



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:39 PM UTC

PDB ID : 1WDL / pdb_00001wdl
Title : fatty acid beta-oxidation multienzyme complex from *Pseudomonas fragi*, form II (native4)
Authors : Ishikawa, M.; Tsuchiya, D.; Oyama, T.; Tsunaka, Y.; Morikawa, K.
Deposited on : 2004-05-17
Resolution : 3.50 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

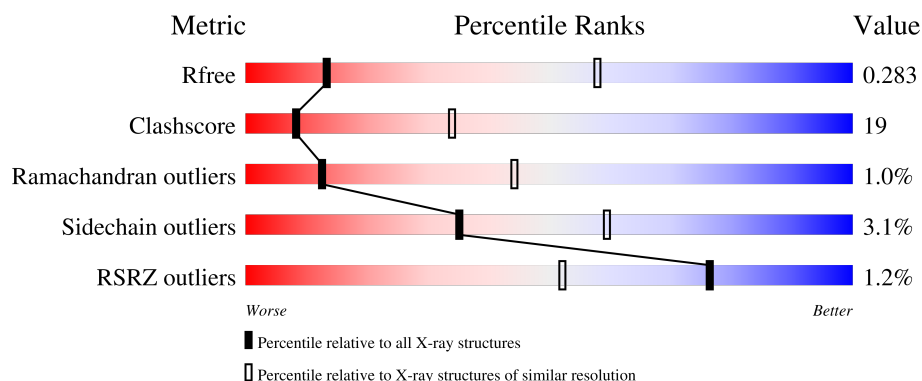
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	715	2% 61% 36% .
1	B	715	2% 60% 37% ..
2	C	390	63% 35% .
2	D	390	64% 35% .

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 16610 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.

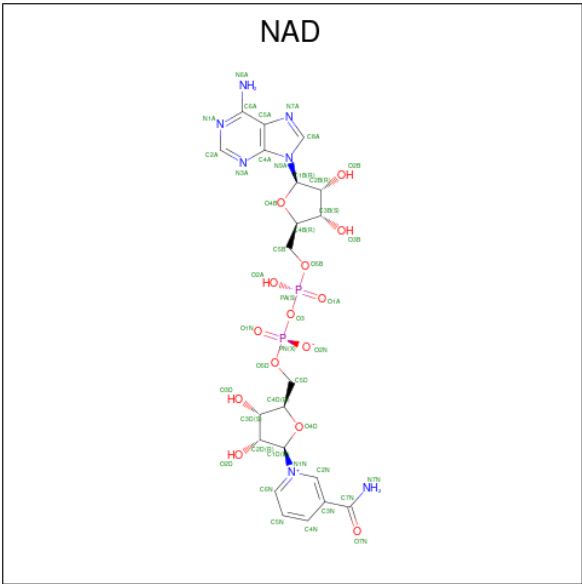
- Molecule 1 is a protein called Fatty oxidation complex alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	715	Total	C	N	O	S	0	0	0
			5361	3420	906	1008	27			
1	B	706	Total	C	N	O	S	0	0	0
			5241	3340	879	995	27			

- Molecule 2 is a protein called 3-ketoacyl-CoA thiolase.

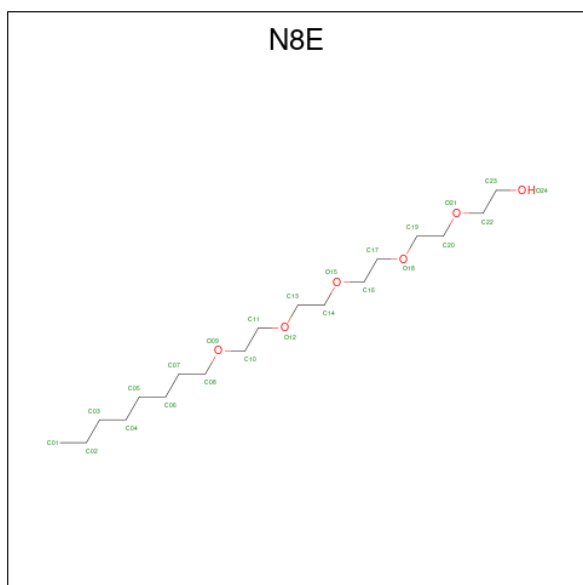
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	390	Total	C	N	O	S	0	0	0
			2885	1795	513	548	29			
2	D	390	Total	C	N	O	S	0	0	0
			2881	1792	512	548	29			

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



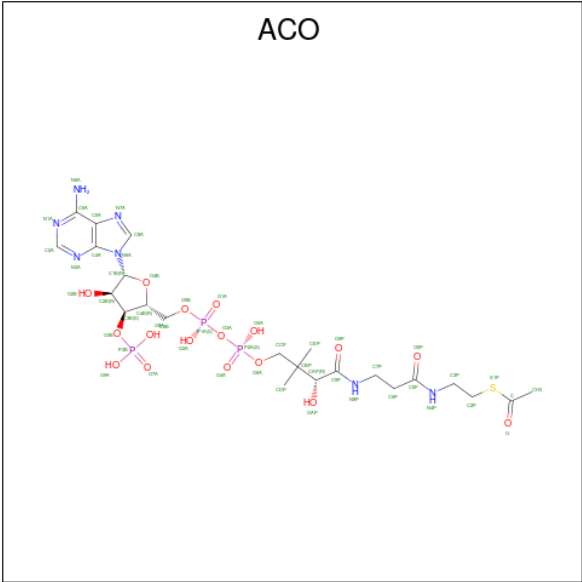
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			35	15	5	13	2		
3	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 4 is 3,6,9,12,15-PENTAOXATRICOSAN-1-OL (CCD ID: N8E) (formula: $C_{18}H_{38}O_6$).

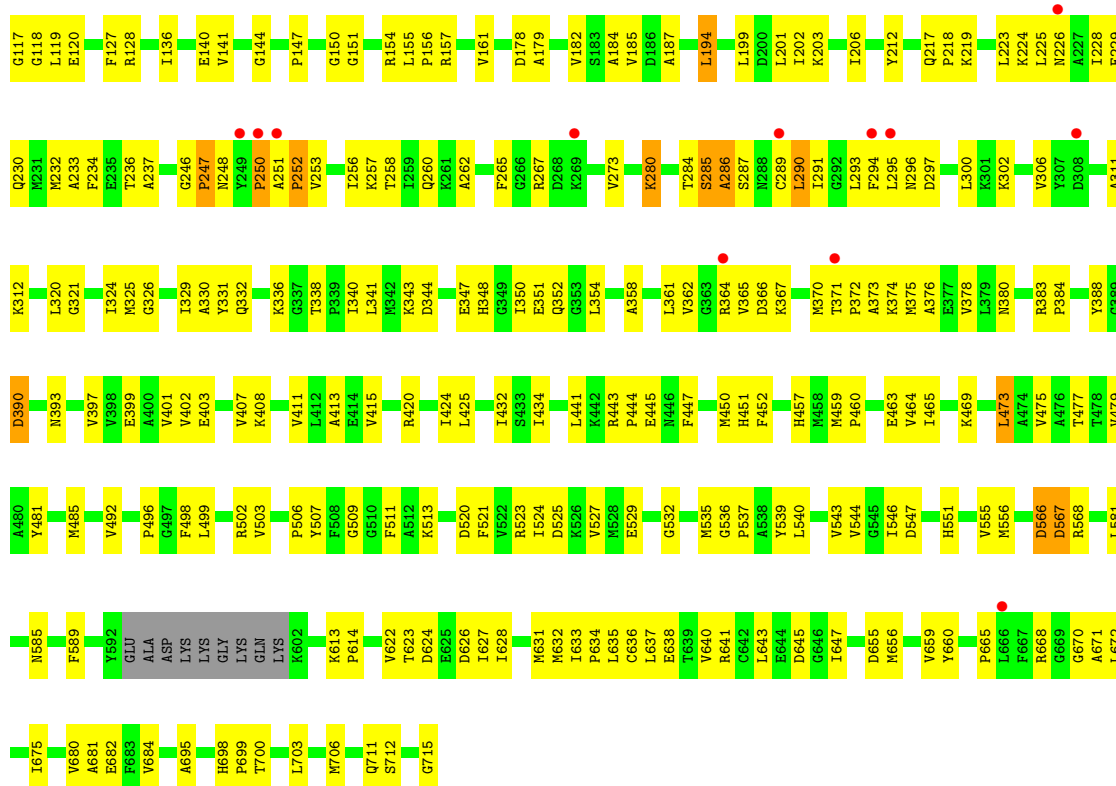


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			24	18	6		
4	A	1	Total	C	O	0	0
			24	18	6		
4	A	1	Total	C	O	0	0
			24	18	6		

- Molecule 5 is ACETYL COENZYME *A (CCD ID: ACO) (formula: $C_{23}H_{38}N_7O_{17}P_3S$).

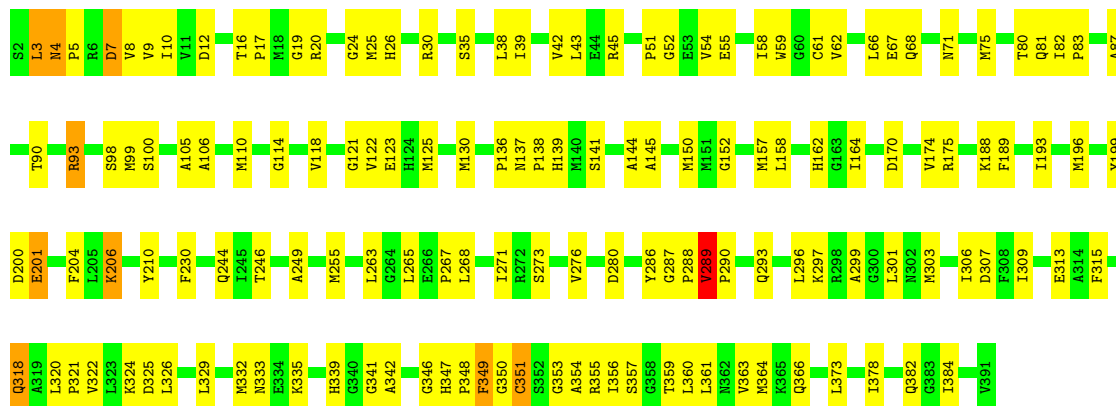


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	C	1	40	16	6	15	3	0	0
5	D	1	51	23	7	17	3	1	0



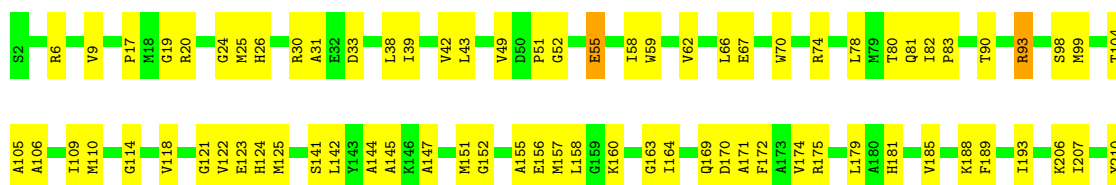
• Molecule 2: 3-ketoacyl-CoA thiolase

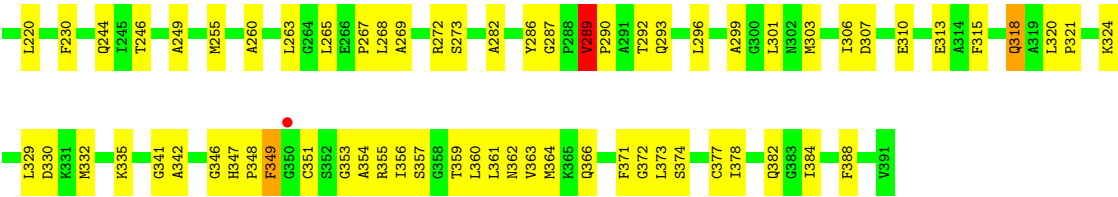
Chain C: 63% 35% .



• Molecule 2: 3-ketoacyl-CoA thiolase

Chain D: 64% 35% .





