



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:36 PM UTC

PDB ID : 1WDM / pdb_00001wdm
Title : fatty acid beta-oxidation multienzyme complex from *Pseudomonas fragi*, form I (native3)
Authors : Ishikawa, M.; Tsuchiya, D.; Oyama, T.; Tsunaka, Y.; Morikawa, K.
Deposited on : 2004-05-17
Resolution : 3.80 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

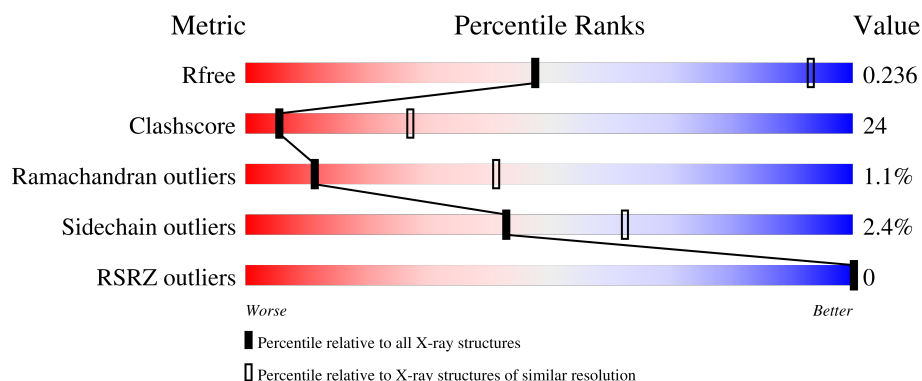
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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	1065 (3.96-3.64)
Clashscore	190562	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
Sidechain outliers	187428	1043 (3.96-3.64)
RSRZ outliers	180081	1064 (3.96-3.64)

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	 60% 38% ..
1	B	715	 58% 40% ..
2	C	390	 55% 43% .
2	D	390	 54% 43% .

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16541 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	707	Total	C	N	O	S	0	0	0
			5257	3355	878	997	27			
1	B	710	Total	C	N	O	S	0	0	0
			5302	3383	889	1003	27			

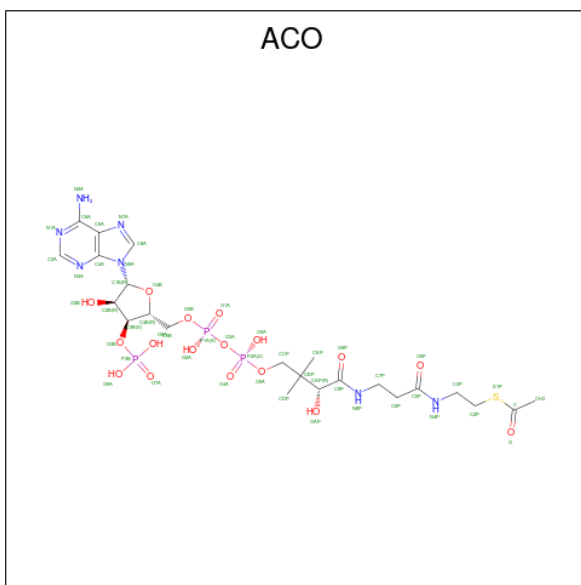
- Molecule 2 is a protein called 3-ketoacyl-CoA thiolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	390	Total	C	N	O	S	0	0	0
			2871	1786	508	548	29			
2	D	390	Total	C	N	O	S	0	0	0
			2869	1785	510	545	29			

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

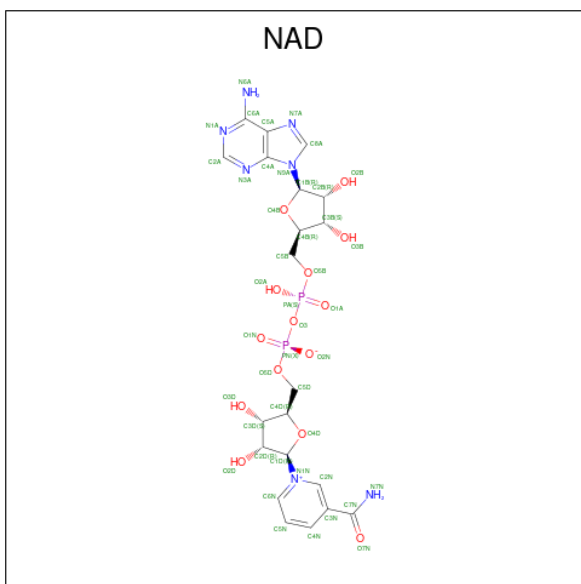
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is ACETYL COENZYME *A (CCD ID: ACO) (formula: C₂₃H₃₈N₇O₁₇P₃S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total 51	C 23	N 7	O 17	P 3	S 1	0	0
4	C	1	Total 51	C 23	N 7	O 17	P 3	S 1	0	0
4	D	1	Total 51	C 23	N 7	O 17	P 3	S 1	0	0

- Molecule 5 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).

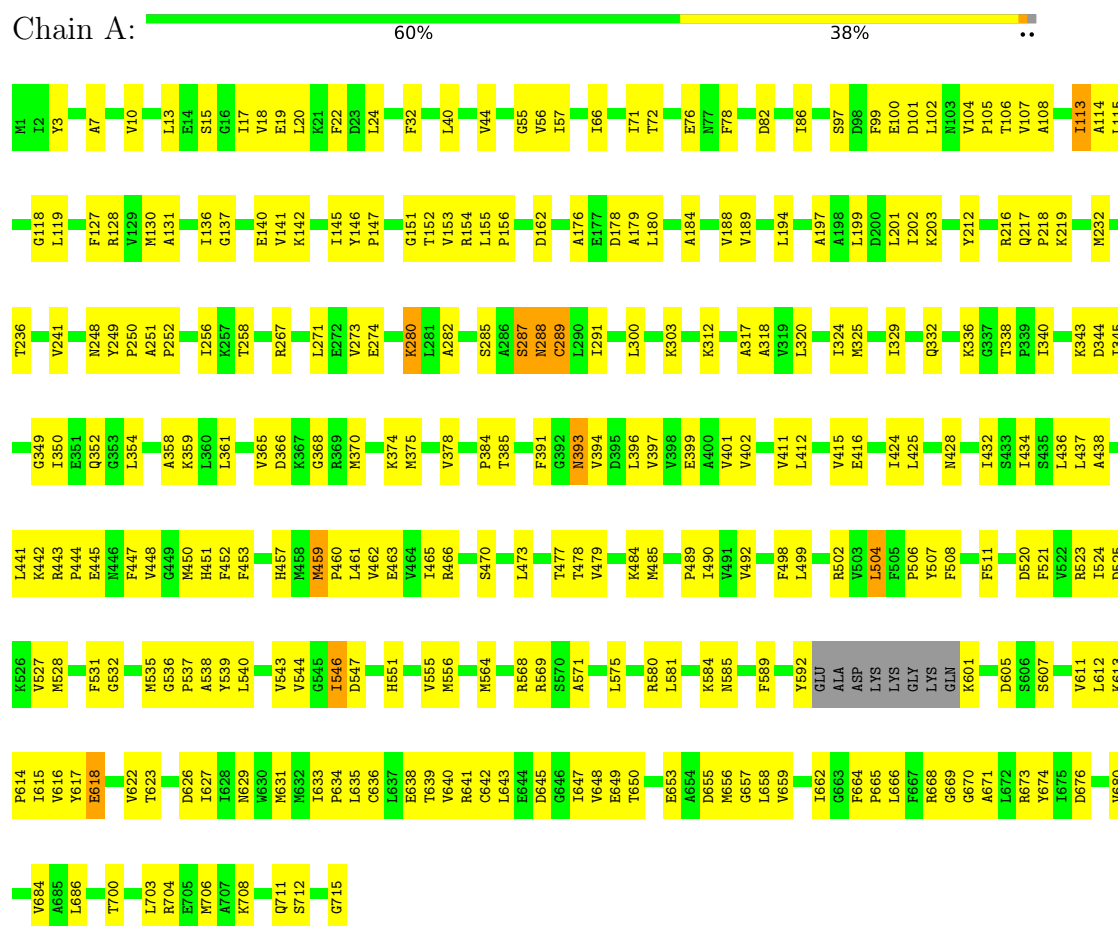


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
5	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

