	ASP	6.8
1	B	133	ILE	6.7
1	A	104	VAL	6.4
1	A	266	PHE	6.4
1	A	259	TRP	5.8
1	A	328	GLY	5.8
1	A	132	PRO	5.8
1	B	104	VAL	5.7
1	B	322	VAL	5.7
1	B	261	ALA	5.6
1	B	132	PRO	5.4
1	A	133	ILE	5.4
1	B	131	ILE	5.4
1	B	260	ASP	5.3
1	B	267	TYR	5.2
1	B	140	ALA	5.1
1	A	131	ILE	5.1
1	B	321	GLY	5.1
1	A	283	PHE	5.1
1	A	287	ASP	5.0
1	B	165	CYS	5.0
1	B	263	ASP	5.0
1	A	136	LEU	5.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	327	ARG	4.9
1	A	134	ALA	4.9
1	B	283	PHE	4.8
1	A	320	GLY	4.8
1	B	134	ALA	4.6
1	A	207	LEU	4.5
1	B	164	ALA	4.5
1	A	255	GLY	4.4
1	A	284	LEU	4.4
1	B	139	ALA	4.3
1	A	140	ALA	4.3
1	A	139	ALA	4.2
1	A	203	THR	4.1
1	B	288	PRO	4.1
1	B	262	SER	4.1
1	A	322	VAL	4.1
1	A	164	ALA	4.0
1	B	102	ILE	4.0
1	A	138	CYS	4.0
1	A	291	PHE	4.0
1	A	285	GLU	4.0
1	B	109	PHE	4.0
1	B	285	GLU	4.0
1	B	106	CYS	3.9
1	B	157	GLU	3.9
1	A	262	SER	3.9
1	B	203	THR	3.9
1	B	138	CYS	3.9
1	A	103	TYR	3.8
1	B	346	TRP	3.8
1	A	105	SER	3.8
1	B	105	SER	3.8
1	B	264	LEU	3.8
1	B	91	ALA	3.7
1	A	106	CYS	3.7
1	A	324	GLU	3.7
1	A	325	GLY	3.7
1	A	109	PHE	3.6
1	B	266	PHE	3.6
1	B	93	LEU	3.6
1	B	323	GLU	3.6
1	A	163	VAL	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	143	ALA	3.5
1	A	135	GLN	3.5
1	A	323	GLU	3.5
1	A	165	CYS	3.5
1	A	280	LEU	3.4
1	A	263	ASP	3.4
1	B	247	ALA	3.4
1	B	110	MET	3.4
1	A	252	GLU	3.4
1	B	163	VAL	3.3
1	B	144	ALA	3.3
1	B	141	GLY	3.3
1	B	307	ALA	3.3
1	B	284	LEU	3.3
1	B	158	ALA	3.3
1	B	92	GLU	3.3
1	A	110	MET	3.3
1	A	108	GLY	3.2
1	A	102	ILE	3.2
1	A	206	ARG	3.2
1	B	136	LEU	3.2
1	A	333	PHE	3.2
1	A	144	ALA	3.2
1	B	208	GLU	3.2
1	B	137	GLY	3.2
1	B	115	THR	3.2
1	B	348	THR	3.2
1	B	281	SER	3.1
1	A	113	SER	3.1
1	B	94	LEU	3.1
1	B	103	TYR	3.0
1	A	272	GLY	3.0