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	95.66Å 118.41Å 191.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 3.50 12.00 – 3.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (12.00-3.50) 96.8 (12.00-3.50)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.18 (at 3.52Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.233 , 0.283 0.236 , 0.283	Depositor DCC
R_{free} test set	1914 reflections (6.88%)	wwPDB-VP
Wilson B-factor (Å ²)	40.9	Xtriage
Anisotropy	0.507	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 31.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	16610	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.70% 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: N8E, NAD, ACO

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	0.30	0/5448	0.91	16/7364 (0.2%)
1	B	0.29	0/5325	0.88	10/7213 (0.1%)
2	C	0.30	1/2933 (0.0%)	0.82	4/3959 (0.1%)
2	D	0.31	1/2929 (0.0%)	0.81	3/3955 (0.1%)
All	All	0.30	2/16635 (0.0%)	0.87	33/22491 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	289	VAL	CA-CB	5.79	1.57	1.54
2	C	289	VAL	CA-CB	5.20	1.56	1.54

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	310	ILE	N-CA-C	-14.99	99.47	113.71
1	B	568	ARG	N-CA-C	-10.82	87.75	110.80
1	A	290	LEU	N-CA-C	-10.69	100.29	113.97
1	B	290	LEU	N-CA-C	-9.90	101.13	113.02
1	A	601	LYS	N-CA-C	7.66	121.89	109.40
1	A	246	GLY	CA-C-N	6.96	128.54	119.84
1	A	246	GLY	C-N-CA	6.96	128.54	119.84
1	B	286	ALA	N-CA-C	-6.58	96.78	110.80
1	A	308	ASP	N-CA-C	6.49	118.90	111.11
2	D	93	ARG	N-CA-C	-6.37	102.90	110.41
1	A	715	GLY	N-CA-C	-6.21	95.30	113.30
1	B	246	GLY	CA-C-N	6.20	127.59	119.84
1	B	246	GLY	C-N-CA	6.20	127.59	119.84
1	B	715	GLY	N-CA-C	-5.99	95.92	113.30
1	A	184	ALA	N-CA-C	-5.94	104.75	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	93	ARG	N-CA-C	-5.84	103.51	110.41
1	A	289	CYS	N-CA-C	5.76	123.07	110.80
1	A	309	LYS	N-CA-C	5.76	119.99	111.87
1	A	589	PHE	N-CA-C	-5.73	105.55	112.54
1	B	184	ALA	N-CA-C	-5.60	105.18	112.23
1	B	71	ILE	N-CA-C	5.56	119.90	111.89
2	C	268	LEU	N-CA-C	-5.39	106.83	113.41
1	A	594	ALA	N-CA-C	5.39	118.33	109.76
2	D	66	LEU	CB-CA-C	-5.37	109.93	117.23
2	C	66	LEU	CB-CA-C	-5.36	109.94	117.23
2	D	268	LEU	N-CA-C	-5.34	106.90	113.41
1	B	589	PHE	N-CA-C	-5.32	105.64	111.82
1	A	506	PRO	N-CA-C	-5.28	106.52	113.65
1	A	530	LYS	N-CA-C	-5.27	106.81	113.18
1	A	666	LEU	N-CA-C	5.25	117.43	111.02
2	C	326	LEU	N-CA-C	-5.22	106.88	113.20
1	A	632	MET	N-CA-C	5.12	116.55	111.07
1	B	285	SER	N-CA-C	5.11	121.68	110.80

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	5361	0	5415	230	0
1	B	5241	0	5227	194	0
2	C	2885	0	2881	116	0
2	D	2881	0	2870	122	0
3	A	35	0	19	0	0
3	B	44	0	26	1	0
4	A	72	0	114	6	0
5	C	40	0	21	0	0
5	D	51	0	34	4	0
All	All	16610	0	16607	638	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 19.