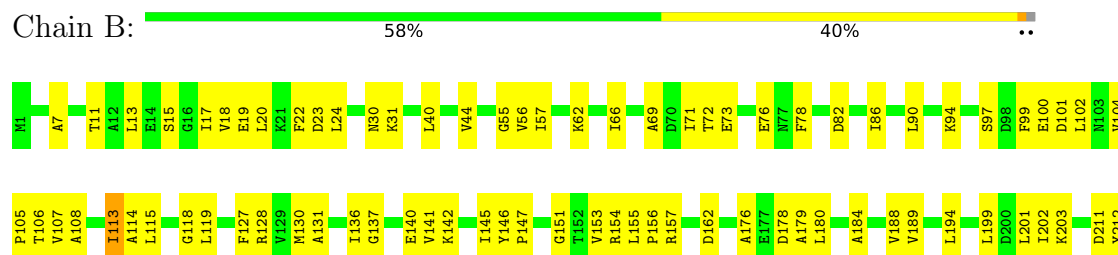
3 Residue-property plots

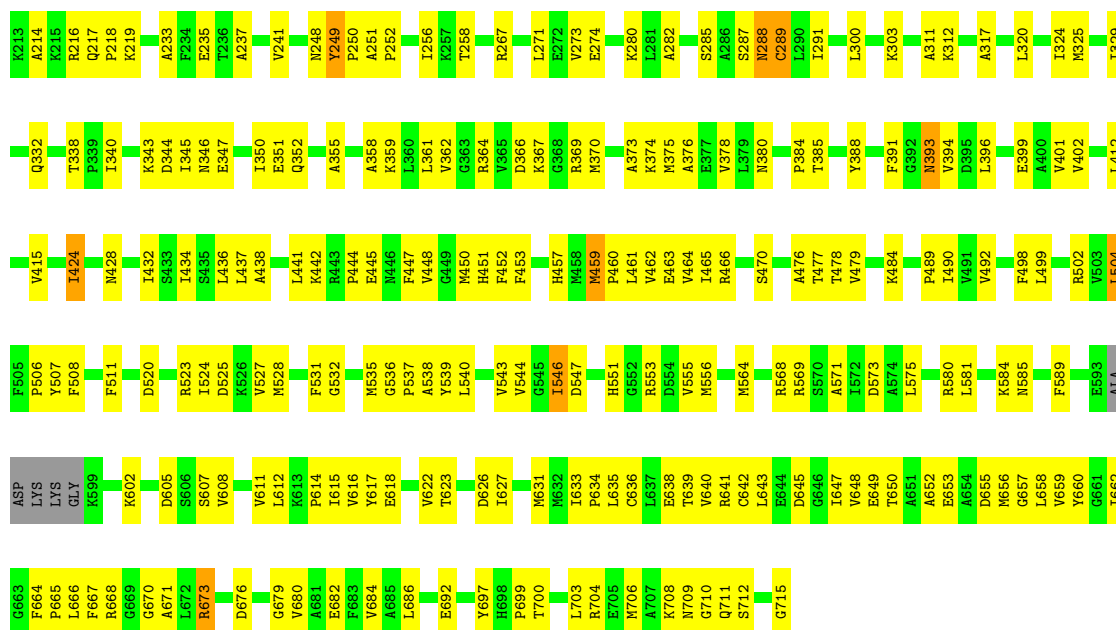
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Fatty oxidation complex alpha subunit



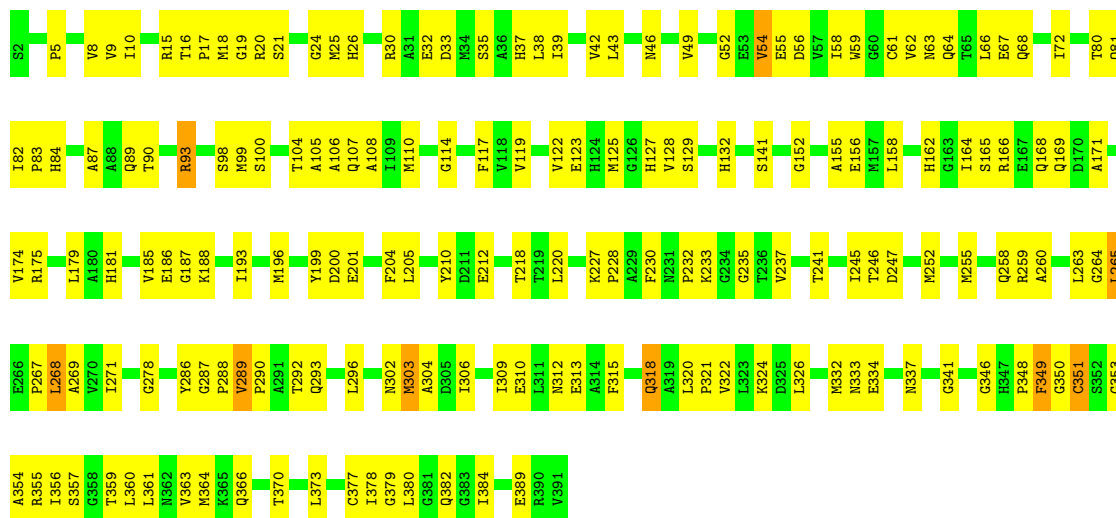
• Molecule 1: Fatty oxidation complex alpha subunit





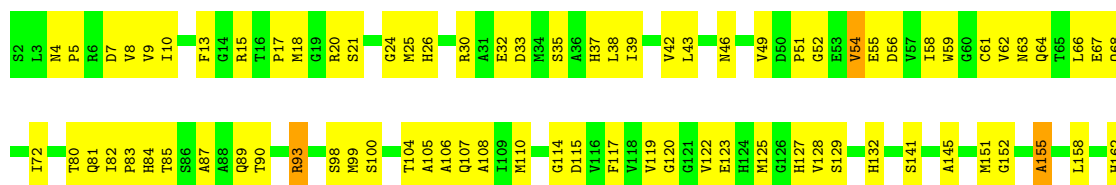
• Molecule 2: 3-ketoacyl-CoA thiolase

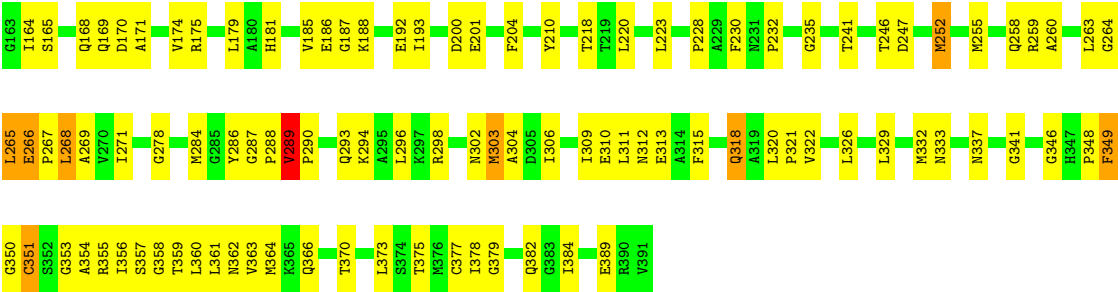
Chain C: 55% 43%



• Molecule 2: 3-ketoacyl-CoA thiolase

Chain D: 54% 43%





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	181.45Å 95.46Å 161.32Å 90.00° 111.79° 90.00°	Depositor
Resolution (Å)	20.00 – 3.80 20.00 – 3.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-3.80) 97.7 (20.00-3.80)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.39 (at 3.82Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.214 , 0.262 0.194 , 0.236	Depositor DCC
R_{free} test set	1710 reflections (6.87%)	wwPDB-VP
Wilson B-factor (Å ²)	63.5	Xtriage
Anisotropy	0.272	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 23.1	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	0.92	EDS
Total number of atoms	16541	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% 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: ZN, 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	0.35	0/5343	0.85	7/7237 (0.1%)
1	B	0.35	0/5388	0.84	6/7291 (0.1%)
2	C	0.38	0/2919	0.84	3/3944 (0.1%)
2	D	0.38	1/2917 (0.0%)	0.84	6/3941 (0.2%)
All	All	0.36	1/16567 (0.0%)	0.84	22/22413 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	289	VAL	CA-CB	5.07	1.57	1.54