1	B	130	GLN	3.0
1	A	261	ALA	3.0
1	B	147	ARG	3.0
1	B	344	GLY	3.0
1	B	97	ASP	3.0
1	A	267	TYR	3.0
1	B	200	ARG	2.9
1	A	346	TRP	2.9
1	B	306	SER	2.9
1	A	125	ASP	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	309	VAL	2.9
1	A	137	GLY	2.8
1	B	108	GLY	2.8
1	A	338	THR	2.8
1	B	291	PHE	2.8
1	B	305	ALA	2.8
1	A	107	THR	2.7
1	A	115	THR	2.7
1	A	279	ASP	2.7
1	B	274	PRO	2.7
1	B	135	GLN	2.7
1	A	258	GLY	2.7
1	B	3	THR	2.7
1	A	48	ARG	2.7
1	B	259	TRP	2.6
1	A	94	LEU	2.6
1	B	113	SER	2.6
1	A	147	ARG	2.6
1	B	107	THR	2.6
1	A	264	LEU	2.6
1	B	198	ARG	2.6
1	A	209	ARG	2.6
1	B	287	ASP	2.6
1	B	325	GLY	2.6
1	B	101	ILE	2.6
1	A	111	MET	2.5
1	A	200	ARG	2.5
1	B	145	ILE	2.5
1	B	111	MET	2.5
1	B	146	ASN	2.5
1	A	307	ALA	2.4
1	B	254	ALA	2.4
1	B	349	ALA	2.4
1	A	156	PRO	2.4
1	B	282	THR	2.4
1	A	208	GLU	2.4
1	A	201	GLY	2.4
1	B	30	THR	2.4
1	B	162	ILE	2.4
1	B	151	PHE	2.4
1	A	257	HIS	2.3
1	B	293	PHE	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	333	PHE	2.3
1	A	347	GLN	2.3
1	B	286	VAL	2.3
1	B	142	GLY	2.3
1	A	253	LEU	2.3
1	A	141	GLY	2.3
1	A	332	GLY	2.3
1	B	338	THR	2.2
1	B	211	GLY	2.2
1	B	339	ALA	2.2
1	A	171	CYS	2.2
1	A	3	THR	2.2
1	A	154	ALA	2.2
1	B	332	GLY	2.2
1	A	282	THR	2.2
1	B	271	ALA	2.1
1	A	274	PRO	2.1
1	B	320	GLY	2.1
1	B	95	ALA	2.1
1	B	209	ARG	2.1
1	A	265	ASP	2.1
1	A	306	SER	2.1
1	B	335	PRO	2.1
1	A	251	LYS	2.1
1	B	345	CYS	2.1
1	B	289	HIS	2.1
1	A	345	CYS	2.1
1	A	305	ALA	2.1
1	A	198	ARG	2.0
1	A	288	PRO	2.0
1	A	88	LEU	2.0
1	A	231	PHE	2.0
1	A	162	ILE	2.0
1	A	242	THR	2.0
1	B	278	ASP	2.0
1	A	339	ALA	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 [\(i\)](#)

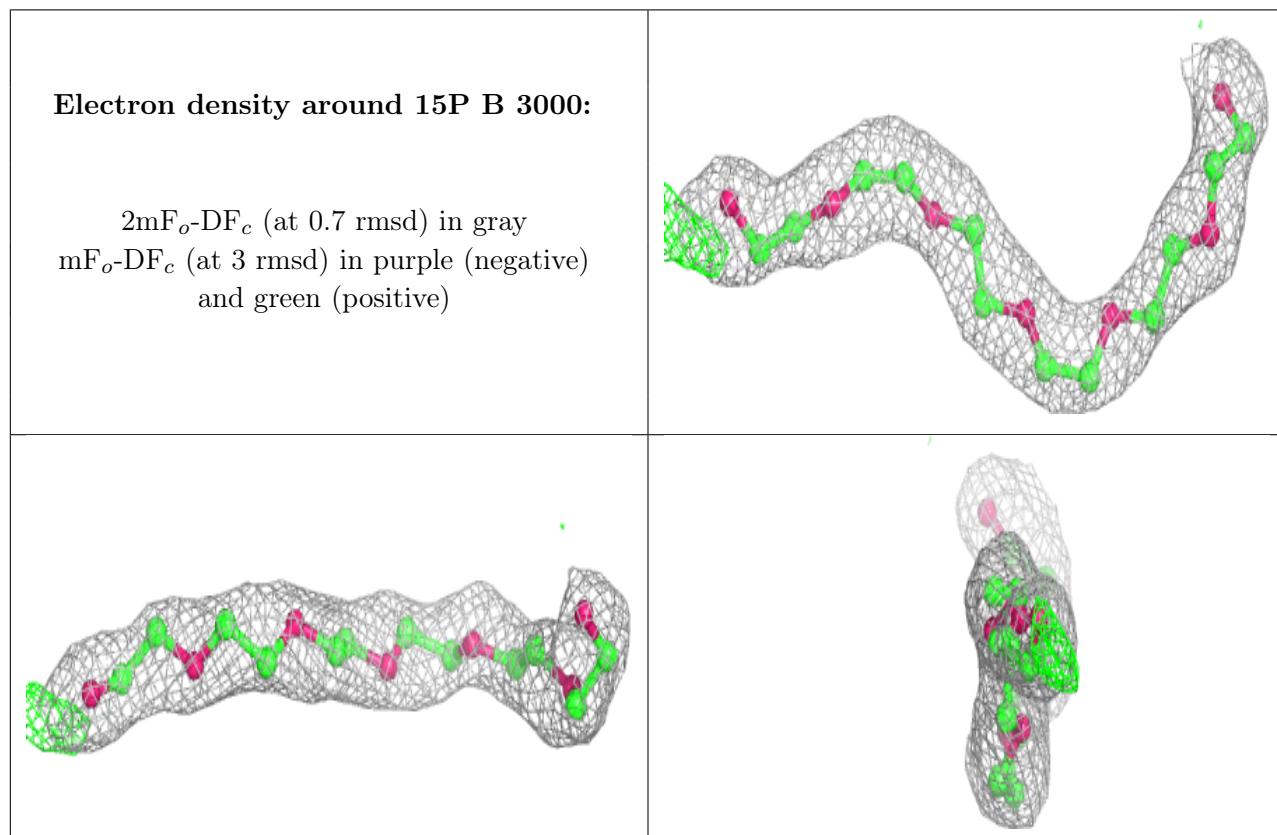
There are no monosaccharides in this entry.