All (638) 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)
2:C:289:VAL:HG13	2:C:290:PRO:HD3	1.49	0.95
2:D:272:ARG:HH12	2:D:301:LEU:HD21	1.33	0.94
2:D:289:VAL:HG13	2:D:290:PRO:HD3	1.49	0.93
1:A:666:LEU:HD12	1:A:666:LEU:H	1.35	0.90
2:D:378:ILE:HB	2:D:382:GLN:HB2	1.57	0.86
1:A:354:LEU:HD13	1:B:380:ASN:HB3	1.56	0.86
2:D:272:ARG:NH1	2:D:301:LEU:HD21	1.93	0.84
1:A:107:VAL:HG22	1:A:127:PHE:HB2	1.59	0.83
1:B:114:ALA:HB3	1:B:136:ILE:HG22	1.59	0.83
1:B:107:VAL:HG22	1:B:127:PHE:HB2	1.59	0.83
1:A:114:ALA:HB3	1:A:136:ILE:HG22	1.61	0.82
2:D:348:PRO:HB2	2:D:351:CYS:HB3	1.59	0.82
2:C:55:GLU:HG3	2:C:114:GLY:HA2	1.64	0.80
1:B:290:LEU:HG	1:B:293:LEU:HD12	1.63	0.80
1:B:320:LEU:HD11	1:B:415:VAL:HG21	1.66	0.78
1:B:144:GLY:HA2	1:B:250:PRO:HB3	1.65	0.77
2:D:263:LEU:HB2	2:D:265:LEU:HD22	1.66	0.77
2:C:306:ILE:HD13	2:C:373:LEU:HB2	1.67	0.77
1:A:465:ILE:HD12	1:A:465:ILE:H	1.49	0.76
1:B:247:PRO:HB3	1:B:529:GLU:O	1.84	0.76
1:B:56:VAL:HB	1:B:106:THR:HG22	1.68	0.76
1:B:99:PHE:HA	1:B:102:LEU:HD13	1.69	0.75
1:A:254:GLU:HG3	1:A:281:LEU:HD21	1.67	0.74
1:A:354:LEU:HD21	1:A:384:PRO:HG3	1.70	0.74
1:B:258:THR:HG23	1:B:273:VAL:HG12	1.71	0.73
1:A:141:VAL:HG12	1:A:251:ALA:HB3	1.71	0.71
1:B:361:LEU:HB3	1:B:375:MET:HG3	1.72	0.71
1:A:232:MET:HA	2:C:157:MET:HE1	1.72	0.71
1:B:566:ASP:O	1:B:567:ASP:HB2	1.90	0.71
1:B:248:ASN:HB3	1:B:532:GLY:O	1.90	0.71
2:D:55:GLU:HG3	2:D:114:GLY:HA2	1.72	0.71
1:A:404:ASN:HD21	4:A:1004:N8E:H031	1.54	0.70
1:B:248:ASN:O	1:B:250:PRO:HD3	1.91	0.70
1:A:296:ASN:HD21	1:A:650:THR:HB	1.56	0.70
1:B:141:VAL:HG12	1:B:251:ALA:HB3	1.73	0.70
2:D:306:ILE:HD13	2:D:373:LEU:HB2	1.71	0.70
1:B:680:VAL:HG21	1:B:712:SER:HA	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:LYS:HG3	1:A:485:MET:HA	1.74	0.69
2:C:123:GLU:HG2	2:C:349:PHE:HB2	1.73	0.69
1:A:361:LEU:HB3	1:A:375:MET:HG3	1.74	0.69
1:B:336:LYS:HG3	1:B:485:MET:HA	1.75	0.69
1:A:680:VAL:HG21	1:A:712:SER:HA	1.74	0.68
1:A:626:ASP:HA	1:A:629:ASN:HD22	1.59	0.68
1:B:465:ILE:HD12	1:B:465:ILE:H	1.59	0.68
2:C:348:PRO:HB2	2:C:351:CYS:HB3	1.75	0.68
1:A:581:LEU:HB2	1:A:585:ASN:HB2	1.77	0.67
2:C:137:ASN:HD21	2:C:139:HIS:HB2	1.59	0.67
2:C:263:LEU:HB2	2:C:265:LEU:HD22	1.76	0.67
1:B:280:LYS:HB2	1:B:280:LYS:NZ	2.10	0.67
2:C:62:VAL:HG21	2:C:349:PHE:HB3	1.77	0.67
1:A:186:ASP:CG	1:A:215:LYS:NZ	2.53	0.66
1:A:504:LEU:HD12	1:A:662:ILE:HG22	1.76	0.66
1:B:537:PRO:HG2	1:B:631:MET:HE3	1.77	0.66
1:A:537:PRO:HG2	1:A:631:MET:HE3	1.76	0.66
2:C:17:PRO:HB2	2:C:25:MET:HE1	1.78	0.66
2:D:62:VAL:HG21	2:D:349:PHE:HB3	1.78	0.66
2:C:201:GLU:CD	2:C:201:GLU:H	2.04	0.65
2:D:125:MET:HE2	2:D:348:PRO:HA	1.78	0.65
1:B:262:ALA:HA	1:B:265:PHE:HD1	1.62	0.64
2:C:10:ILE:HD11	2:C:271:ILE:HG13	1.77	0.64
1:B:31:LYS:HD2	1:B:70:ASP:HB2	1.79	0.64
2:D:98:SER:HB3	2:D:354:ALA:H	1.63	0.64
1:B:547:ASP:HB3	1:B:581:LEU:HD22	1.79	0.64
1:B:633:ILE:HB	1:B:634:PRO:HD3	1.78	0.64
1:B:32:PHE:HE2	1:B:40:LEU:HD12	1.62	0.64
2:C:43:LEU:HD11	2:C:82:ILE:HD11	1.80	0.64
1:A:633:ILE:HB	1:A:634:PRO:HD3	1.79	0.63
1:B:613:LYS:HB3	1:B:614:PRO:HD3	1.81	0.63
1:B:706:MET:HB2	1:B:711:GLN:HB2	1.79	0.63
2:C:51:PRO:HB3	2:C:82:ILE:HD13	1.80	0.63
2:D:289:VAL:HG23	2:D:293:GLN:NE2	2.13	0.63
1:A:89:ASN:N	1:A:89:ASN:HD22	1.95	0.63
1:A:145:ILE:HD13	1:A:290:LEU:HD11	1.80	0.62
1:A:330:ALA:HA	1:A:340:ILE:HD13	1.80	0.62
2:C:125:MET:HE2	2:C:348:PRO:HA	1.81	0.62
2:D:313:GLU:CD	2:D:341:GLY:HA3	2.23	0.62
2:C:289:VAL:O	2:C:293:GLN:HG3	1.99	0.62
1:A:338:THR:HG21	1:A:481:TYR:HE1	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:500:VAL:HG13	1:A:662:ILE:HG23	1.81	0.62
2:C:320:LEU:HB2	2:C:321:PRO:HD3	1.80	0.62
2:D:320:LEU:HB2	2:D:321:PRO:HD3	1.81	0.62
2:D:342:ALA:HB1	2:D:347:HIS:HB2	1.82	0.62
2:C:93:ARG:NH1	2:C:276:VAL:HG11	2.15	0.62
2:C:315:PHE:O	2:C:318:GLN:HG3	2.00	0.62
1:A:226:ASN:CG	1:A:228:ILE:HG22	2.26	0.61
1:A:502:ARG:HA	1:A:556:MET:HE2	1.82	0.61
1:A:592:TYR:HA	1:A:601:LYS:O	2.01	0.60
2:C:125:MET:HE3	2:C:246:THR:H	1.65	0.60
1:B:354:LEU:HD21	1:B:384:PRO:HG3	1.84	0.60
1:B:388:TYR:CE2	1:B:415:VAL:HG22	2.37	0.59
2:C:3:LEU:HG	2:C:3:LEU:O	2.02	0.59
2:D:30:ARG:HB2	2:D:33:ASP:OD2	2.01	0.59
1:A:289:CYS:HB2	1:A:714:PHE:O	2.02	0.59
1:B:330:ALA:HA	1:B:340:ILE:HD13	1.83	0.59
2:D:188:LYS:HD2	2:D:366:GLN:OE1	2.03	0.59
1:B:393:ASN:HA	1:B:420:ARG:HH12	1.67	0.59
2:C:296:LEU:HD21	2:C:306:ILE:HD11	1.85	0.59
2:D:272:ARG:HH11	2:D:371:PHE:HE2	1.50	0.59
1:A:343:LYS:HD3	1:A:344:ASP:N	2.17	0.59
1:B:581:LEU:HB2	1:B:585:ASN:HB2	1.85	0.59
1:B:656:MET:HE3	1:B:660:TYR:HE1	1.68	0.59
1:A:302:LYS:O	1:A:306:VAL:HG23	2.03	0.59
1:A:141:VAL:HG23	1:A:142:LYS:HD2	1.84	0.59
1:A:228:ILE:HG21	2:C:280:ASP:CG	2.27	0.59
1:A:362:VAL:HG21	1:B:373:ALA:HA	1.85	0.59
1:B:521:PHE:HA	1:B:524:ILE:HD12	1.85	0.59
1:A:109:ALA:HB1	1:A:194:LEU:HD22	1.83	0.59
1:A:226:ASN:OD1	1:A:228:ILE:HG22	2.03	0.58
1:A:669:GLY:HA3	1:A:673:ARG:HD3	1.84	0.58
1:A:212:TYR:OH	1:A:213:LYS:HE2	2.04	0.58
1:B:311:ALA:HB1	1:B:477:THR:HA	1.84	0.58
2:D:125:MET:HE3	2:D:246:THR:H	1.68	0.58
1:A:511:PHE:HB2	1:A:631:MET:HE1	1.86	0.58
1:A:186:ASP:CG	1:A:215:LYS:HZ1	2.10	0.58
1:A:533:TRP:HH2	1:A:662:ILE:HD12	1.69	0.58
1:B:228:ILE:HG22	2:D:282:ALA:HB3	1.85	0.58
1:B:535:MET:HE3	1:B:540:LEU:HG	1.84	0.58
1:B:622:VAL:HG23	1:B:626:ASP:HB2	1.86	0.58
2:C:287:GLY:O	2:C:290:PRO:HD2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:359:THR:O	2:D:363:VAL:HG23	2.03	0.57
1:A:521:PHE:HA	1:A:524:ILE:HD12	1.86	0.57
2:C:378:ILE:HB	2:C:382:GLN:HB2	1.85	0.57
1:A:233:ALA:HB2	2:C:145:ALA:HB2	1.85	0.57
1:A:144:GLY:HA2	1:A:250:PRO:HB3	1.86	0.57
1:A:525:ASP:HB3	1:A:536:GLY:HA3	1.86	0.57
1:B:33:ASN:HB2	1:B:73:GLU:OE1	2.05	0.57
1:B:320:LEU:HD13	1:B:411:VAL:HG12	1.87	0.57
2:D:287:GLY:O	2:D:290:PRO:HD2	2.04	0.57
1:B:388:TYR:HE2	1:B:415:VAL:HG22	1.68	0.57
2:D:39:ILE:HG23	2:D:118:VAL:HG11	1.87	0.57
2:D:377:CYS:SG	5:D:4001:ACO:HH31	2.44	0.57
1:A:361:LEU:HD21	1:A:378:VAL:HG11	1.86	0.56
1:B:343:LYS:HD3	1:B:344:ASP:N	2.20	0.56
1:B:638:GLU:HA	1:B:641:ARG:HH11	1.70	0.56
1:B:671:ALA:O	1:B:675:ILE:HG13	2.05	0.56
1:A:633:ILE:HD11	1:A:686:LEU:HD22	1.88	0.56
1:B:424:ILE:HD12	1:B:424:ILE:N	2.21	0.56
1:B:511:PHE:HB2	1:B:631:MET:HE1	1.87	0.56
1:B:109:ALA:HB1	1:B:194:LEU:HD22	1.85	0.56
1:B:217:GLN:HB3	1:B:218:PRO:HD3	1.87	0.56
2:C:342:ALA:HB1	2:C:347:HIS:HB2	1.86	0.56
1:A:290:LEU:O	1:A:290:LEU:HD23	2.06	0.56
2:C:52:GLY:HA2	2:C:83:PRO:HG2	1.88	0.56
1:B:434:ILE:HD13	1:B:465:ILE:HG21	1.87	0.56
1:B:67:VAL:O	1:B:68:GLY:O	2.23	0.55
2:C:318:GLN:C	2:C:321:PRO:HD2	2.31	0.55
2:D:356:ILE:HG13	2:D:357:SER:N	2.21	0.55
1:A:31:LYS:HD2	1:A:70:ASP:HB2	1.87	0.55
2:C:130:MET:O	2:D:70:TRP:HZ2	1.89	0.55
2:D:315:PHE:O	2:D:318:GLN:HG3	2.06	0.55
1:A:209:GLU:OE2	2:D:206:LYS:HB2	2.07	0.55
1:A:466:ARG:HG3	1:A:470:SER:HB2	1.87	0.55
2:D:51:PRO:HB3	2:D:82:ILE:HD13	1.86	0.55
1:B:525:ASP:HB2	1:B:536:GLY:HA3	1.88	0.55
1:A:465:ILE:HD12	1:A:465:ILE:N	2.19	0.55
1:B:347:GLU:O	1:B:351:GLU:HG2	2.06	0.55
2:C:152:GLY:HA3	2:C:230:PHE:CD2	2.41	0.55
1:A:375:MET:HE2	1:B:375:MET:HE2	1.88	0.55
2:C:80:THR:HG22	2:C:81:GLN:N	2.22	0.55
1:A:451:HIS:HB3	1:A:463:GLU:HB2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:GLY:HA3	1:B:154:ARG:NH1	2.23	0.54
2:D:17:PRO:HB2	2:D:25:MET:HE1	1.89	0.54
1:A:450:MET:HG2	1:A:452:PHE:CE1	2.42	0.54
1:A:292:GLY:HA3	1:A:714:PHE:C	2.32	0.54
1:B:361:LEU:HD21	1:B:378:VAL:HG11	1.89	0.54
1:B:397:VAL:HB	1:B:425:LEU:HD23	1.90	0.54
1:A:341:LEU:HD23	1:A:383:ARG:HB2	1.89	0.54
1:B:101:ASP:CG	1:B:267:ARG:HH22	2.15	0.54
1:B:155:LEU:HB3	1:B:156:PRO:HD3	1.90	0.54
2:D:172:PHE:HE2	2:D:313:GLU:HG2	1.72	0.54
1:A:246:GLY:HA3	1:A:668:ARG:HH22	1.73	0.54
1:A:502:ARG:HD3	1:A:642:CYS:SG	2.48	0.54
2:D:318:GLN:C	2:D:321:PRO:HD2	2.33	0.54
1:A:503:VAL:HG12	1:A:635:LEU:HG	1.89	0.53
1:B:413:ALA:HA	1:B:441:LEU:HD23	1.91	0.53
2:D:156:GLU:O	2:D:160:LYS:HG2	2.08	0.53
1:A:153:VAL:HG21	1:A:271:LEU:HD23	1.91	0.53
1:A:539:TYR:O	1:A:543:VAL:HG23	2.08	0.53
1:A:553:ARG:HH12	1:A:573:ASP:CG	2.15	0.53
2:C:359:THR:O	2:C:363:VAL:HG23	2.07	0.53
1:A:434:ILE:HD13	1:A:465:ILE:HG21	1.89	0.53
1:A:375:MET:HE1	1:B:372:PRO:O	2.08	0.53
1:A:706:MET:HB2	1:A:711:GLN:HB2	1.90	0.53
1:B:289:CYS:C	1:B:291:ILE:H	2.11	0.53
1:B:229:GLU:O	2:D:145:ALA:HB2	2.09	0.53
2:C:4:ASN:HB2	2:C:7:ASP:OD2	2.09	0.53
1:A:258:THR:HG23	1:A:273:VAL:HG12	1.90	0.52
1:A:292:GLY:O	1:A:296:ASN:HB2	2.09	0.52
1:A:457:HIS:CE1	1:A:458:MET:HG2	2.44	0.52
1:B:117:GLY:HA2	1:B:120:GLU:OE1	2.09	0.52
2:D:80:THR:HG22	2:D:81:GLN:N	2.23	0.52
2:D:272:ARG:NH1	2:D:371:PHE:HE2	2.08	0.52
1:B:280:LYS:HB2	1:B:280:LYS:HZ3	1.74	0.52
1:B:450:MET:HG2	1:B:452:PHE:CE1	2.45	0.52
2:C:164:ILE:N	2:C:164:ILE:HD12	2.24	0.52
1:A:248:ASN:O	1:A:250:PRO:HD3	2.08	0.52
1:B:507:TYR:HB2	1:B:635:LEU:HD12	1.91	0.52
2:D:175:ARG:HE	2:D:179:LEU:HD12	1.74	0.52
1:B:445:GLU:CD	1:B:445:GLU:H	2.16	0.52
2:D:106:ALA:O	2:D:110:MET:HG3	2.10	0.52
1:A:32:PHE:CE1	1:A:66:ILE:HG21	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:ILE:O	1:B:206:ILE:HG13	2.10	0.52
1:A:251:ALA:N	1:A:252:PRO:CD	2.73	0.52
2:D:25:MET:HE2	2:D:26:HIS:NE2	2.25	0.52
2:D:38:LEU:O	2:D:42:VAL:HG23	2.10	0.52
2:D:246:THR:OG1	2:D:346:GLY:HA3	2.10	0.52
1:A:265:PHE:HB3	1:A:269:LYS:HB3	1.90	0.52
1:A:671:ALA:O	1:A:675:ILE:HG13	2.09	0.52
2:C:255:MET:HE1	2:C:263:LEU:HD12	1.92	0.52
2:D:255:MET:HE2	2:D:260:ALA:HA	1.92	0.52
1:A:155:LEU:HB3	1:A:156:PRO:HD3	1.92	0.52
1:B:325:MET:HG3	3:B:2001:NAD:O4D	2.09	0.52
1:B:348:HIS:O	1:B:352:GLN:HG2	2.10	0.52