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	249	TYR	CA-C-N	7.23	126.73	118.85
1	A	249	TYR	C-N-CA	7.23	126.73	118.85
1	B	249	TYR	CA-C-N	7.16	126.65	118.85
1	B	249	TYR	C-N-CA	7.16	126.65	118.85
2	C	93	ARG	N-CA-C	-6.19	102.87	110.61
1	A	589	PHE	N-CA-C	-6.10	104.75	111.82
2	D	93	ARG	N-CA-C	-6.00	103.11	110.61
1	B	589	PHE	N-CA-C	-5.95	104.87	111.36
1	A	184	ALA	N-CA-C	-5.94	104.75	112.23
1	B	184	ALA	N-CA-C	-5.85	104.86	112.23
1	B	459	MET	CA-C-N	5.63	125.24	119.56
1	B	459	MET	C-N-CA	5.63	125.24	119.56
2	C	268	LEU	N-CA-C	-5.62	106.27	113.23
1	A	459	MET	CA-C-N	5.56	125.18	119.56
1	A	459	MET	C-N-CA	5.56	125.18	119.56
2	C	66	LEU	CB-CA-C	-5.48	110.23	116.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	268	LEU	N-CA-C	-5.33	106.62	113.23
2	D	266	GLU	CA-C-N	5.29	125.23	119.78
2	D	266	GLU	C-N-CA	5.29	125.23	119.78
1	A	674	TYR	N-CA-C	-5.05	105.96	111.82
2	D	155	ALA	N-CA-C	-5.02	105.48	112.45
2	D	66	LEU	CB-CA-C	-5.00	110.78	116.54

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	5257	0	5243	230	0
1	B	5302	0	5314	248	0
2	C	2871	0	2848	154	0
2	D	2869	0	2849	165	0
3	A	1	0	0	0	0
4	A	51	0	34	2	0
4	C	51	0	34	0	0
4	D	51	0	34	0	0
5	A	44	0	26	1	0
5	B	44	0	26	1	0
All	All	16541	0	16408	776	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 24.