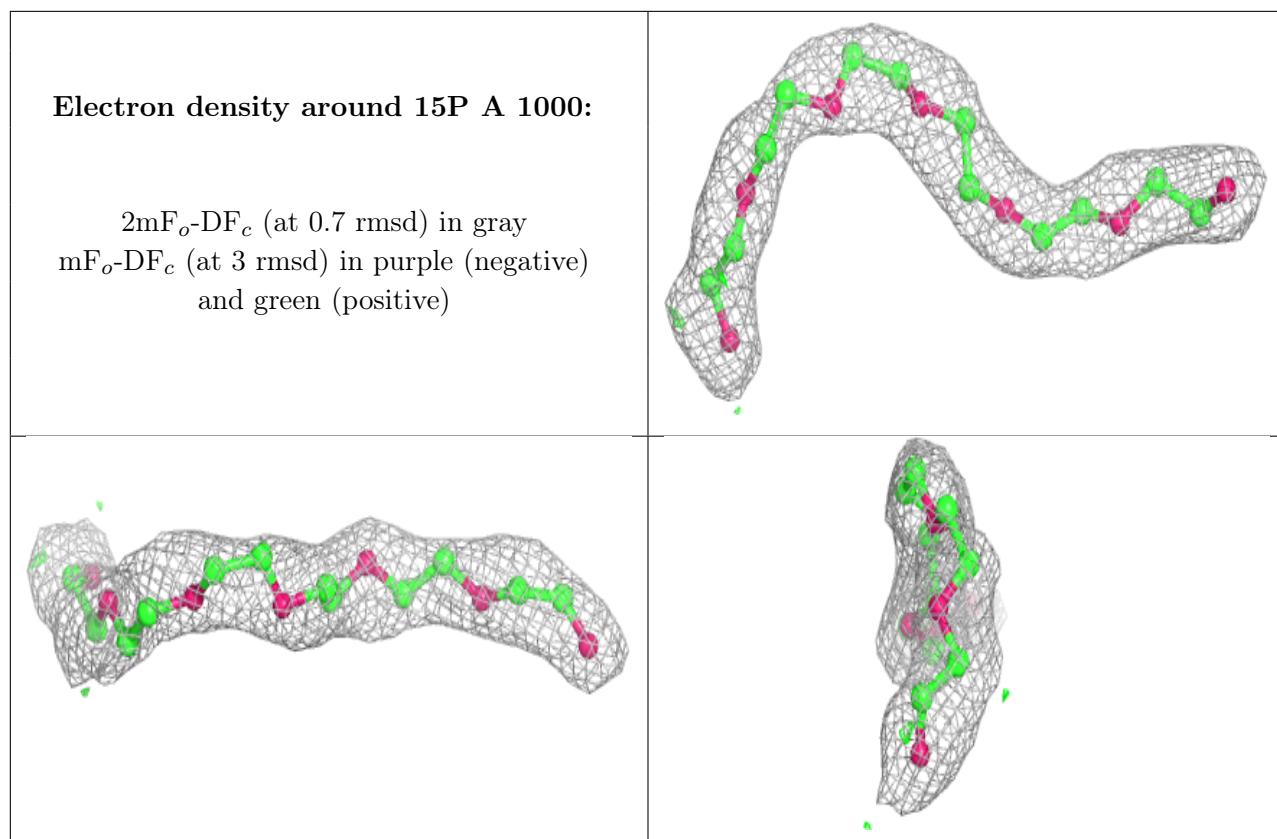
6.4 Ligands [\(i\)](#)

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	B	3000	19/104	0.80	0.20	38,47,53,54	0
2	15P	A	1000	19/104	0.81	0.23	43,47,57,58	0
3	GOL	A	2000	6/6	0.91	0.18	35,44,47,49	0
3	GOL	B	4000	6/6	0.94	0.16	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.





6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.