2:C:25:MET:HE2	2:C:26:HIS:NE2	2.25	0.52
2:C:246:THR:OG1	2:C:346:GLY:HA3	2.10	0.52
2:D:189:PHE:HB3	2:D:193:ILE:CD1	2.40	0.52
1:B:523:ARG:O	1:B:527:VAL:HG23	2.09	0.52
1:A:525:ASP:CB	1:A:536:GLY:HA3	2.40	0.51
1:B:364:ARG:NH2	1:B:370:MET:HE3	2.24	0.51
2:C:20:ARG:O	2:C:24:GLY:HA3	2.10	0.51
1:B:330:ALA:HA	1:B:340:ILE:HG21	1.93	0.51
2:C:10:ILE:HD12	2:C:10:ILE:N	2.25	0.51
1:A:312:LYS:NZ	1:A:422:ASP:HB2	2.25	0.51
1:B:393:ASN:HA	1:B:420:ARG:NH1	2.26	0.51
1:B:475:VAL:O	1:B:479:VAL:HG23	2.10	0.51
2:D:122:VAL:HG23	2:D:249:ALA:HB2	1.91	0.51
2:C:360:LEU:HG	2:C:364:MET:HE2	1.91	0.51
1:A:292:GLY:HA3	1:A:714:PHE:O	2.11	0.51
2:C:99:MET:HB3	2:C:384:ILE:HD13	1.93	0.51
1:B:141:VAL:HG12	1:B:251:ALA:CB	2.39	0.50
2:D:80:THR:HG22	2:D:81:GLN:H	1.76	0.50
1:A:507:TYR:HB2	1:A:635:LEU:HD12	1.94	0.50
1:B:525:ASP:CB	1:B:536:GLY:HA3	2.42	0.50
2:D:9:VAL:HG13	2:D:267:PRO:HB3	1.94	0.50
2:D:310:GLU:HG3	2:D:360:LEU:HB2	1.93	0.50
1:A:523:ARG:O	1:A:527:VAL:HG23	2.12	0.50
1:B:262:ALA:HA	1:B:265:PHE:CD1	2.44	0.50
2:D:313:GLU:O	2:D:342:ALA:HB3	2.11	0.50
1:A:186:ASP:CG	1:A:215:LYS:HZ3	2.20	0.50
1:A:199:LEU:HD11	1:A:203:LYS:HE3	1.94	0.50
1:A:228:ILE:HD13	2:C:280:ASP:HB2	1.93	0.50
1:A:645:ASP:HB2	1:A:647:ILE:HD13	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:312:LYS:HG3	1:B:473:LEU:HD21	1.92	0.50
2:D:17:PRO:HB3	2:D:210:TYR:O	2.11	0.50
2:D:164:ILE:HD12	2:D:164:ILE:N	2.27	0.50
2:D:265:LEU:H	2:D:265:LEU:HD23	1.76	0.50
1:A:157:ARG:HD2	1:A:219:LYS:HA	1.93	0.50
1:A:246:GLY:HA3	1:A:668:ARG:HH12	1.76	0.50
1:A:638:GLU:HA	1:A:641:ARG:HH11	1.76	0.50
2:D:58:ILE:HD12	2:D:105:ALA:HB2	1.93	0.50
1:A:82:ASP:O	1:A:86:ILE:HG13	2.12	0.49
1:A:255:ALA:O	1:A:259:ILE:HG13	2.12	0.49
1:A:424:ILE:HD12	1:A:424:ILE:N	2.27	0.49
1:B:287:SER:OG	1:B:668:ARG:NH1	2.45	0.49
2:D:255:MET:HE1	2:D:263:LEU:HD12	1.93	0.49
1:A:350:ILE:HG21	1:A:384:PRO:HB3	1.94	0.49
1:A:580:ARG:CZ	1:A:608:VAL:HG22	2.41	0.49
2:C:12:ASP:CG	2:C:45:ARG:HH21	2.19	0.49
2:D:98:SER:CB	2:D:354:ALA:H	2.25	0.49
1:A:574:ALA:HB2	1:A:615:ILE:HD11	1.94	0.49
1:B:108:ALA:HB3	1:B:128:ARG:HG2	1.93	0.49
1:B:302:LYS:O	1:B:306:VAL:HG23	2.13	0.49
1:B:401:VAL:HG12	1:B:402:VAL:N	2.27	0.49
2:C:8:VAL:HG11	2:C:271:ILE:HD12	1.94	0.49
1:B:199:LEU:HD11	1:B:203:LYS:HE3	1.92	0.49
1:B:465:ILE:HD12	1:B:465:ILE:N	2.25	0.49
2:C:273:SER:HB3	2:C:299:ALA:HB2	1.94	0.49
1:A:325:MET:O	1:A:329:ILE:HG13	2.11	0.49
2:C:55:GLU:HG3	2:C:114:GLY:CA	2.40	0.49
1:A:413:ALA:HA	1:A:441:LEU:HD23	1.93	0.49
1:B:399:GLU:HG2	1:B:401:VAL:HG23	1.93	0.49
1:B:520:ASP:O	1:B:524:ILE:HG13	2.12	0.49
2:D:20:ARG:O	2:D:24:GLY:HA3	2.12	0.49
1:A:371:THR:HG22	1:A:373:ALA:H	1.76	0.49
1:A:465:ILE:H	1:A:465:ILE:CD1	2.24	0.49
1:B:104:VAL:HG22	1:B:105:PRO:HD2	1.95	0.49
1:B:161:VAL:HG21	1:B:225:LEU:HD22	1.94	0.49
1:B:465:ILE:HA	1:B:492:VAL:O	2.12	0.49
1:B:655:ASP:O	1:B:659:VAL:HG23	2.11	0.49
2:D:19:GLY:O	2:D:246:THR:HG23	2.13	0.49
2:C:355:ARG:NH2	2:C:356:ILE:HG22	2.28	0.49
1:A:404:ASN:HD21	4:A:1004:N8E:C03	2.25	0.49
1:B:622:VAL:CG2	1:B:626:ASP:HB2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:170:ASP:O	2:D:174:VAL:HG23	2.13	0.49
2:C:17:PRO:HB3	2:C:210:TYR:O	2.13	0.48
2:D:125:MET:HE3	2:D:246:THR:N	2.27	0.48
1:B:503:VAL:HG12	1:B:635:LEU:HG	1.95	0.48
2:D:377:CYS:SG	5:D:4001:ACO:CH3	3.01	0.48
1:A:443:ARG:N	1:A:444:PRO:HD3	2.28	0.48
1:B:232:MET:N	2:D:157:MET:HE1	2.27	0.48
1:A:658:LEU:HD22	1:A:662:ILE:HD13	1.94	0.48
1:A:700:THR:OG1	1:A:703:LEU:HB2	2.13	0.48
2:C:9:VAL:HG13	2:C:267:PRO:HB3	1.94	0.48
2:C:158:LEU:HD23	2:C:158:LEU:O	2.13	0.48
2:D:163:GLY:C	2:D:164:ILE:HD12	2.38	0.48
2:D:244:GLN:HB2	2:D:346:GLY:HA2	1.96	0.48
1:A:228:ILE:HG23	1:A:229:GLU:N	2.27	0.48
1:A:288:ASN:O	1:A:289:CYS:SG	2.68	0.48
1:A:499:LEU:O	1:A:503:VAL:HG23	2.13	0.48
2:C:162:HIS:HB3	2:C:324:LYS:HZ1	1.78	0.48
2:C:313:GLU:O	2:C:342:ALA:HB3	2.13	0.48
2:C:38:LEU:O	2:C:42:VAL:HG23	2.13	0.48
2:D:255:MET:HE2	2:D:260:ALA:CA	2.44	0.48
1:B:157:ARG:HG2	1:B:223:LEU:HD23	1.96	0.48
2:D:125:MET:CE	2:D:246:THR:H	2.26	0.48
1:A:358:ALA:O	1:A:362:VAL:HG23	2.14	0.48
1:A:537:PRO:HG2	1:A:631:MET:CE	2.43	0.48
1:B:331:TYR:HE1	1:B:361:LEU:HG	1.79	0.48
2:D:360:LEU:HG	2:D:364:MET:HE2	1.95	0.48
1:A:111:ASN:HA	1:A:194:LEU:HD11	1.95	0.48
1:A:130:MET:SD	1:A:185:VAL:HG21	2.53	0.48
1:A:580:ARG:HG2	1:A:587:LYS:HB3	1.96	0.48
2:C:99:MET:HE2	2:C:357:SER:OG	2.14	0.48
2:C:289:VAL:CG1	2:C:290:PRO:HD3	2.33	0.48
1:A:293:LEU:HD23	1:A:714:PHE:CE2	2.48	0.48
1:A:503:VAL:C	1:A:506:PRO:HD2	2.38	0.48
2:C:30:ARG:NH1	2:C:67:GLU:HG2	2.29	0.48
1:A:451:HIS:HB2	1:A:465:ILE:HD11	1.96	0.47
1:A:676:ASP:OD2	1:A:712:SER:HB3	2.14	0.47
1:B:338:THR:HG21	1:B:481:TYR:HE1	1.79	0.47
1:A:464:VAL:HG11	1:A:475:VAL:HG13	1.96	0.47
1:B:695:ALA:HA	1:B:698:HIS:ND1	2.29	0.47
2:D:357:SER:O	2:D:360:LEU:HB3	2.14	0.47
2:C:8:VAL:HG21	2:C:106:ALA:HB1	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:125:MET:HE3	2:C:246:THR:N	2.29	0.47
1:B:41:ARG:HD2	1:B:95:ILE:HG12	1.95	0.47
1:B:294:PHE:HA	1:B:297:ASP:HB3	1.97	0.47
2:C:98:SER:HB3	2:C:353:GLY:HA3	1.96	0.47
2:D:289:VAL:CG1	2:D:290:PRO:HD3	2.33	0.47
2:D:307:ASP:O	2:D:335:LYS:HB2	2.14	0.47
1:A:110:ILE:HB	1:A:130:MET:HG3	1.95	0.47
2:C:200:ASP:OD2	2:C:204:PHE:HB2	2.15	0.47
2:C:303:MET:CE	2:C:306:ILE:HD12	2.44	0.47
2:D:164:ILE:HG22	2:D:169:GLN:HG3	1.97	0.47
1:A:502:ARG:NH1	1:A:647:ILE:HG12	2.30	0.47
2:C:9:VAL:CG1	2:C:267:PRO:HB3	2.45	0.47
1:A:499:LEU:HD13	1:A:499:LEU:C	2.40	0.47
1:B:116:GLY:HA2	1:B:140:GLU:OE1	2.14	0.47
1:B:624:ASP:O	1:B:628:ILE:HG13	2.14	0.47
2:D:360:LEU:HD22	2:D:374:SER:HB3	1.97	0.47
1:A:618:GLU:OE2	1:A:620:ARG:HD2	2.15	0.47
1:B:350:ILE:HG21	1:B:384:PRO:HB3	1.95	0.47
1:B:623:THR:O	1:B:627:ILE:HG13	2.15	0.47
2:D:99:MET:HB3	2:D:384:ILE:HD13	1.95	0.47
1:A:289:CYS:SG	1:A:714:PHE:O	2.73	0.47
1:B:499:LEU:HD13	1:B:499:LEU:C	2.40	0.47
1:A:22:PHE:CD2	1:A:66:ILE:HD11	2.49	0.47
1:A:249:TYR:HD1	1:A:249:TYR:O	1.98	0.47
1:A:320:LEU:HD13	1:A:411:VAL:HG12	1.96	0.47
1:B:105:PRO:HG3	1:B:212:TYR:CD2	2.50	0.47
1:A:23:ASP:OD2	1:A:62:LYS:HE2	2.15	0.46
1:A:130:MET:HB2	1:A:185:VAL:HG11	1.97	0.46
1:A:228:ILE:HD13	2:C:280:ASP:CB	2.45	0.46
1:A:304:ALA:O	1:A:308:ASP:HB2	2.15	0.46
1:A:416:GLU:OE1	1:A:442:LYS:HG2	2.14	0.46
1:A:421:GLU:HA	1:A:443:ARG:CZ	2.45	0.46
1:A:506:PRO:HG2	1:A:638:GLU:HG2	1.97	0.46
1:A:666:LEU:HD12	1:A:666:LEU:N	2.18	0.46
1:B:253:VAL:O	1:B:257:LYS:HG3	2.15	0.46
1:B:341:LEU:HD23	1:B:383:ARG:HB2	1.97	0.46
2:C:93:ARG:HG2	2:C:378:ILE:HD13	1.96	0.46
2:C:137:ASN:ND2	2:C:139:HIS:HB2	2.27	0.46
1:A:37:LEU:HD22	1:A:95:ILE:HD12	1.95	0.46
1:A:140:GLU:HG3	1:A:147:PRO:HD3	1.97	0.46
1:A:401:VAL:HG12	1:A:402:VAL:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:59:TRP:HE1	2:D:122:VAL:HB	1.80	0.46
2:D:74:ARG:NH2	2:D:78:LEU:HD21	2.30	0.46
2:D:98:SER:HB2	2:D:353:GLY:HA3	1.97	0.46
1:A:459:MET:HA	1:A:460:PRO:HD3	1.74	0.46
1:B:79:LYS:HA	1:B:284:THR:HG23	1.97	0.46
1:B:150:GLY:HA3	1:B:154:ARG:HH12	1.81	0.46
1:B:251:ALA:N	1:B:252:PRO:CD	2.78	0.46
2:D:175:ARG:NE	2:D:179:LEU:HD12	2.30	0.46
1:A:18:VAL:CG1	1:A:56:VAL:HG22	2.46	0.46
1:A:461:LEU:HB2	1:A:660:TYR:HB3	1.97	0.46
1:A:209:GLU:O	2:D:207:ILE:HD12	2.15	0.46
1:B:358:ALA:O	1:B:362:VAL:HG23	2.16	0.46
1:B:411:VAL:O	1:B:415:VAL:HG23	2.15	0.46
2:D:272:ARG:NH1	2:D:371:PHE:CE2	2.83	0.46
1:B:443:ARG:N	1:B:444:PRO:HD3	2.30	0.46
1:A:407:VAL:O	1:A:411:VAL:HG23	2.15	0.46
2:C:244:GLN:HB2	2:C:346:GLY:HA2	1.97	0.46
1:A:507:TYR:CE1	1:A:631:MET:HB3	2.51	0.46
1:B:502:ARG:HA	1:B:556:MET:HE2	1.98	0.46
2:C:200:ASP:HB2	2:C:201:GLU:OE2	2.14	0.46
1:A:246:GLY:HA3	1:A:668:ARG:NH2	2.31	0.46
1:B:81:PRO:HD2	1:B:84:GLU:HB2	1.96	0.46
2:C:4:ASN:HD22	2:C:4:ASN:HA	1.58	0.46
2:C:17:PRO:HB2	2:C:25:MET:CE	2.45	0.46
2:C:93:ARG:HH12	2:C:276:VAL:HG11	1.80	0.46
1:A:355:ALA:O	1:A:359:LYS:HG3	2.16	0.45
1:A:465:ILE:HA	1:A:492:VAL:O	2.16	0.45
1:B:147:PRO:HB3	1:B:151:GLY:HA3	1.98	0.45
2:C:80:THR:HG22	2:C:81:GLN:H	1.80	0.45
1:B:407:VAL:O	1:B:411:VAL:HG23	2.15	0.45
2:D:9:VAL:CG1	2:D:267:PRO:HB3	2.46	0.45
1:A:374:LYS:O	1:A:378:VAL:HG23	2.16	0.45
1:A:691:ALA:HB1	1:A:698:HIS:CE1	2.52	0.45
1:B:66:ILE:O	1:B:118:GLY:HA3	2.16	0.45
1:A:321:GLY:O	1:A:326:GLY:HA3	2.17	0.45
1:B:320:LEU:HB2	1:B:399:GLU:HA	1.97	0.45
1:A:157:ARG:HG2	1:A:157:ARG:HH11	1.81	0.45
1:A:520:ASP:O	1:A:524:ILE:HG13	2.16	0.45
1:A:532:GLY:C	1:A:665:PRO:HG3	2.40	0.45
2:C:87:ALA:HB1	2:D:93:ARG:HH21	1.81	0.45
2:D:364:MET:SD	2:D:372:GLY:HA3	2.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:ASN:HD22	1:A:248:ASN:HA	1.49	0.45
1:A:396:LEU:HD23	1:A:397:VAL:N	2.31	0.45
1:A:501:ASN:HD22	4:A:1002:N8E:H013	1.82	0.45
1:B:136:ILE:HD11	1:B:179:ALA:HB1	1.98	0.45
1:B:665:PRO:HB2	1:B:668:ARG:HD2	1.98	0.45
1:B:13:LEU:HB2	1:B:17:ILE:O	2.17	0.45
2:C:188:LYS:HD2	2:C:366:GLN:OE1	2.17	0.45
1:A:262:ALA:HB2	1:A:273:VAL:HG21	1.99	0.45
1:B:232:MET:O	1:B:236:THR:HG23	2.17	0.45
2:C:329:LEU:HD23	2:C:329:LEU:O	2.17	0.45
2:D:52:GLY:HA2	2:D:83:PRO:HG2	1.99	0.45
1:A:502:ARG:HH11	1:A:647:ILE:HG12	1.82	0.45
1:A:666:LEU:H	1:A:666:LEU:CD1	2.12	0.45
1:B:637:LEU:O	1:B:641:ARG:HG3	2.17	0.45
1:A:56:VAL:HB	1:A:106:THR:HG22	1.99	0.45
1:A:288:ASN:C	1:A:289:CYS:SG	2.99	0.45
1:A:325:MET:HE3	1:A:428:ASN:HD21	1.82	0.45
2:C:71:ASN:O	2:C:75:MET:HG2	2.17	0.45
1:B:364:ARG:HH21	1:B:370:MET:HE3	1.80	0.44
1:A:147:PRO:HB3	1:A:151:GLY:HA3	1.98	0.44
1:A:412:LEU:HB3	1:A:441:LEU:HD21	1.99	0.44
1:B:300:LEU:HD11	1:B:656:MET:HG3	1.98	0.44