All (776) 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:525:ASP:HB2	1:A:536:GLY:HA3	1.34	1.09
1:B:525:ASP:HB2	1:B:536:GLY:HA3	1.36	1.07
2:D:17:PRO:HB2	2:D:25:MET:HE1	1.54	0.89
2:D:289:VAL:HG13	2:D:290:PRO:HD3	1.55	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:125:MET:HE2	2:C:348:PRO:HA	1.58	0.85
2:D:98:SER:HB3	2:D:353:GLY:HA3	1.59	0.85
1:A:375:MET:HE2	1:B:375:MET:HE2	1.57	0.84
1:B:401:VAL:HG12	1:B:402:VAL:H	1.42	0.84
2:C:289:VAL:HG13	2:C:290:PRO:HD3	1.60	0.83
2:D:125:MET:HE2	2:D:348:PRO:HA	1.59	0.82
1:B:673:ARG:HB2	1:B:673:ARG:HH11	1.43	0.82
2:C:360:LEU:HG	2:C:364:MET:HE2	1.62	0.81
1:A:401:VAL:HG12	1:A:402:VAL:H	1.45	0.81
1:B:537:PRO:HG2	1:B:631:MET:HE3	1.60	0.81
2:C:378:ILE:HB	2:C:382:GLN:HB2	1.62	0.80
1:A:71:ILE:HD11	1:A:291:ILE:HG23	1.64	0.80
2:C:287:GLY:O	2:C:290:PRO:HD2	1.80	0.80
2:C:17:PRO:HB2	2:C:25:MET:HE1	1.64	0.80
2:D:306:ILE:HD13	2:D:373:LEU:HB2	1.63	0.79
1:A:537:PRO:HG2	1:A:631:MET:HE3	1.66	0.78
2:D:378:ILE:HB	2:D:382:GLN:HB2	1.66	0.77
1:A:251:ALA:HB3	1:A:252:PRO:HD3	1.67	0.76
1:B:71:ILE:HD11	1:B:291:ILE:HG23	1.66	0.76
1:A:343:LYS:HD3	1:A:344:ASP:N	2.01	0.76
1:A:416:GLU:OE1	1:A:442:LYS:HG2	1.85	0.76
2:D:287:GLY:O	2:D:290:PRO:HD2	1.85	0.76
2:C:98:SER:HB3	2:C:353:GLY:HA3	1.67	0.76
1:B:361:LEU:HD21	1:B:378:VAL:HG11	1.67	0.75
1:A:130:MET:HE3	1:A:176:ALA:HA	1.69	0.74
1:A:581:LEU:HB2	1:A:585:ASN:HB2	1.69	0.74
1:A:113:ILE:H	1:A:113:ILE:CD1	2.01	0.74
1:B:343:LYS:HD3	1:B:344:ASP:N	2.02	0.73
1:B:502:ARG:HA	1:B:556:MET:HE2	1.71	0.73
2:C:8:VAL:HG21	2:C:106:ALA:HB1	1.69	0.73
2:D:80:THR:HG22	2:D:81:GLN:H	1.53	0.73
1:B:241:VAL:HG21	1:B:256:ILE:HD11	1.72	0.72
1:B:251:ALA:HB3	1:B:252:PRO:HD3	1.69	0.72
1:B:581:LEU:HB2	1:B:585:ASN:HB2	1.71	0.72
1:A:361:LEU:HD21	1:A:378:VAL:HG11	1.71	0.72
2:C:306:ILE:HD13	2:C:373:LEU:HB2	1.71	0.72
1:A:350:ILE:HG21	1:A:384:PRO:HB3	1.72	0.71
2:D:43:LEU:HD11	2:D:82:ILE:HD11	1.71	0.71
2:C:255:MET:HE2	2:C:260:ALA:HA	1.70	0.71
1:A:241:VAL:HG21	1:A:256:ILE:HD11	1.71	0.71
1:A:199:LEU:HD11	1:A:203:LYS:HE3	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:296:LEU:HD21	2:C:306:ILE:HD11	1.72	0.70
2:D:8:VAL:HG21	2:D:106:ALA:HB1	1.72	0.70
1:A:450:MET:HG2	1:A:452:PHE:CE1	2.26	0.69
1:A:504:LEU:HD13	4:A:1002:ACO:HH33	1.73	0.69
1:B:130:MET:CE	1:B:176:ALA:HA	2.22	0.69
2:D:152:GLY:HA3	2:D:230:PHE:CE2	2.27	0.69
1:A:673:ARG:HH11	1:A:673:ARG:HB2	1.55	0.69
2:C:46:ASN:O	2:C:49:VAL:HG22	1.92	0.69
1:B:325:MET:HE2	1:B:428:ASN:HD21	1.55	0.69
1:B:350:ILE:HG21	1:B:384:PRO:HB3	1.75	0.69
2:C:55:GLU:HG3	2:C:114:GLY:HA2	1.74	0.69
1:A:401:VAL:HG12	1:A:402:VAL:N	2.06	0.69
1:B:546:ILE:HD12	1:B:546:ILE:H	1.58	0.69
2:C:80:THR:HG22	2:C:81:GLN:H	1.57	0.69
1:A:180:LEU:HD23	1:A:180:LEU:O	1.93	0.69
1:B:130:MET:HE3	1:B:176:ALA:HA	1.74	0.69
1:B:450:MET:HG2	1:B:452:PHE:CE1	2.28	0.69
2:C:43:LEU:HD11	2:C:82:ILE:HD11	1.75	0.69
1:A:108:ALA:HB3	1:A:128:ARG:HG2	1.74	0.68
2:C:188:LYS:HD3	2:C:366:GLN:OE1	1.94	0.68
2:D:360:LEU:HG	2:D:364:MET:HE2	1.74	0.68
1:B:401:VAL:HG12	1:B:402:VAL:N	2.07	0.68
1:A:546:ILE:HD12	1:A:546:ILE:H	1.57	0.67
1:A:113:ILE:N	1:A:113:ILE:HD12	2.09	0.67
1:A:130:MET:CE	1:A:176:ALA:HA	2.24	0.67
1:A:320:LEU:HD11	1:A:415:VAL:HG21	1.76	0.67
2:C:289:VAL:HG23	2:C:293:GLN:HE21	1.59	0.67
2:D:55:GLU:HG3	2:D:114:GLY:HA2	1.77	0.67
2:D:289:VAL:HG23	2:D:293:GLN:HE21	1.59	0.67
1:B:320:LEU:HD11	1:B:415:VAL:HG21	1.77	0.67
2:C:54:VAL:HG21	2:C:82:ILE:HD12	1.76	0.67
1:B:199:LEU:HD11	1:B:203:LYS:HE3	1.76	0.66
1:B:130:MET:HE1	1:B:179:ALA:HB3	1.76	0.66
2:D:152:GLY:HA3	2:D:230:PHE:CD2	2.30	0.66
2:D:348:PRO:HB2	2:D:351:CYS:HB3	1.77	0.66
2:D:98:SER:HB3	2:D:353:GLY:CA	2.26	0.66
1:A:113:ILE:H	1:A:113:ILE:HD12	1.61	0.66
1:B:153:VAL:HG21	1:B:271:LEU:HD23	1.77	0.65
1:B:108:ALA:HB3	1:B:128:ARG:HG2	1.77	0.65
2:C:255:MET:HE2	2:C:260:ALA:CA	2.25	0.65
1:B:539:TYR:O	1:B:543:VAL:HG23	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:54:VAL:HG21	2:D:82:ILE:HD12	1.79	0.65
2:C:361:LEU:HA	2:C:364:MET:HE3	1.77	0.65
2:C:89:GLN:HB3	2:D:93:ARG:NH1	2.11	0.65
1:A:56:VAL:HB	1:A:106:THR:HG22	1.77	0.65
1:B:325:MET:CE	1:B:428:ASN:HD21	2.08	0.65
2:D:21:SER:HA	2:D:247:ASP:OD2	1.96	0.65
1:A:546:ILE:HD12	1:A:546:ILE:N	2.11	0.65
1:B:180:LEU:O	1:B:180:LEU:HD23	1.96	0.65
1:B:502:ARG:NH1	1:B:647:ILE:HG12	2.12	0.64
1:A:130:MET:HE1	1:A:179:ALA:CB	2.28	0.64
1:B:706:MET:HB2	1:B:711:GLN:HB2	1.80	0.64
2:D:98:SER:HB2	2:D:350:GLY:O	1.98	0.64
2:D:361:LEU:HA	2:D:364:MET:HE3	1.79	0.64
2:C:35:SER:O	2:C:39:ILE:HG13	1.97	0.64
1:A:502:ARG:HA	1:A:556:MET:HE2	1.79	0.64
1:B:300:LEU:HD11	1:B:656:MET:HG3	1.80	0.64
2:C:63:ASN:HB3	2:C:128:VAL:HG11	1.80	0.64
2:D:46:ASN:O	2:D:49:VAL:HG22	1.96	0.64
1:A:424:ILE:HD12	1:A:424:ILE:N	2.13	0.63
2:C:9:VAL:HG13	2:C:267:PRO:HB3	1.80	0.63
2:C:252:MET:HE3	2:C:354:ALA:HB1	1.80	0.63
1:A:101:ASP:CG	1:A:267:ARG:HH22	2.05	0.63
2:D:313:GLU:CD	2:D:341:GLY:HA3	2.23	0.63
1:B:113:ILE:HD13	1:B:113:ILE:N	2.14	0.63