1:B:374:LYS:O	1:B:378:VAL:HG23	2.17	0.44
1:B:566:ASP:CG	1:B:567:ASP:H	2.24	0.44
2:C:59:TRP:O	2:C:90:THR:HA	2.17	0.44
2:D:171:ALA:HA	2:D:220:LEU:HD21	1.98	0.44
2:D:348:PRO:O	2:D:349:PHE:C	2.60	0.44
2:D:364:MET:HE1	2:D:388:PHE:HB2	1.99	0.44
1:B:459:MET:HA	1:B:460:PRO:HD3	1.75	0.44
2:D:98:SER:OG	2:D:121:GLY:HA3	2.16	0.44
2:D:289:VAL:HG23	2:D:293:GLN:HE21	1.79	0.44
2:D:359:THR:HA	2:D:362:ASN:HD22	1.81	0.44
1:A:401:VAL:HG21	1:A:411:VAL:HG21	1.98	0.44
1:B:233:ALA:HB2	2:D:145:ALA:HB2	1.98	0.44
1:B:636:CYS:O	1:B:640:VAL:HG23	2.18	0.44
2:C:106:ALA:O	2:C:110:MET:HG3	2.18	0.44
1:B:199:LEU:HD13	1:B:199:LEU:C	2.43	0.44
1:B:234:PHE:CZ	1:B:260:GLN:HA	2.53	0.44
2:C:175:ARG:NH1	2:C:333:ASN:OD1	2.50	0.44
2:C:348:PRO:O	2:C:349:PHE:C	2.60	0.44
2:D:299:ALA:O	2:D:301:LEU:HG	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:303:MET:O	2:D:303:MET:HE3	2.17	0.44
1:A:466:ARG:HH22	1:A:649:GLU:CD	2.26	0.44
1:A:570:SER:HA	1:A:615:ILE:HG23	2.00	0.44
1:A:622:VAL:HG23	1:A:626:ASP:HB2	1.98	0.44
1:A:655:ASP:O	1:A:659:VAL:HG23	2.18	0.44
1:B:237:ALA:HB1	1:B:256:ILE:HD13	1.99	0.44
1:B:332:GLN:OE1	1:B:457:HIS:HA	2.17	0.44
2:C:35:SER:O	2:C:39:ILE:HG13	2.17	0.44
2:C:265:LEU:HD23	2:C:265:LEU:H	1.83	0.44
2:C:273:SER:CB	2:C:299:ALA:HB2	2.47	0.44
2:C:286:TYR:O	2:C:289:VAL:HG13	2.17	0.44
2:D:152:GLY:HA3	2:D:230:PHE:CD2	2.53	0.44
1:A:161:VAL:HG21	1:A:225:LEU:HD22	2.00	0.44
1:A:445:GLU:HA	1:A:469:LYS:O	2.17	0.44
1:B:80:LEU:HB3	1:B:81:PRO:CD	2.47	0.44
1:A:234:PHE:CZ	1:A:260:GLN:HA	2.53	0.44
1:A:523:ARG:HH22	1:A:622:VAL:HG13	1.83	0.44
1:A:684:VAL:HG22	1:A:703:LEU:HD22	2.00	0.44
2:C:288:PRO:HB2	2:C:322:VAL:HG11	1.99	0.44
2:C:318:GLN:O	2:C:322:VAL:HG23	2.18	0.44
2:C:303:MET:HE2	2:C:309:ILE:HD11	2.00	0.43
1:A:289:CYS:CB	1:A:714:PHE:O	2.64	0.43
1:A:680:VAL:O	1:A:684:VAL:HG23	2.19	0.43
1:B:290:LEU:HD23	1:B:294:PHE:HE1	1.83	0.43
1:B:499:LEU:O	1:B:503:VAL:HG23	2.18	0.43
2:C:98:SER:HB3	2:C:353:GLY:CA	2.48	0.43
2:D:59:TRP:O	2:D:90:THR:HA	2.18	0.43
1:B:232:MET:HG3	2:D:147:ALA:HB3	2.00	0.43
1:B:321:GLY:O	1:B:326:GLY:HA3	2.17	0.43
1:B:551:HIS:O	1:B:555:VAL:HG23	2.18	0.43
1:A:246:GLY:HA3	1:A:668:ARG:NH1	2.33	0.43
1:A:595:ASP:OD1	1:A:595:ASP:C	2.62	0.43
1:B:624:ASP:HA	1:B:627:ILE:HD12	2.00	0.43
2:C:141:SER:HA	2:C:144:ALA:O	2.18	0.43
2:D:286:TYR:O	2:D:289:VAL:HG13	2.18	0.43
2:C:122:VAL:HG23	2:C:249:ALA:HB2	2.00	0.43
2:C:136:PRO:O	2:C:138:PRO:HD3	2.18	0.43
1:A:71:ILE:HG22	1:A:71:ILE:O	2.19	0.43
1:B:226:ASN:HB3	1:B:229:GLU:H	1.84	0.43
2:C:313:GLU:CD	2:C:341:GLY:HA3	2.44	0.43
2:D:151:MET:HE3	5:D:4001:ACO:H21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:ALA:HA	1:A:667:PHE:HB2	2.01	0.43
1:B:465:ILE:HG12	1:B:498:PHE:CE2	2.54	0.43
1:B:532:GLY:C	1:B:665:PRO:HG3	2.44	0.43
1:B:684:VAL:HG13	1:B:699:PRO:HG2	2.00	0.43
2:C:93:ARG:HD2	2:C:100:SER:OG	2.19	0.43
2:C:170:ASP:O	2:C:174:VAL:HG23	2.17	0.43
2:C:339:HIS:CD2	2:C:363:VAL:HG22	2.54	0.43
1:A:350:ILE:CG2	1:A:384:PRO:HB3	2.49	0.43
1:B:465:ILE:HG12	1:B:498:PHE:CZ	2.54	0.43
1:B:546:ILE:N	1:B:546:ILE:HD12	2.34	0.43
2:C:58:ILE:HD12	2:C:105:ALA:HB2	2.00	0.43
2:D:123:GLU:HG2	2:D:349:PHE:HB2	2.00	0.43
1:A:622:VAL:CG2	1:A:626:ASP:HB2	2.49	0.43
1:B:296:ASN:N	1:B:296:ASN:HD22	2.15	0.43
1:B:645:ASP:HB2	1:B:647:ILE:HD13	2.00	0.43
2:D:141:SER:HA	2:D:144:ALA:O	2.19	0.43
1:A:67:VAL:O	1:A:68:GLY:O	2.37	0.43
1:A:635:LEU:C	1:A:635:LEU:HD23	2.43	0.43
2:C:19:GLY:O	2:C:246:THR:HG23	2.18	0.43
2:D:98:SER:HB3	2:D:354:ALA:N	2.30	0.43
2:D:98:SER:HB2	2:D:353:GLY:CA	2.49	0.43
2:D:105:ALA:O	2:D:109:ILE:HG13	2.18	0.43
1:A:67:VAL:O	1:A:68:GLY:C	2.61	0.42
1:A:330:ALA:HA	1:A:340:ILE:HG21	2.01	0.42
1:B:107:VAL:HG23	1:B:202:ILE:CD1	2.48	0.42
1:B:224:LYS:HB2	2:D:142:LEU:O	2.18	0.42
1:B:233:ALA:HB2	2:D:145:ALA:CB	2.49	0.42
1:B:451:HIS:HB3	1:B:463:GLU:HB2	2.01	0.42
1:B:503:VAL:C	1:B:506:PRO:HD2	2.44	0.42
1:A:304:ALA:HB1	1:A:483:LYS:NZ	2.34	0.42
1:B:18:VAL:HG12	1:B:55:GLY:O	2.18	0.42
1:B:67:VAL:C	1:B:68:GLY:O	2.63	0.42
1:A:89:ASN:ND2	4:A:1003:N8E:H132	2.34	0.42
1:A:226:ASN:OD1	1:A:227:ALA:N	2.51	0.42
1:B:1:MET:SD	1:B:4:GLU:HB2	2.59	0.42
2:C:324:LYS:NZ	2:C:324:LYS:HB3	2.34	0.42
2:D:30:ARG:NH1	2:D:67:GLU:HG2	2.35	0.42
1:A:404:ASN:HB3	1:A:407:VAL:HB	2.01	0.42
1:A:408:LYS:HD2	1:A:432:ILE:HD12	2.02	0.42
1:B:178:ASP:O	1:B:182:VAL:HG22	2.19	0.42
1:B:507:TYR:CE1	1:B:631:MET:HB3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:628:ILE:O	1:B:632:MET:HG2	2.20	0.42
2:C:189:PHE:HB3	2:C:193:ILE:CD1	2.49	0.42
2:D:31:ALA:HB2	2:D:124:HIS:HB2	2.01	0.42
1:A:638:GLU:HA	1:A:641:ARG:NH1	2.35	0.42
1:B:32:PHE:CE1	1:B:66:ILE:HG21	2.55	0.42
1:B:56:VAL:O	1:B:106:THR:HA	2.20	0.42
2:C:357:SER:O	2:C:360:LEU:HB3	2.19	0.42
2:D:49:VAL:O	2:D:49:VAL:HG23	2.20	0.42
1:A:120:GLU:CD	1:A:149:PHE:HB2	2.44	0.42
1:A:358:ALA:HB1	1:B:376:ALA:HB1	2.00	0.42
1:A:475:VAL:O	1:A:479:VAL:HG23	2.18	0.42
2:C:286:TYR:CZ	2:C:289:VAL:HG11	2.55	0.42
2:D:292:THR:O	2:D:296:LEU:HG	2.19	0.42
1:A:111:ASN:HA	1:A:194:LEU:CD1	2.49	0.42
1:A:226:ASN:HB3	1:A:229:GLU:H	1.84	0.42
1:A:628:ILE:O	1:A:632:MET:HG2	2.20	0.42
1:B:77:ASN:O	1:B:85:LEU:HD13	2.18	0.42
1:A:104:VAL:HG22	1:A:105:PRO:HD2	2.02	0.42
1:A:176:ALA:HB1	1:A:188:VAL:HG11	2.01	0.42
1:A:401:VAL:HG11	1:A:407:VAL:HG12	2.01	0.42
1:B:434:ILE:HG23	1:B:447:PHE:CE2	2.55	0.42
2:D:269:ALA:HB2	2:D:361:LEU:HD22	2.02	0.42
1:A:297:ASP:CG	1:A:301:LYS:HE3	2.44	0.42
1:A:546:ILE:HD12	1:A:546:ILE:N	2.35	0.42
1:B:325:MET:O	1:B:329:ILE:HG13	2.19	0.42
2:C:299:ALA:O	2:C:301:LEU:HG	2.20	0.42
2:D:296:LEU:HD21	2:D:306:ILE:HD11	2.02	0.42
1:A:464:VAL:HG21	1:A:479:VAL:HG22	2.01	0.42
1:A:702:LYS:O	1:A:706:MET:HG2	2.20	0.42
1:B:700:THR:OG1	1:B:703:LEU:HB2	2.20	0.42
1:A:57:ILE:HG12	1:A:202:ILE:HG13	2.02	0.41
1:A:89:ASN:N	1:A:89:ASN:ND2	2.63	0.41
1:A:157:ARG:HG2	1:A:223:LEU:HD23	2.02	0.41
1:A:658:LEU:HB3	1:A:662:ILE:HD11	2.01	0.41
1:B:509:GLY:O	1:B:513:LYS:HG3	2.20	0.41
1:B:540:LEU:HD23	1:B:544:VAL:HG23	2.02	0.41
2:C:39:ILE:HG23	2:C:118:VAL:HG11	2.02	0.41
2:D:6:ARG:HB3	2:D:110:MET:HA	2.02	0.41
2:D:43:LEU:HD11	2:D:82:ILE:HD11	2.01	0.41
1:B:655:ASP:HB3	1:B:670:GLY:HA3	2.02	0.41
2:D:313:GLU:OE2	2:D:341:GLY:HA3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:VAL:HG12	1:A:55:GLY:O	2.20	0.41
1:A:146:TYR:HB2	1:A:147:PRO:HD2	2.01	0.41
1:A:350:ILE:HD11	1:A:386:LEU:HG	2.01	0.41
1:B:157:ARG:NH1	1:B:223:LEU:HG	2.35	0.41
2:D:329:LEU:HD23	2:D:329:LEU:O	2.20	0.41
1:B:672:LEU:HA	1:B:675:ILE:HD12	2.02	0.41
2:C:307:ASP:O	2:C:335:LYS:HB2	2.20	0.41
1:A:93:ASN:OD1	1:A:149:PHE:HA	2.19	0.41
1:A:525:ASP:OD2	1:A:538:ALA:HB3	2.20	0.41
1:B:185:VAL:HG12	1:B:187:ALA:H	1.85	0.41
1:B:464:VAL:HG11	1:B:475:VAL:HG13	2.03	0.41
2:D:273:SER:OG	2:D:299:ALA:HB2	2.21	0.41
1:A:56:VAL:O	1:A:106:THR:HA	2.21	0.41
1:A:141:VAL:HG12	1:A:251:ALA:CB	2.46	0.41
1:A:502:ARG:HA	1:A:556:MET:CE	2.49	0.41
2:C:293:GLN:O	2:C:297:LYS:HG3	2.20	0.41
2:C:357:SER:O	2:C:361:LEU:HG	2.21	0.41
2:D:172:PHE:CE2	2:D:313:GLU:HG2	2.54	0.41
1:A:338:THR:OG1	1:A:484:LYS:HE3	2.21	0.41
1:A:384:PRO:HB2	1:B:383:ARG:HD3	2.02	0.41
1:A:461:LEU:HB2	1:A:660:TYR:CB	2.50	0.41
1:B:127:PHE:CD2	1:B:201:LEU:HD21	2.56	0.41
1:B:157:ARG:HD2	1:B:219:LYS:HA	2.02	0.41
1:A:344:ASP:OD1	1:A:345:ILE:N	2.52	0.41
1:B:525:ASP:O	1:B:529:GLU:HG3	2.19	0.41
1:B:681:ALA:HB3	1:B:682:GLU:OE1	2.21	0.41
1:A:342:MET:HE1	1:A:354:LEU:N	2.36	0.41
1:B:228:ILE:HG22	2:D:282:ALA:CB	2.50	0.41
1:B:289:CYS:C	1:B:291:ILE:N	2.75	0.41
1:B:371:THR:HG22	1:B:373:ALA:H	1.85	0.41
1:B:408:LYS:HD2	1:B:432:ILE:HD12	2.02	0.41
2:C:93:ARG:HG2	2:C:93:ARG:O	2.21	0.41
2:C:199:TYR:HA	2:C:204:PHE:O	2.21	0.41
2:D:158:LEU:HD23	2:D:318:GLN:HA	2.03	0.41
2:D:164:ILE:CG2	2:D:169:GLN:HG3	2.51	0.41
2:D:181:HIS:O	2:D:185:VAL:HG23	2.20	0.41
1:A:70:ASP:HA	1:A:294:PHE:HZ	1.86	0.41
1:A:320:LEU:HB2	1:A:399:GLU:HA	2.02	0.41
1:A:445:GLU:CD	1:A:445:GLU:H	2.30	0.41
1:B:20:LEU:HD23	1:B:20:LEU:C	2.45	0.41
1:B:78:PHE:HA	1:B:85:LEU:HD13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:365:VAL:C	1:B:367:LYS:H	2.29	0.41
1:B:403:GLU:HA	1:B:408:LYS:HE2	2.03	0.41
2:C:201:GLU:CD	2:C:201:GLU:N	2.74	0.41
2:C:206:LYS:HB2	2:C:206:LYS:NZ	2.36	0.41
2:D:347:HIS:CD2	5:D:4001:ACO:S1P	3.14	0.41
1:A:404:ASN:ND2	4:A:1004:N8E:H031	2.31	0.40
2:C:61:CYS:SG	2:C:68:GLN:HB3	2.60	0.40
2:C:98:SER:HB3	2:C:354:ALA:H	1.86	0.40
2:D:58:ILE:HD13	2:D:104:THR:HB	2.02	0.40
1:A:20:LEU:HD23	1:A:20:LEU:C	2.46	0.40
1:A:473:LEU:HD23	1:A:473:LEU:C	2.47	0.40
1:B:539:TYR:O	1:B:543:VAL:HG23	2.21	0.40
2:D:155:ALA:HB2	2:D:315:PHE:CD2	2.57	0.40
1:A:288:ASN:C	1:A:289:CYS:HG	2.25	0.40
1:A:386:LEU:HB2	1:B:390:ASP:OD1	2.20	0.40
1:B:445:GLU:HA	1:B:469:LYS:O	2.21	0.40
2:C:121:GLY:HA3	2:C:350:GLY:O	2.21	0.40
1:A:105:PRO:HG3	1:A:212:TYR:CD2	2.57	0.40
1:A:140:GLU:OE2	4:A:1003:N8E:H051	2.21	0.40
1:A:388:TYR:CE2	1:A:415:VAL:HG22	2.55	0.40
1:A:443:ARG:HA	1:A:445:GLU:OE2	2.21	0.40
2:C:122:VAL:HG22	2:C:123:GLU:N	2.35	0.40
1:A:127:PHE:CD2	1:A:201:LEU:HD21	2.56	0.40
1:B:226:ASN:O	1:B:230:GLN:HG3	2.20	0.40
2:C:16:THR:HG22	2:C:196:MET:HE1	2.03	0.40
2:C:189:PHE:HB3	2:C:193:ILE:HD12	2.03	0.40
2:D:74:ARG:CZ	2:D:78:LEU:HD21	2.52	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	713/715 (100%)	652 (91%)	52 (7%)	9 (1%)	9	39
1	B	702/715 (98%)	637 (91%)	56 (8%)	9 (1%)	9	39
2	C	388/390 (100%)	353 (91%)	32 (8%)	3 (1%)	16	49
2	D	388/390 (100%)	350 (90%)	36 (9%)	2 (0%)	24	57
All	All	2191/2210 (99%)	1992 (91%)	176 (8%)	23 (1%)	12	44