1:B:303:LYS:HE3	1:B:650:THR:HG21	1.80	0.63
1:A:592:TYR:HA	1:A:601:LYS:O	1.99	0.63
2:D:9:VAL:HG13	2:D:267:PRO:HB3	1.80	0.63
2:D:255:MET:HE2	2:D:260:ALA:HA	1.80	0.63
1:B:525:ASP:CB	1:B:536:GLY:HA3	2.22	0.62
1:B:631:MET:O	1:B:634:PRO:HD2	1.99	0.62
1:B:285:SER:O	1:B:289:CYS:HB2	1.98	0.62
1:B:622:VAL:CG2	1:B:626:ASP:HB2	2.29	0.62
2:C:246:THR:OG1	2:C:346:GLY:HA3	1.98	0.62
1:A:633:ILE:HB	1:A:634:PRO:HD3	1.80	0.62
1:A:525:ASP:CB	1:A:536:GLY:HA3	2.20	0.62
1:A:130:MET:HE1	1:A:179:ALA:HB3	1.82	0.62
2:C:348:PRO:HB2	2:C:351:CYS:HB3	1.82	0.62
1:A:189:VAL:HG21	1:A:194:LEU:HA	1.82	0.62
1:A:706:MET:HB2	1:A:711:GLN:HB2	1.80	0.62
2:C:87:ALA:HB1	2:D:93:ARG:HH21	1.64	0.61
1:B:424:ILE:HD12	1:B:424:ILE:N	2.14	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:58:ILE:HD12	2:C:105:ALA:HB2	1.81	0.61
2:D:188:LYS:HD2	2:D:366:GLN:OE1	2.01	0.61
2:C:25:MET:HE2	2:C:26:HIS:NE2	2.16	0.61
1:A:465:ILE:N	1:A:465:ILE:HD12	2.15	0.61
1:B:56:VAL:HB	1:B:106:THR:HG22	1.82	0.61
2:C:18:MET:HB3	2:C:246:THR:HG21	1.81	0.61
2:D:35:SER:O	2:D:39:ILE:HG13	2.00	0.61
2:D:296:LEU:HD21	2:D:306:ILE:HD11	1.82	0.61
1:A:40:LEU:HD23	1:A:40:LEU:O	2.01	0.61
1:B:130:MET:HE1	1:B:179:ALA:CB	2.30	0.61
2:C:152:GLY:HA3	2:C:230:PHE:CE2	2.36	0.61
2:C:25:MET:HE2	2:C:26:HIS:CE1	2.35	0.61
1:B:288:ASN:N	1:B:288:ASN:HD22	1.97	0.61
2:C:265:LEU:N	2:C:265:LEU:HD23	2.16	0.61
1:A:546:ILE:H	1:A:546:ILE:CD1	2.13	0.61
2:D:18:MET:HB3	2:D:246:THR:HG21	1.83	0.61
1:B:546:ILE:HD12	1:B:546:ILE:N	2.16	0.60
2:D:58:ILE:HD12	2:D:105:ALA:HB2	1.83	0.60
2:C:21:SER:HA	2:C:247:ASP:OD2	2.01	0.60
1:A:82:ASP:O	1:A:86:ILE:HG13	2.01	0.60
2:C:174:VAL:HG22	2:C:218:THR:HG22	1.81	0.60
1:A:537:PRO:HG2	1:A:631:MET:CE	2.32	0.60
1:B:155:LEU:HB3	1:B:156:PRO:HD3	1.84	0.60
1:A:465:ILE:HG12	1:A:498:PHE:CE2	2.37	0.60
1:B:622:VAL:HG23	1:B:626:ASP:HB2	1.84	0.60
1:B:673:ARG:HB2	1:B:673:ARG:NH1	2.17	0.60
1:A:40:LEU:HD23	1:A:44:VAL:HG23	1.84	0.60
1:A:285:SER:O	1:A:289:CYS:HB2	2.01	0.60
1:A:511:PHE:HB2	1:A:631:MET:HE1	1.82	0.60
2:D:62:VAL:HG21	2:D:349:PHE:HB3	1.83	0.60
2:D:175:ARG:NE	2:D:179:LEU:HD12	2.16	0.60
1:B:22:PHE:CD2	1:B:66:ILE:HD11	2.37	0.59
1:B:105:PRO:HG3	1:B:212:TYR:CD2	2.37	0.59
1:A:680:VAL:O	1:A:684:VAL:HG23	2.01	0.59
1:A:97:SER:HB3	1:A:267:ARG:NH1	2.18	0.59
1:B:40:LEU:HD23	1:B:44:VAL:HG23	1.84	0.59
2:C:313:GLU:CD	2:C:341:GLY:HA3	2.26	0.59
1:B:101:ASP:CG	1:B:267:ARG:HH22	2.10	0.59
2:C:315:PHE:O	2:C:318:GLN:HG3	2.02	0.59
2:C:20:ARG:O	2:C:24:GLY:HA3	2.02	0.59
2:D:246:THR:OG1	2:D:346:GLY:HA3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:622:VAL:CG2	1:A:626:ASP:HB2	2.33	0.59
1:B:465:ILE:HG12	1:B:498:PHE:CE2	2.38	0.59
2:C:93:ARG:HH21	2:D:87:ALA:HB1	1.66	0.58
1:B:40:LEU:HD23	1:B:40:LEU:O	2.02	0.58
1:B:668:ARG:HH11	1:B:668:ARG:HG2	1.67	0.58
2:C:106:ALA:O	2:C:110:MET:HG3	2.03	0.58
2:C:255:MET:HE1	2:C:263:LEU:HD12	1.84	0.58
2:C:30:ARG:HB2	2:C:33:ASP:OD2	2.03	0.58
2:C:62:VAL:HG21	2:C:349:PHE:HB3	1.84	0.58
2:D:255:MET:HE1	2:D:263:LEU:HD12	1.84	0.58
1:A:338:THR:OG1	1:A:484:LYS:HE3	2.03	0.58
2:C:98:SER:HB2	2:C:350:GLY:O	2.04	0.58
1:A:361:LEU:HB3	1:A:375:MET:HG3	1.86	0.58
2:D:255:MET:HE2	2:D:260:ALA:CA	2.33	0.58
1:B:399:GLU:HG2	1:B:401:VAL:HG23	1.84	0.58
1:A:55:GLY:HA2	1:A:104:VAL:HG13	1.84	0.57
2:D:63:ASN:HB3	2:D:128:VAL:HG11	1.86	0.57
2:D:265:LEU:HD23	2:D:265:LEU:N	2.19	0.57
1:B:249:TYR:OH	1:B:666:LEU:HB2	2.04	0.57
2:D:329:LEU:HD23	2:D:329:LEU:O	2.04	0.57
1:A:631:MET:O	1:A:634:PRO:HD2	2.05	0.57
1:B:338:THR:OG1	1:B:484:LYS:HE3	2.04	0.57
1:B:461:LEU:HD12	1:B:462:VAL:H	1.69	0.57
1:B:465:ILE:HD12	1:B:465:ILE:N	2.20	0.57
1:B:649:GLU:HB3	1:B:653:GLU:OE1	2.05	0.57
1:A:673:ARG:HB2	1:A:673:ARG:NH1	2.20	0.57
1:B:645:ASP:HB2	1:B:647:ILE:HD13	1.86	0.57
2:D:125:MET:HE3	2:D:246:THR:N	2.19	0.57
2:D:38:LEU:O	2:D:42:VAL:HG23	2.05	0.57
1:A:399:GLU:HG2	1:A:401:VAL:HG23	1.87	0.56
2:C:98:SER:HB3	2:C:353:GLY:CA	2.32	0.56
1:B:465:ILE:HG12	1:B:498:PHE:CZ	2.40	0.56
2:C:152:GLY:HA3	2:C:230:PHE:CD2	2.39	0.56
2:D:359:THR:O	2:D:363:VAL:HG23	2.05	0.56
1:A:155:LEU:HB3	1:A:156:PRO:HD3	1.85	0.56
1:A:704:ARG:O	1:A:708:LYS:HG3	2.05	0.56
1:B:99:PHE:HA	1:B:102:LEU:HD13	1.86	0.56
1:B:140:GLU:HB2	1:B:146:TYR:HA	1.86	0.56
2:C:61:CYS:SG	2:C:68:GLN:HB3	2.46	0.56
2:C:255:MET:HE3	2:C:259:ARG:CG	2.35	0.56
1:B:684:VAL:HG22	1:B:703:LEU:HD22	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:10:ILE:N	2:D:10:ILE:HD12	2.19	0.56
2:D:33:ASP:O	2:D:37:HIS:HB2	2.06	0.56
1:A:146:TYR:HB2	1:A:147:PRO:HD2	1.87	0.56
2:C:38:LEU:O	2:C:42:VAL:HG23	2.04	0.56
2:D:252:MET:HE3	2:D:354:ALA:HB1	1.88	0.56
2:D:320:LEU:HB2	2:D:321:PRO:HD3	1.86	0.56
1:A:288:ASN:N	1:A:288:ASN:HD22	2.04	0.56
1:A:523:ARG:O	1:A:527:VAL:HG23	2.06	0.56
1:B:569:ARG:O	1:B:615:ILE:HD12	2.06	0.56
2:D:80:THR:HG22	2:D:81:GLN:N	2.20	0.56
1:B:107:VAL:HG22	1:B:127:PHE:HB2	1.88	0.55
2:C:318:GLN:C	2:C:321:PRO:HD2	2.31	0.55
1:B:708:LYS:C	1:B:710:GLY:H	2.13	0.55
1:B:502:ARG:HA	1:B:556:MET:CE	2.36	0.55