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	68	GLY
1	A	250	PRO
1	B	250	PRO
1	B	286	ALA
1	B	68	GLY
1	B	566	ASP
1	B	567	ASP
2	C	349	PHE
1	A	289	CYS
1	A	597	LYS
2	C	332	MET
2	D	349	PHE
1	A	65	PHE
1	A	252	PRO
1	B	285	SER
2	D	332	MET
1	A	500	VAL
1	B	324	ILE
1	B	496	PRO
2	C	54	VAL
1	A	324	ILE
1	A	161	VAL
1	B	252	PRO

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	547/562 (97%)	524 (96%)	23 (4%)	26	52
1	B	530/562 (94%)	517 (98%)	13 (2%)	42	63
2	C	305/307 (99%)	294 (96%)	11 (4%)	31	57
2	D	304/307 (99%)	298 (98%)	6 (2%)	48	67
All	All	1686/1738 (97%)	1633 (97%)	53 (3%)	35	59

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	A	40	LEU
1	A	48	LYS
1	A	77	ASN
1	A	89	ASN
1	A	102	LEU
1	A	104	VAL
1	A	140	GLU
1	A	158	LEU
1	A	194	LEU
1	A	199	LEU
1	A	217	GLN
1	A	247	PRO
1	A	248	ASN
1	A	280	LYS
1	A	290	LEU
1	A	296	ASN
1	A	298	GLN
1	A	366	ASP
1	A	421	GLU
1	A	445	GLU
1	A	525	ASP
1	A	540	LEU
1	B	38	ASN
1	B	40	LEU
1	B	90	LEU
1	B	104	VAL
1	B	119	LEU
1	B	194	LEU
1	B	247	PRO
1	B	280	LYS
1	B	295	LEU
1	B	366	ASP

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Mol	Chain	Res	Type
1	B	390	ASP
1	B	473	LEU
1	B	643	LEU
2	C	3	LEU
2	C	4	ASN
2	C	5	PRO
2	C	7	ASP
2	C	150	MET
2	C	201	GLU
2	C	206	LYS
2	C	289	VAL
2	C	318	GLN
2	C	325	ASP
2	C	351	CYS
2	D	55	GLU
2	D	289	VAL
2	D	318	GLN
2	D	324	LYS
2	D	330	ASP
2	D	355	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	A	77	ASN
1	A	89	ASN
1	A	174	ASN
1	A	217	GLN
1	A	230	GLN
1	A	244	GLN
1	A	296	ASN
1	A	298	GLN
1	A	316	GLN
1	A	380	ASN
1	A	404	ASN
1	A	501	ASN
1	A	550	HIS
1	A	629	ASN
1	A	698	HIS
1	B	38	ASN
1	B	42	GLN

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Mol	Chain	Res	Type
1	B	103	ASN
1	B	296	ASN
1	B	629	ASN
2	C	4	ASN
2	C	113	ASN
2	C	132	HIS
2	C	162	HIS
2	C	169	GLN
2	C	197	GLN
2	C	202	ASN
2	C	231	ASN
2	C	244	GLN
2	C	258	GLN
2	C	312	ASN
2	D	4	ASN
2	D	84	HIS
2	D	162	HIS
2	D	197	GLN
2	D	258	GLN
2	D	293	GLN
2	D	333	ASN
2	D	362	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

7 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	N8E	A	1002	-	23,23,23	0.42	0	22,22,22	0.43	0
5	ACO	C	3001	-	40,42,53	0.80	1 (2%)	62,66,79	0.56	0
4	N8E	A	1003	-	23,23,23	0.40	0	22,22,22	0.43	0
4	N8E	A	1004	-	23,23,23	0.44	0	22,22,22	0.42	0
5	ACO	D	4001	-	51,53,53	0.82	0	73,79,79	0.59	1 (1%)
3	NAD	A	1001	-	38,38,48	0.70	0	53,58,73	0.45	0
3	NAD	B	2001	-	46,48,48	1.43	4 (8%)	64,73,73	1.36	4 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	N8E	A	1002	-	-	11/21/21/21	-
5	ACO	C	3001	-	-	6/37/54/67	0/3/3/3
4	N8E	A	1003	-	-	14/21/21/21	-
4	N8E	A	1004	-	-	9/21/21/21	-
5	ACO	D	4001	-	-	8/51/67/67	0/3/3/3
3	NAD	A	1001	-	-	1/22/51/62	0/4/4/5
3	NAD	B	2001	-	-	6/30/62/62	0/5/5/5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2001	NAD	C3N-C7N	5.34	1.58	1.50
3	B	2001	NAD	C2N-N1N	4.25	1.39	1.35
3	B	2001	NAD	C6N-N1N	3.52	1.43	1.35
3	B	2001	NAD	C4N-C3N	3.32	1.44	1.39
5	C	3001	ACO	CCP-CBP	2.05	1.56	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2001	NAD	C5N-C4N-C3N	-6.79	113.69	120.36
3	B	2001	NAD	C6N-C5N-C4N	5.60	127.52	119.45
3	B	2001	NAD	C5N-C6N-N1N	-3.95	114.99	120.38
3	B	2001	NAD	C2N-C3N-C4N	3.02	121.77	118.26
5	D	4001	ACO	C2P-S1P-C	2.67	114.27	101.42

There are no chirality outliers.

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	2001	NAD	C2N-C3N-C7N-O7N
3	B	2001	NAD	C2N-C3N-C7N-N7N
5	C	3001	ACO	CCP-O6A-P2A-O3A
5	C	3001	ACO	CCP-O6A-P2A-O4A
5	C	3001	ACO	CCP-O6A-P2A-O5A
5	D	4001	ACO	S1P-C2P-C3P-N4P
5	D	4001	ACO	C3P-C2P-S1P-C
5	D	4001	ACO	O-C-S1P-C2P
5	D	4001	ACO	CH3-C-S1P-C2P
3	B	2001	NAD	C4N-C3N-C7N-O7N
3	B	2001	NAD	C4N-C3N-C7N-N7N
5	C	3001	ACO	C3B-C4B-C5B-O5B
4	A	1002	N8E	O15-C16-C17-O18
4	A	1004	N8E	O12-C13-C14-O15
4	A	1003	N8E	O12-C13-C14-O15
4	A	1002	N8E	O18-C19-C20-O21
5	C	3001	ACO	O4B-C4B-C5B-O5B
4	A	1003	N8E	O09-C10-C11-O12
4	A	1002	N8E	C06-C07-C08-O09
4	A	1003	N8E	C06-C07-C08-O09
5	D	4001	ACO	C3B-C4B-C5B-O5B
4	A	1003	N8E	C04-C05-C06-C07
4	A	1003	N8E	C03-C04-C05-C06
4	A	1002	N8E	C03-C04-C05-C06
4	A	1003	N8E	C05-C06-C07-C08
4	A	1002	N8E	C01-C02-C03-C04
5	D	4001	ACO	O4B-C4B-C5B-O5B
3	B	2001	NAD	C3B-C4B-C5B-O5B
4	A	1003	N8E	O15-C16-C17-O18
4	A	1002	N8E	C14-C13-O12-C11
4	A	1003	N8E	C19-C20-O21-C22
4	A	1004	N8E	C13-C14-O15-C16
3	B	2001	NAD	O4B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
4	A	1003	N8E	C01-C02-C03-C04
4	A	1004	N8E	C04-C05-C06-C07
4	A	1004	N8E	C11-C10-O09-C08
4	A	1003	N8E	C16-C17-O18-C19
4	A	1002	N8E	C07-C08-O09-C10
4	A	1003	N8E	C20-C19-O18-C17
4	A	1003	N8E	C10-C11-O12-C13
4	A	1003	N8E	C13-C14-O15-C16
4	A	1002	N8E	C05-C06-C07-C08
4	A	1002	N8E	C13-C14-O15-C16
4	A	1004	N8E	C06-C07-C08-O09
4	A	1002	N8E	C10-C11-O12-C13
4	A	1004	N8E	O18-C19-C20-O21
5	D	4001	ACO	O5P-C5P-C6P-C7P
4	A	1004	N8E	C02-C03-C04-C05
4	A	1004	N8E	O15-C16-C17-O18
5	C	3001	ACO	CBP-CCP-O6A-P2A
5	D	4001	ACO	C5P-C6P-C7P-N8P
4	A	1003	N8E	C11-C10-O09-C08
4	A	1002	N8E	O09-C10-C11-O12
4	A	1004	N8E	O09-C10-C11-O12
3	A	1001	NAD	O4B-C4B-C5B-O5B