2:C:17:PRO:HB3	2:C:210:TYR:O	2.06	0.55
2:D:93:ARG:HD2	2:D:100:SER:OG	2.06	0.55
1:A:712:SER:OG	1:A:715:GLY:HA3	2.07	0.55
2:C:320:LEU:HB2	2:C:321:PRO:HD3	1.87	0.55
2:D:17:PRO:HB3	2:D:210:TYR:O	2.07	0.55
1:A:676:ASP:OD2	1:A:712:SER:HB2	2.07	0.55
1:B:40:LEU:O	1:B:44:VAL:HG23	2.07	0.55
1:B:180:LEU:HD12	1:B:188:VAL:HG23	1.88	0.55
2:C:181:HIS:O	2:C:185:VAL:HG23	2.07	0.55
1:A:502:ARG:NH1	1:A:647:ILE:HG12	2.22	0.55
1:A:686:LEU:O	1:A:686:LEU:HD23	2.06	0.55
2:C:52:GLY:HA2	2:C:83:PRO:HG2	1.87	0.55
1:A:194:LEU:C	1:A:194:LEU:HD23	2.32	0.55
1:A:401:VAL:CG1	1:A:402:VAL:H	2.19	0.55
1:B:546:ILE:H	1:B:546:ILE:CD1	2.19	0.55
2:C:67:GLU:OE2	2:C:127:HIS:HB3	2.07	0.55
2:D:67:GLU:OE2	2:D:127:HIS:HB3	2.07	0.55
1:B:680:VAL:O	1:B:684:VAL:HG23	2.07	0.55
1:A:525:ASP:OD2	1:A:538:ALA:HB3	2.07	0.54
1:A:547:ASP:OD2	1:A:584:LYS:HD2	2.08	0.54
1:B:66:ILE:O	1:B:118:GLY:HA3	2.07	0.54
2:D:286:TYR:O	2:D:289:VAL:HG13	2.06	0.54
1:B:347:GLU:O	1:B:351:GLU:HG2	2.08	0.54
1:B:464:VAL:HG21	1:B:479:VAL:HG22	1.89	0.54
1:B:140:GLU:HG3	1:B:147:PRO:N	2.22	0.54
1:B:504:LEU:HG	1:B:662:ILE:HD11	1.90	0.54
2:C:16:THR:HG22	2:C:196:MET:HE1	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:30:ARG:NH1	2:C:32:GLU:OE1	2.41	0.54
1:A:66:ILE:O	1:A:118:GLY:HA3	2.08	0.54
1:A:140:GLU:HB2	1:A:146:TYR:HA	1.89	0.54
1:A:520:ASP:O	1:A:524:ILE:HG13	2.07	0.54
2:C:10:ILE:HD12	2:C:10:ILE:N	2.23	0.54
2:D:59:TRP:CZ3	2:D:120:GLY:HA3	2.42	0.54
2:D:99:MET:HE2	2:D:357:SER:OG	2.07	0.54
2:D:165:SER:OG	2:D:168:GLN:HG3	2.07	0.54
1:A:40:LEU:O	1:A:44:VAL:HG23	2.07	0.54
1:B:537:PRO:HG2	1:B:631:MET:CE	2.35	0.54
2:C:33:ASP:O	2:C:37:HIS:HB2	2.06	0.54
1:A:668:ARG:HG2	1:A:668:ARG:HH11	1.72	0.54
1:B:623:THR:O	1:B:627:ILE:HG13	2.08	0.54
2:D:20:ARG:O	2:D:24:GLY:HA3	2.06	0.54
1:A:490:ILE:HD12	1:A:657:GLY:HA2	1.90	0.54
1:B:525:ASP:OD2	1:B:538:ALA:HB3	2.07	0.54
1:A:300:LEU:HD11	1:A:656:MET:HG3	1.89	0.54
2:C:185:VAL:C	2:C:187:GLY:H	2.16	0.54
1:B:686:LEU:HD23	1:B:686:LEU:O	2.07	0.53
2:D:181:HIS:O	2:D:185:VAL:HG23	2.08	0.53
2:C:255:MET:HE2	2:C:260:ALA:N	2.23	0.53
2:D:246:THR:HB	2:D:348:PRO:HG3	1.90	0.53
1:A:22:PHE:CD2	1:A:66:ILE:HD11	2.44	0.53
1:B:146:TYR:HB2	1:B:147:PRO:HD2	1.90	0.53
2:C:246:THR:HB	2:C:348:PRO:HG3	1.90	0.53
2:D:125:MET:HE3	2:D:246:THR:H	1.74	0.53
2:D:58:ILE:HB	2:D:119:VAL:HG12	1.91	0.53
2:C:348:PRO:O	2:C:349:PHE:C	2.51	0.53
1:B:31:LYS:HB2	1:B:69:ALA:HA	1.91	0.53
2:D:106:ALA:O	2:D:110:MET:HG3	2.09	0.53
1:B:13:LEU:HD11	1:B:19:GLU:HB2	1.91	0.53
2:D:348:PRO:O	2:D:349:PHE:C	2.51	0.53
1:B:55:GLY:HA2	1:B:104:VAL:HG13	1.89	0.53
2:C:125:MET:HE3	2:C:246:THR:N	2.23	0.53
2:D:318:GLN:O	2:D:322:VAL:HG23	2.08	0.53
1:B:523:ARG:NH2	1:B:627:ILE:HD11	2.24	0.53
2:C:359:THR:O	2:C:363:VAL:HG23	2.09	0.53
1:A:506:PRO:HG3	1:A:564:MET:CE	2.39	0.53
1:B:535:MET:SD	1:B:543:VAL:HG21	2.49	0.53
1:B:658:LEU:O	1:B:662:ILE:HG22	2.09	0.53
1:A:412:LEU:HB3	1:A:441:LEU:HD21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:539:TYR:O	1:A:543:VAL:HG23	2.09	0.52
1:A:611:VAL:O	1:A:614:PRO:HD2	2.09	0.52
1:B:343:LYS:HD3	1:B:344:ASP:H	1.73	0.52
1:A:465:ILE:HA	1:A:492:VAL:O	2.09	0.52
1:B:20:LEU:HD23	1:B:20:LEU:C	2.35	0.52
1:B:393:ASN:HD22	1:B:393:ASN:C	2.17	0.52
2:C:93:ARG:HD2	2:C:100:SER:OG	2.10	0.52
1:A:194:LEU:HD23	1:A:194:LEU:O	2.10	0.52
1:A:280:LYS:HB2	1:A:280:LYS:NZ	2.25	0.52
2:C:58:ILE:HB	2:C:119:VAL:HG12	1.92	0.52
1:A:622:VAL:HG23	1:A:626:ASP:HB2	1.91	0.52
1:B:532:GLY:C	1:B:665:PRO:HG3	2.34	0.52
2:D:318:GLN:C	2:D:321:PRO:HD2	2.35	0.52
1:B:465:ILE:HA	1:B:492:VAL:O	2.09	0.52
2:D:52:GLY:HA2	2:D:83:PRO:HG2	1.90	0.52
1:B:401:VAL:CG1	1:B:402:VAL:H	2.19	0.52
2:C:122:VAL:HG22	2:C:123:GLU:N	2.25	0.52
2:C:286:TYR:CE1	2:C:289:VAL:HG11	2.45	0.52
2:D:315:PHE:O	2:D:318:GLN:HG3	2.09	0.52
1:A:147:PRO:HB3	1:A:151:GLY:HA3	1.92	0.52
1:B:72:THR:O	1:B:76:GLU:HG3	2.09	0.52
1:B:618:GLU:CD	1:B:618:GLU:H	2.18	0.52
1:A:180:LEU:HD12	1:A:188:VAL:HG23	1.93	0.51
1:B:147:PRO:HB3	1:B:151:GLY:HA3	1.92	0.51
2:C:59:TRP:HE1	2:C:122:VAL:HB	1.75	0.51
1:B:189:VAL:HG21	1:B:194:LEU:HA	1.92	0.51
2:C:252:MET:CE	2:C:354:ALA:HB1	2.40	0.51
2:C:292:THR:HG23	2:C:373:LEU:HD21	1.92	0.51
1:A:571:ALA:HB1	1:A:612:LEU:HD22	1.93	0.51
1:B:391:PHE:HA	1:B:394:VAL:HG23	1.91	0.51
1:B:633:ILE:HB	1:B:634:PRO:HD3	1.90	0.51
2:D:175:ARG:HE	2:D:179:LEU:HD12	1.75	0.51
1:A:317:ALA:O	1:A:340:ILE:HA	2.10	0.51
1:B:312:LYS:O	1:B:477:THR:HG23	2.10	0.51
2:D:228:PRO:HB3	2:D:235:GLY:HA3	1.92	0.51
2:D:286:TYR:CZ	2:D:289:VAL:HG11	2.46	0.51
1:A:568:ARG:HD2	1:A:617:TYR:CE1	2.46	0.51
1:A:613:LYS:HB3	1:A:614:PRO:HD3	1.91	0.51
1:A:684:VAL:HG22	1:A:703:LEU:HD22	1.92	0.51
1:B:57:ILE:HG12	1:B:202:ILE:HG13	1.91	0.51
1:A:32:PHE:CE1	1:A:66:ILE:HG21	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:174:VAL:HG22	2:D:218:THR:HG22	1.93	0.51
1:B:448:VAL:HG12	1:B:470:SER:HB3	1.92	0.51
1:A:99:PHE:HA	1:A:102:LEU:HD13	1.93	0.51
1:A:391:PHE:HA	1:A:394:VAL:HG23	1.93	0.51