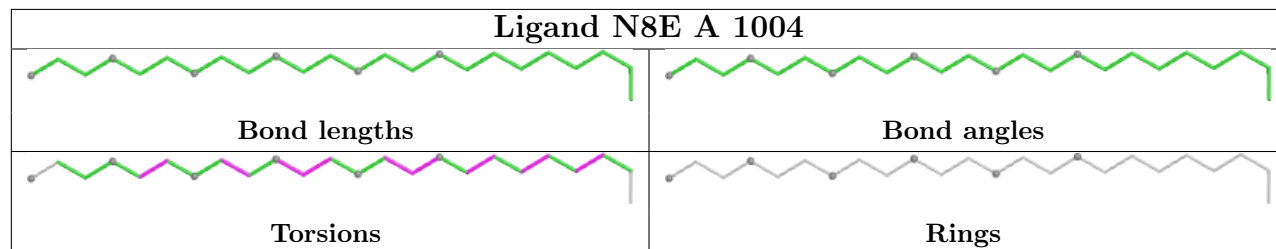
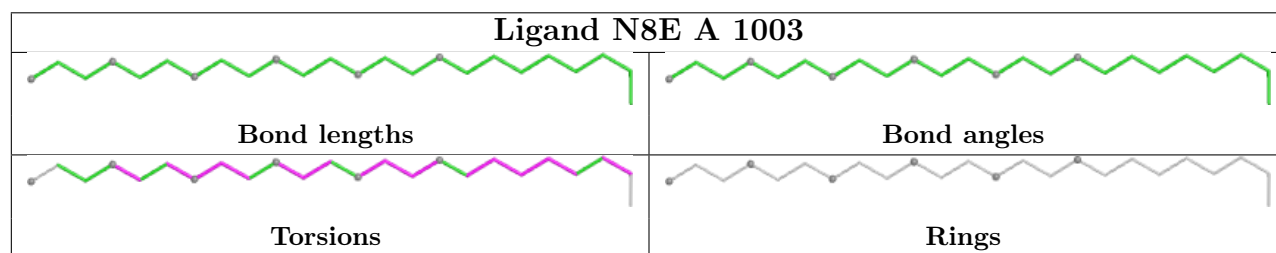
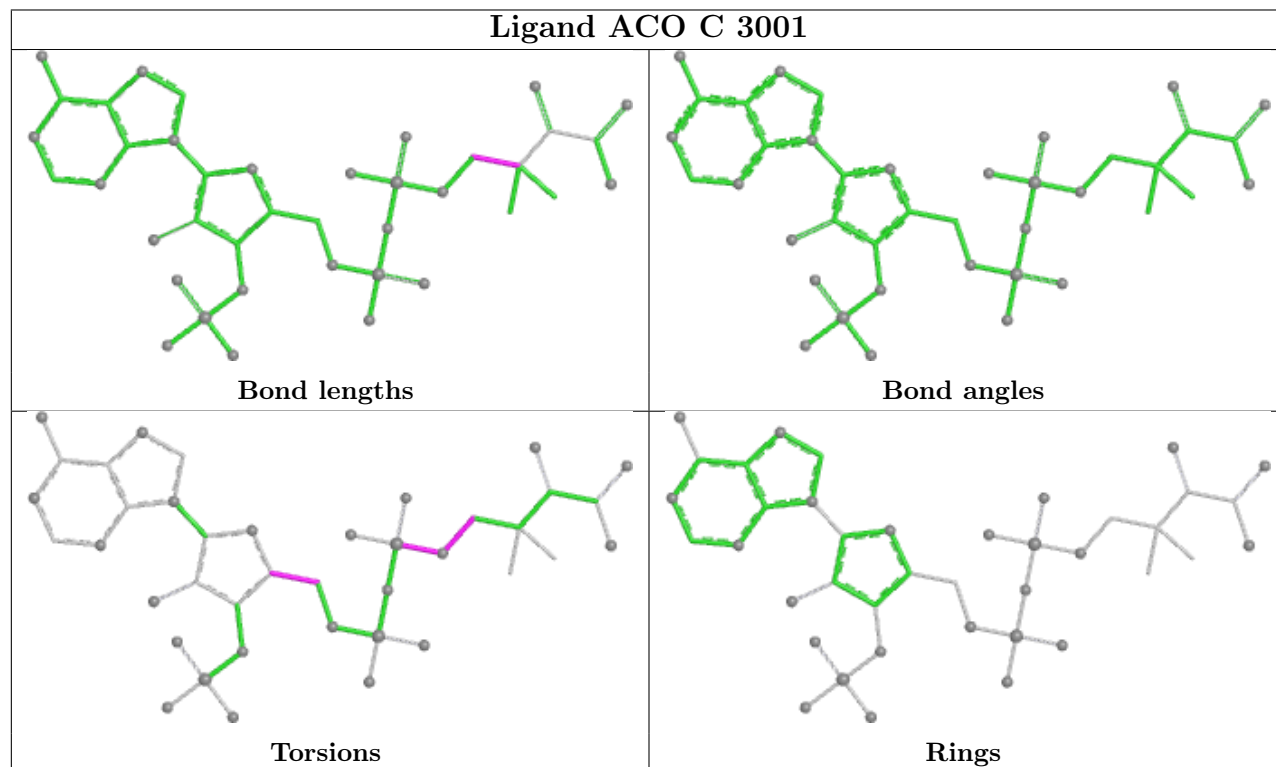
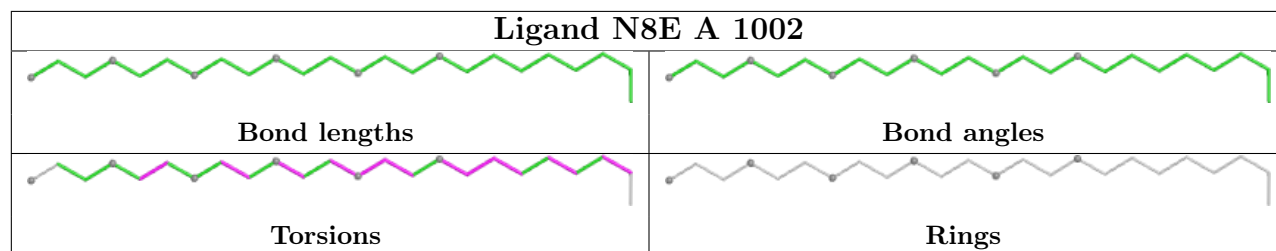
There are no ring outliers.

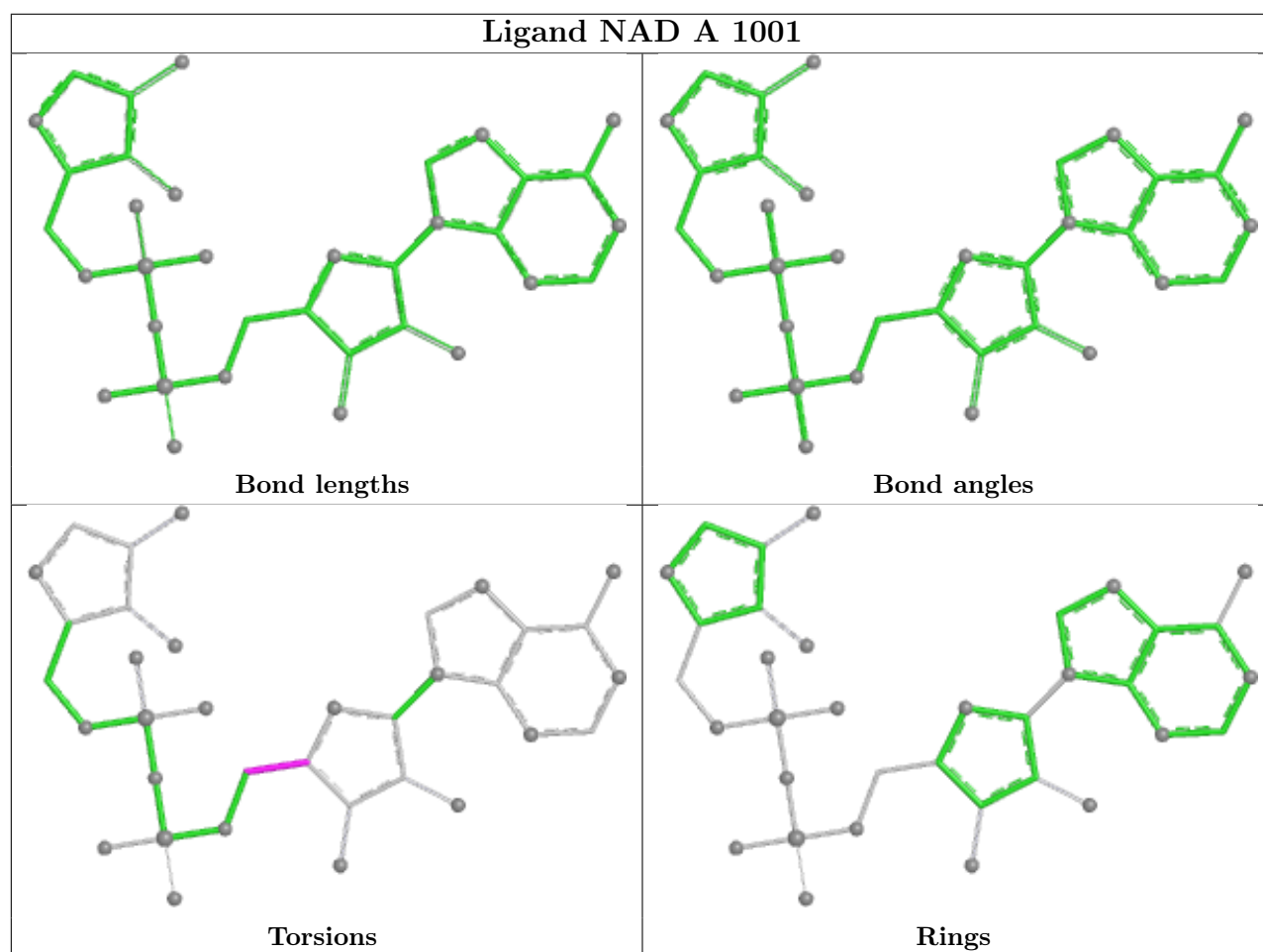
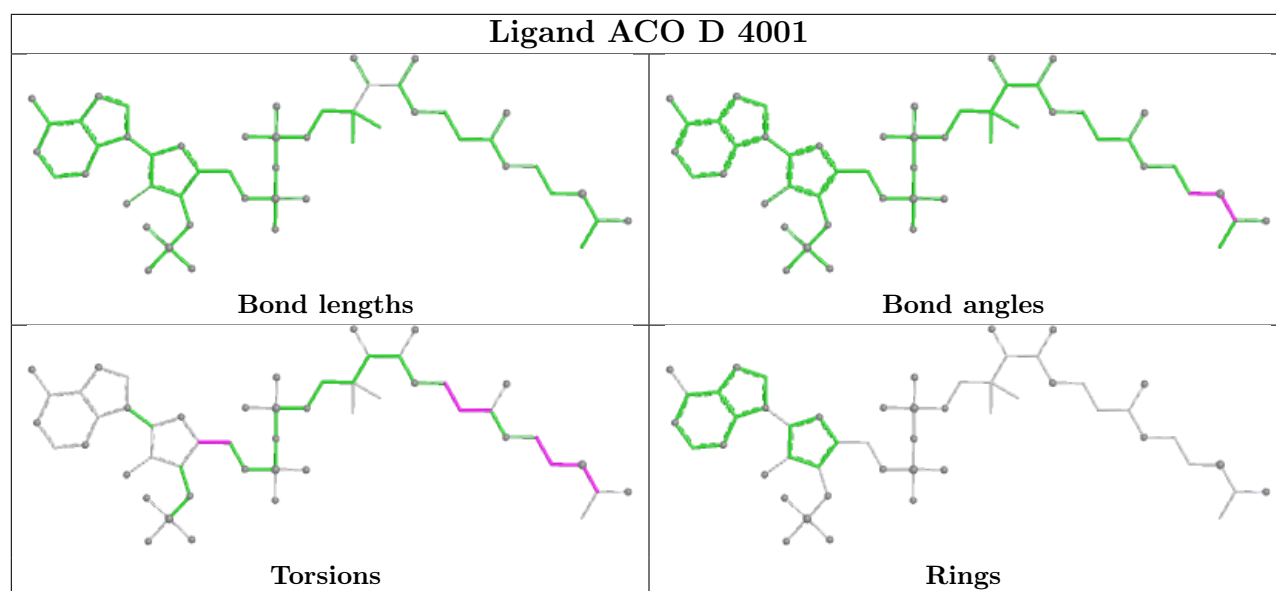
5 monomers are involved in 11 short contacts:

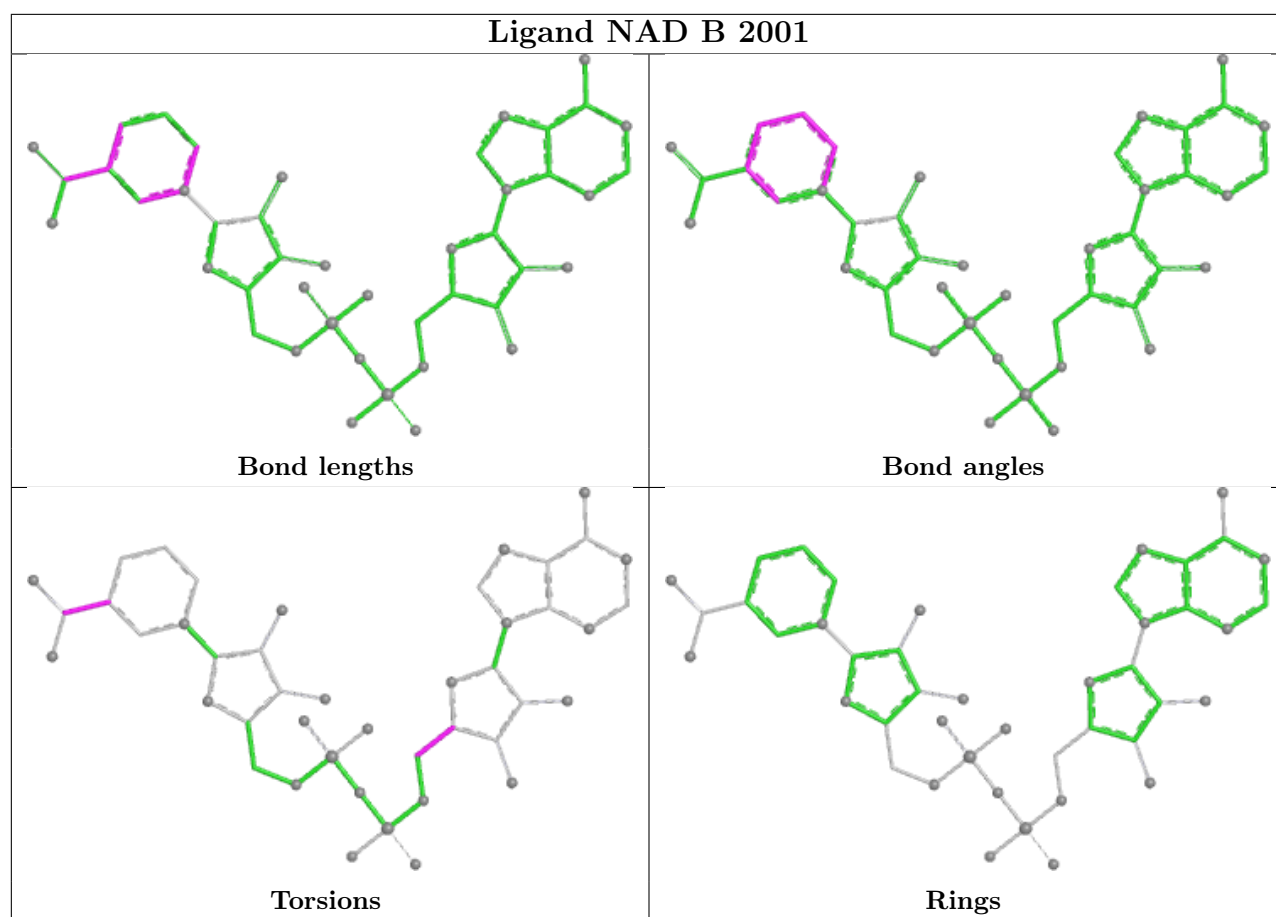
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1002	N8E	1	0
4	A	1003	N8E	2	0
4	A	1004	N8E	3	0
5	D	4001	ACO	4	0
3	B	2001	NAD	1	0

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	715/715 (100%)	-0.08	11 (1%) 72 47	1, 8, 48, 139	0
1	B	706/715 (98%)	0.09	14 (1%) 65 39	1, 25, 71, 130	0
2	C	390/390 (100%)	-0.23	0 100 100	1, 4, 27, 70	0
2	D	390/390 (100%)	-0.21	1 (0%) 90 76	1, 3, 30, 91	0
All	All	2201/2210 (99%)	-0.07	26 (1%) 76 52	1, 9, 58, 139	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	251	ALA	4.0
1	A	598	GLY	3.8
1	B	251	ALA	3.6
1	A	250	PRO	3.5
1	A	245	ALA	3.1
1	B	249	TYR	3.0
1	A	289	CYS	2.9
1	B	308	ASP	2.9
1	B	68	GLY	2.9
1	A	248	ASN	2.8
1	B	289	CYS	2.8
1	A	249	TYR	2.7
1	B	250	PRO	2.6
1	A	599	LYS	2.6
2	D	350	GLY	2.5
1	B	269	LYS	2.5
1	A	597	LYS	2.4
1	B	364	ARG	2.4
1	B	72	THR	2.3
1	B	295	LEU	2.3
1	B	666	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	368	GLY	2.3
1	B	226	ASN	2.2
1	B	294	PHE	2.1
1	A	587	LYS	2.0
1	B	371	THR	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](#)

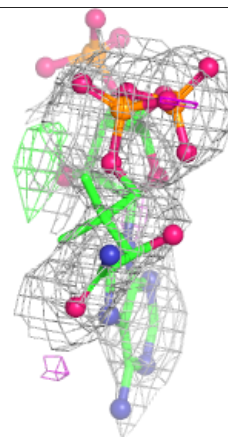
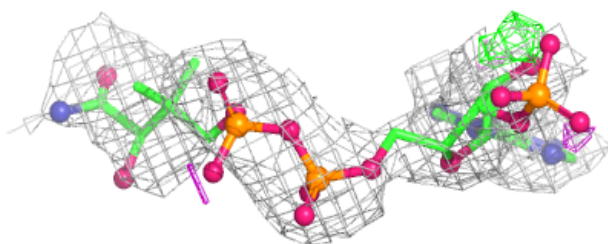
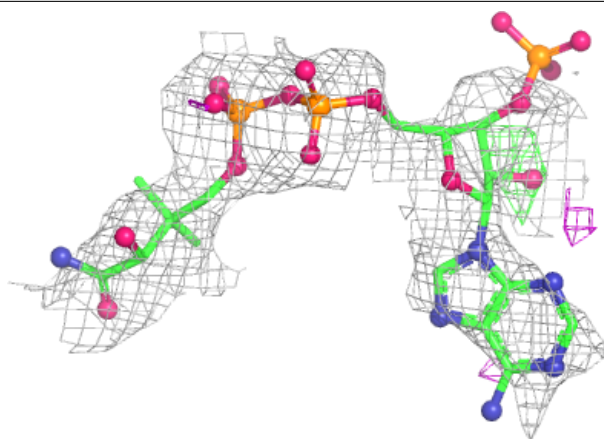
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	ACO	C	3001	40/51	0.64	0.19	67,80,128,128	0
4	N8E	A	1002	24/24	0.67	0.15	23,23,23,23	0
4	N8E	A	1004	24/24	0.69	0.16	26,58,77,77	0
5	ACO	D	4001	51/51	0.69	0.16	62,68,133,133	0
3	NAD	B	2001	44/44	0.77	0.14	43,56,93,93	0
4	N8E	A	1003	24/24	0.82	0.12	15,15,15,15	0
3	NAD	A	1001	35/44	0.86	0.12	20,44,116,116	0

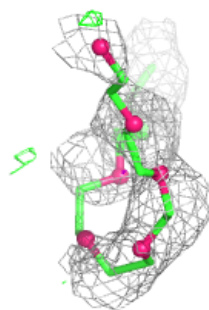
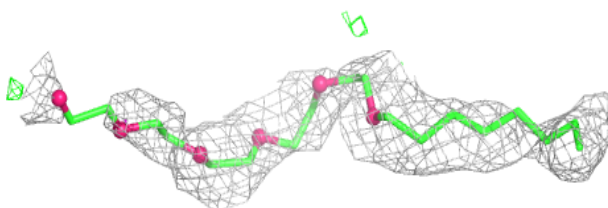
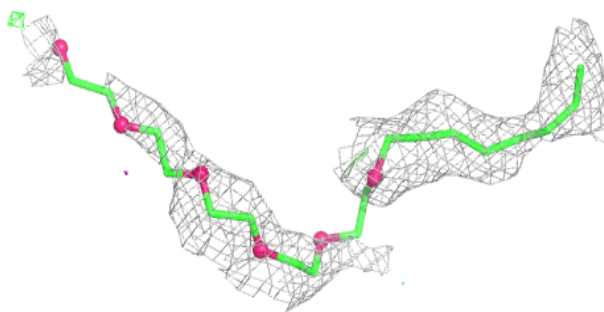
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ACO C 3001:

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

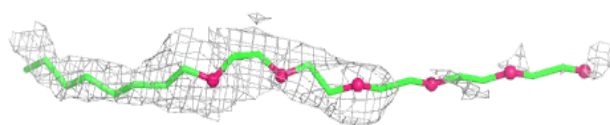
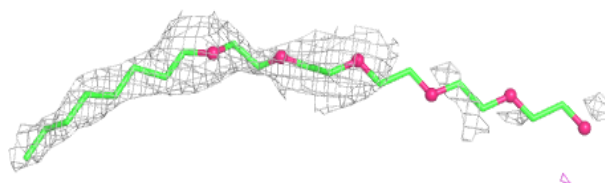
**Electron density around N8E A 1002:**

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

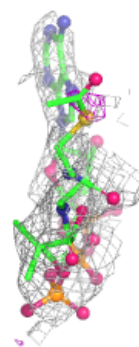
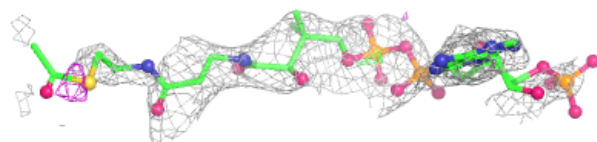
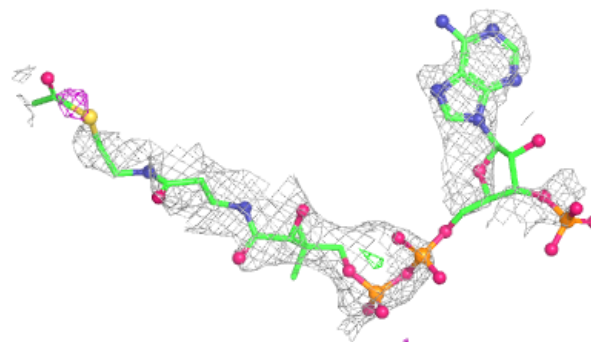


Electron density around N8E A 1004:

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

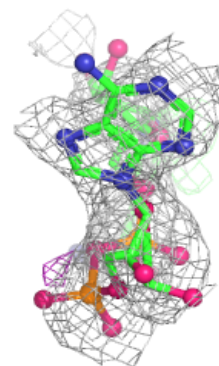
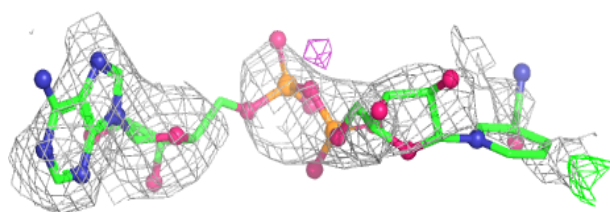
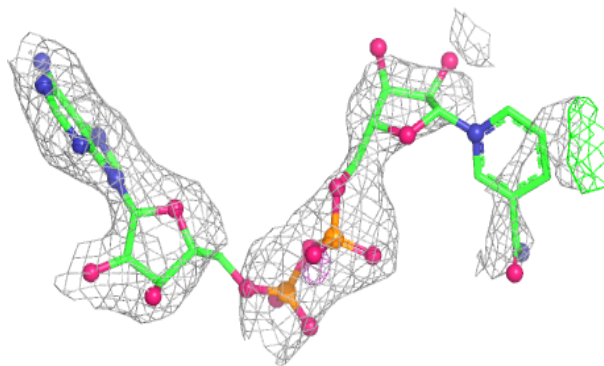
**Electron density around ACO D 4001:**

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

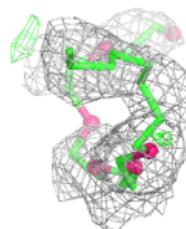
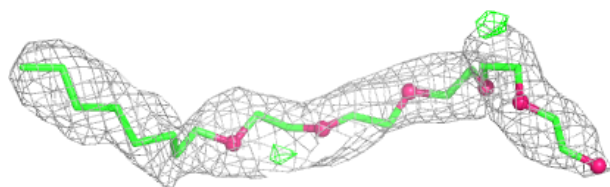


Electron density around NAD B 2001:

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

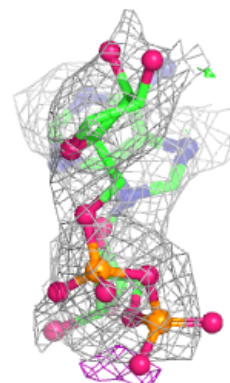
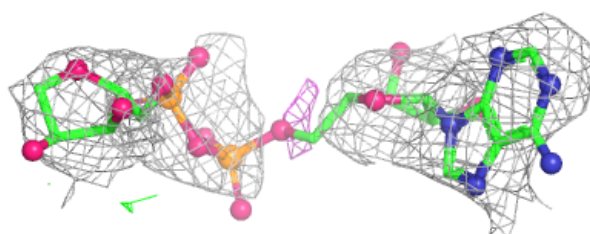
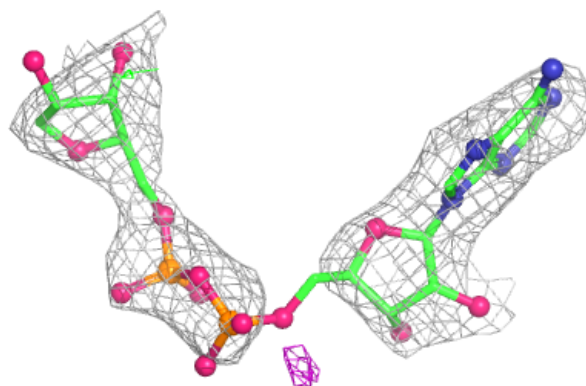
**Electron density around N8E A 1003:**

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



Electron density around NAD A 1001:

$2mF_o - DF_c$ (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.