1:A:465:ILE:HG12	1:A:498:PHE:CZ	2.46	0.51
1:B:113:ILE:HD13	1:B:113:ILE:H	1.74	0.51
1:B:445:GLU:CD	1:B:445:GLU:H	2.19	0.51
1:B:568:ARG:HD2	1:B:617:TYR:CE1	2.46	0.51
2:C:312:ASN:HB2	2:C:356:ILE:HD13	1.93	0.51
1:A:374:LYS:O	1:A:378:VAL:HG23	2.11	0.51
1:A:504:LEU:O	1:A:507:TYR:HB3	2.11	0.50
1:A:436:LEU:HD23	1:A:436:LEU:O	2.11	0.50
2:D:151:MET:HE1	2:D:284:MET:SD	2.51	0.50
1:B:370:MET:HE1	1:B:378:VAL:HG21	1.92	0.50
2:C:80:THR:HG22	2:C:81:GLN:N	2.24	0.50
1:A:72:THR:O	1:A:76:GLU:HG3	2.11	0.50
1:A:180:LEU:HD23	1:A:180:LEU:C	2.36	0.50
1:B:237:ALA:O	1:B:241:VAL:HG23	2.10	0.50
1:A:461:LEU:HD12	1:A:462:VAL:H	1.75	0.50
1:A:643:LEU:HD23	1:A:643:LEU:O	2.12	0.50
1:B:451:HIS:HB3	1:B:463:GLU:HB2	1.93	0.50
2:C:93:ARG:NH1	2:D:89:GLN:HB3	2.26	0.50
2:C:310:GLU:OE2	2:C:337:ASN:HA	2.12	0.50
2:D:192:GLU:HB3	2:D:362:ASN:ND2	2.27	0.50
1:A:13:LEU:HD11	1:A:19:GLU:HB2	1.93	0.50
2:C:99:MET:HE2	2:C:357:SER:OG	2.11	0.50
2:C:171:ALA:HA	2:C:220:LEU:HD21	1.92	0.50
1:A:57:ILE:HG12	1:A:202:ILE:HG13	1.93	0.50
1:B:105:PRO:HG3	1:B:212:TYR:CE2	2.47	0.50
1:B:479:VAL:HG13	1:B:489:PRO:CG	2.42	0.50
1:A:645:ASP:HB2	1:A:647:ILE:HD13	1.93	0.50
1:B:194:LEU:HD23	1:B:194:LEU:O	2.12	0.50
2:D:169:GLN:HB3	2:D:241:THR:HG21	1.94	0.50
1:A:199:LEU:CD1	1:A:203:LYS:HE3	2.42	0.49
1:A:647:ILE:HG22	1:A:648:VAL:HG23	1.94	0.49
1:B:154:ARG:HD3	1:B:219:LYS:HD2	1.93	0.49
1:B:194:LEU:HD23	1:B:194:LEU:C	2.37	0.49
1:B:547:ASP:HB3	1:B:581:LEU:HD22	1.94	0.49
1:B:622:VAL:HG22	1:B:623:THR:O	2.12	0.49
1:B:643:LEU:O	1:B:643:LEU:HD23	2.12	0.49
2:D:25:MET:HE2	2:D:26:HIS:CE1	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:LEU:C	1:A:199:LEU:HD13	2.38	0.49
1:B:350:ILE:HD11	1:B:385:THR:O	2.13	0.49
1:B:358:ALA:O	1:B:362:VAL:HG23	2.12	0.49
1:B:504:LEU:O	1:B:507:TYR:HB3	2.12	0.49
2:C:56:ASP:CG	2:D:93:ARG:HH22	2.21	0.49
2:C:129:SER:OG	2:C:132:HIS:HB2	2.13	0.49
2:C:200:ASP:OD2	2:C:204:PHE:HB2	2.12	0.49
1:B:396:LEU:C	1:B:396:LEU:HD23	2.37	0.49
1:A:636:CYS:O	1:A:640:VAL:HG23	2.12	0.49
1:B:199:LEU:HD13	1:B:199:LEU:C	2.38	0.49
2:C:99:MET:HB3	2:C:384:ILE:HD13	1.95	0.49
2:C:105:ALA:O	2:C:108:ALA:HB3	2.13	0.49
2:C:175:ARG:NE	2:C:179:LEU:HD12	2.27	0.49
2:D:185:VAL:C	2:D:187:GLY:H	2.19	0.49
1:A:217:GLN:HB3	1:A:218:PRO:HD3	1.94	0.49
1:A:442:LYS:C	1:A:444:PRO:HD3	2.38	0.49
1:B:180:LEU:HD23	1:B:180:LEU:C	2.37	0.49
2:D:122:VAL:HG22	2:D:123:GLU:N	2.28	0.49
1:A:7:ALA:HA	1:A:24:LEU:HA	1.95	0.49
1:A:448:VAL:HG21	1:A:478:THR:OG1	2.13	0.49
1:A:623:THR:O	1:A:627:ILE:HG13	2.13	0.49
1:B:668:ARG:HG2	1:B:668:ARG:NH1	2.28	0.49
2:C:93:ARG:HH22	2:D:56:ASP:CG	2.21	0.49
1:A:325:MET:O	1:A:329:ILE:HG13	2.13	0.49
1:B:82:ASP:O	1:B:86:ILE:HG13	2.13	0.48
1:B:345:ILE:HG13	1:B:346:ASN:N	2.27	0.48
1:B:361:LEU:HB3	1:B:375:MET:HG3	1.94	0.48
1:B:442:LYS:C	1:B:444:PRO:HD3	2.38	0.48
2:C:302:ASN:C	2:C:304:ALA:N	2.71	0.48
2:D:312:ASN:HB2	2:D:356:ILE:HD13	1.95	0.48
1:A:312:LYS:O	1:A:477:THR:HG23	2.13	0.48
1:B:248:ASN:O	1:B:250:PRO:HD3	2.13	0.48
1:B:700:THR:OG1	1:B:703:LEU:HB2	2.13	0.48
2:C:360:LEU:HG	2:C:364:MET:CE	2.39	0.48
1:A:105:PRO:HG3	1:A:212:TYR:CD2	2.48	0.48
1:A:303:LYS:HE3	1:A:650:THR:HG21	1.94	0.48
1:A:451:HIS:HB3	1:A:463:GLU:HB2	1.95	0.48
1:B:436:LEU:O	1:B:436:LEU:HD23	2.13	0.48
2:D:302:ASN:C	2:D:304:ALA:N	2.71	0.48
1:B:271:LEU:O	1:B:274:GLU:HB3	2.14	0.48
1:B:520:ASP:O	1:B:524:ILE:HG13	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:286:TYR:O	2:C:289:VAL:HG13	2.12	0.48
1:A:401:VAL:CG1	1:A:402:VAL:N	2.76	0.48
1:B:652:ALA:O	1:B:656:MET:HG2	2.13	0.48
2:D:302:ASN:O	2:D:304:ALA:N	2.46	0.48
1:A:350:ILE:HD11	1:A:385:THR:O	2.14	0.48
1:A:499:LEU:HD13	1:A:499:LEU:C	2.39	0.48
1:A:605:ASP:OD2	1:A:607:SER:OG	2.32	0.48
1:B:288:ASN:N	1:B:288:ASN:ND2	2.60	0.48
1:B:388:TYR:HE2	1:B:415:VAL:HG22	1.78	0.48
2:C:302:ASN:O	2:C:304:ALA:N	2.47	0.48
2:D:255:MET:HE3	2:D:259:ARG:HG3	1.95	0.48
2:D:370:THR:O	2:D:389:GLU:HA	2.13	0.48
1:A:78:PHE:CD1	1:A:282:ALA:HB1	2.48	0.48
2:C:286:TYR:CZ	2:C:289:VAL:HG11	2.49	0.48
2:D:123:GLU:HG2	2:D:349:PHE:HB2	1.95	0.48
2:D:171:ALA:HA	2:D:220:LEU:HD21	1.94	0.48
1:A:271:LEU:O	1:A:274:GLU:HB3	2.14	0.48
1:A:396:LEU:C	1:A:396:LEU:HD23	2.39	0.48
1:B:114:ALA:HB3	1:B:136:ILE:HG22	1.96	0.48
1:B:367:LYS:C	1:B:369:ARG:H	2.22	0.48
1:B:374:LYS:O	1:B:378:VAL:HG23	2.13	0.48
1:B:285:SER:HA	1:B:288:ASN:HD21	1.79	0.48
1:B:448:VAL:HG21	1:B:478:THR:OG1	2.13	0.48
2:C:8:VAL:HG11	2:C:271:ILE:HD12	1.96	0.48
2:D:129:SER:OG	2:D:132:HIS:HB2	2.14	0.48
1:B:635:LEU:C	1:B:635:LEU:HD23	2.39	0.47
2:C:370:THR:O	2:C:389:GLU:HA	2.14	0.47
1:B:199:LEU:CD1	1:B:203:LYS:HE3	2.43	0.47
1:B:317:ALA:O	1:B:340:ILE:HA	2.14	0.47
2:C:25:MET:HG2	2:C:212:GLU:OE1	2.13	0.47
2:C:169:GLN:HB3	2:C:241:THR:HG21	1.95	0.47
2:C:201:GLU:CD	2:C:201:GLU:H	2.22	0.47
2:C:289:VAL:O	2:C:293:GLN:HG3	2.14	0.47
2:D:59:TRP:HE1	2:D:122:VAL:HB	1.79	0.47
2:D:114:GLY:HA3	2:D:117:PHE:CE1	2.49	0.47
1:B:412:LEU:HB3	1:B:441:LEU:HD21	1.96	0.47
1:B:438:ALA:HB2	1:B:447:PHE:HD2	1.79	0.47
2:C:30:ARG:NH1	2:C:67:GLU:HG2	2.30	0.47
1:A:146:TYR:HB2	1:A:147:PRO:CD	2.45	0.47
1:B:401:VAL:CG1	1:B:402:VAL:N	2.77	0.47
1:B:636:CYS:O	1:B:640:VAL:HG23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:165:SER:OG	2:C:168:GLN:HG3	2.15	0.47
2:D:30:ARG:NH1	2:D:67:GLU:HG2	2.29	0.47
2:D:125:MET:CE	2:D:246:THR:H	2.27	0.47
1:A:453:PHE:HB2	1:A:459:MET:HG3	1.96	0.47
1:A:504:LEU:HG	1:A:662:ILE:HD11	1.95	0.47
1:A:618:GLU:CD	1:A:618:GLU:H	2.22	0.47
1:A:658:LEU:O	1:A:662:ILE:HG22	2.14	0.47
1:B:434:ILE:HG23	1:B:447:PHE:CE2	2.49	0.47
1:B:523:ARG:O	1:B:527:VAL:HG23	2.15	0.47
1:B:655:ASP:O	1:B:659:VAL:HG23	2.14	0.47
2:C:255:MET:HE3	2:C:259:ARG:HG3	1.96	0.47
2:D:286:TYR:CE1	2:D:289:VAL:HG11	2.50	0.47
1:B:511:PHE:HB2	1:B:631:MET:HE1	1.95	0.47
2:D:10:ILE:HD11	2:D:271:ILE:HG13	1.96	0.47
2:D:30:ARG:NH1	2:D:32:GLU:OE1	2.47	0.47
1:A:20:LEU:C	1:A:20:LEU:HD23	2.39	0.47
1:A:287:SER:C	1:A:289:CYS:H	2.23	0.47
1:A:546:ILE:N	1:A:546:ILE:CD1	2.76	0.47
1:B:638:GLU:HA	1:B:641:ARG:HH11	1.78	0.47
1:B:684:VAL:CG2	1:B:703:LEU:HD22	2.45	0.47
1:B:704:ARG:HG2	1:B:704:ARG:HH11	1.80	0.47
2:C:175:ARG:HE	2:C:179:LEU:HD12	1.79	0.47
1:A:700:THR:OG1	1:A:703:LEU:HB2	2.15	0.47
1:B:23:ASP:OD2	1:B:62:LYS:HE2	2.14	0.47
1:B:528:MET:O	1:B:531:PHE:HB3	2.14	0.47
2:C:318:GLN:O	2:C:321:PRO:HD2	2.14	0.47
2:D:361:LEU:HD23	2:D:364:MET:CE	2.45	0.47
1:A:434:ILE:HG23	1:A:447:PHE:CE2	2.50	0.47
1:B:303:LYS:HE3	1:B:650:THR:CG2	2.45	0.47
2:D:17:PRO:HB2	2:D:25:MET:CE	2.35	0.47
2:D:174:VAL:HG13	2:D:218:THR:O	2.15	0.47
1:B:119:LEU:HD23	1:B:119:LEU:O	2.15	0.46
1:B:352:GLN:O	1:B:355:ALA:HB3	2.15	0.46
2:D:255:MET:HE2	2:D:260:ALA:N	2.29	0.46
1:A:635:LEU:C	1:A:635:LEU:HD23	2.39	0.46
1:A:664:PHE:CD2	1:A:670:GLY:HA2	2.50	0.46
2:D:311:LEU:HD13	2:D:375:THR:HG23	1.98	0.46
1:B:7:ALA:HA	1:B:24:LEU:HA	1.96	0.46
2:C:318:GLN:O	2:C:322:VAL:HG23	2.15	0.46
2:D:303:MET:O	2:D:303:MET:HE3	2.15	0.46
2:D:310:GLU:HG3	2:D:360:LEU:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:GLU:O	1:A:216:ARG:HD3	2.16	0.46
1:A:140:GLU:HG3	1:A:147:PRO:N	2.31	0.46
1:A:358:ALA:O	1:A:359:LYS:C	2.58	0.46
1:A:544:VAL:HG21	4:A:1002:ACO:HH32	1.97	0.46
1:A:643:LEU:HD23	1:A:643:LEU:C	2.41	0.46
1:B:617:TYR:HB3	1:B:618:GLU:OE2	2.15	0.46
1:A:504:LEU:O	1:A:504:LEU:HD23	2.15	0.46
2:C:19:GLY:O	2:C:246:THR:HG23	2.14	0.46
1:A:332:GLN:OE1	1:A:457:HIS:HA	2.16	0.46
1:B:571:ALA:HB1	1:B:612:LEU:HD22	1.98	0.46
1:A:114:ALA:HB3	1:A:136:ILE:HG22	1.97	0.46
1:A:445:GLU:CD	1:A:445:GLU:H	2.24	0.46
1:B:217:GLN:HB3	1:B:218:PRO:HD3	1.98	0.46
1:B:575:LEU:HD22	1:B:580:ARG:HD3	1.98	0.46
1:B:642:CYS:O	1:B:647:ILE:HB	2.16	0.46
2:D:105:ALA:O	2:D:108:ALA:HB3	2.15	0.46
1:A:119:LEU:O	1:A:119:LEU:HD23	2.15	0.46
1:B:162:ASP:HB2	2:D:141:SER:HB3	1.98	0.46
1:B:358:ALA:O	1:B:359:LYS:C	2.59	0.46
2:C:63:ASN:HB3	2:C:128:VAL:CG1	2.43	0.46
2:D:59:TRP:O	2:D:90:THR:HA	2.16	0.46
1:B:647:ILE:HG22	1:B:648:VAL:HG23	1.97	0.46
1:A:442:LYS:HG3	1:A:443:ARG:HG3	1.98	0.45
1:B:113:ILE:HG22	1:B:115:LEU:HG	1.97	0.45
1:B:490:ILE:HD12	1:B:657:GLY:HA2	1.97	0.45
1:B:580:ARG:CZ	1:B:608:VAL:HG22	2.46	0.45
2:C:199:TYR:CZ	2:C:205:LEU:HD13	2.51	0.45
2:C:287:GLY:C	2:C:290:PRO:HD2	2.41	0.45
1:A:141:VAL:HA	1:A:145:ILE:O	2.16	0.45
1:A:354:LEU:HD22	1:B:380:ASN:OD1	2.15	0.45
2:D:62:VAL:CG2	2:D:349:PHE:HB3	2.46	0.45
1:A:194:LEU:C	1:A:194:LEU:CD2	2.90	0.45
1:A:197:ALA:HB2	2:D:204:PHE:CE1	2.52	0.45
1:A:532:GLY:C	1:A:665:PRO:HG3	2.41	0.45
1:B:325:MET:HG3	5:B:2001:NAD:O4D	2.17	0.45
2:C:59:TRP:CD1	2:C:122:VAL:HG12	2.52	0.45
2:C:107:GLN:HB3	2:D:107:GLN:HB3	1.99	0.45
2:D:170:ASP:O	2:D:174:VAL:HG23	2.17	0.45
1:A:638:GLU:HA	1:A:641:ARG:HH11	1.81	0.45
1:B:128:ARG:HG3	1:B:128:ARG:HH11	1.82	0.45
1:B:130:MET:HE1	1:B:176:ALA:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:459:MET:HA	1:B:460:PRO:HD3	1.74	0.45
2:C:378:ILE:HG22	2:C:379:GLY:N	2.32	0.45
1:B:141:VAL:HA	1:B:145:ILE:O	2.16	0.45
1:B:350:ILE:CG2	1:B:384:PRO:HB3	2.45	0.45
1:B:450:MET:HE3	1:B:478:THR:CG2	2.46	0.45
2:C:166:ARG:HG2	2:C:166:ARG:HH11	1.82	0.45
1:B:664:PHE:CD2	1:B:670:GLY:HA2	2.51	0.45
2:C:288:PRO:HD3	2:C:377:CYS:HB3	1.99	0.45
1:A:107:VAL:HG23	1:A:202:ILE:CD1	2.47	0.45
1:A:432:ILE:HG21	1:A:437:LEU:HD21	1.98	0.45
1:A:443:ARG:N	1:A:444:PRO:HD3	2.32	0.45
1:B:551:HIS:O	1:B:555:VAL:HG23	2.17	0.45
1:B:639:THR:HG21	1:B:671:ALA:HB3	1.99	0.45
1:A:459:MET:HA	1:A:460:PRO:HD3	1.75	0.45
1:A:528:MET:O	1:A:531:PHE:HB3	2.17	0.45
1:B:525:ASP:HB3	1:B:537:PRO:HD2	1.99	0.45
2:C:9:VAL:CG1	2:C:267:PRO:HB3	2.47	0.45
1:A:569:ARG:O	1:A:615:ILE:HD12	2.17	0.45
1:B:146:TYR:HB2	1:B:147:PRO:CD	2.47	0.45
2:C:49:VAL:HG23	2:C:49:VAL:O	2.17	0.45
2:C:93:ARG:NH2	2:D:87:ALA:HB1	2.32	0.45
1:B:605:ASP:OD2	1:B:607:SER:OG	2.34	0.45
2:C:322:VAL:HG12	2:C:326:LEU:HD12	1.99	0.45
2:D:269:ALA:CB	2:D:361:LEU:HD22	2.47	0.45
2:D:302:ASN:C	2:D:304:ALA:H	2.26	0.45
1:B:100:GLU:O	1:B:216:ARG:HD3	2.16	0.44
1:B:666:LEU:C	1:B:668:ARG:H	2.24	0.44
2:C:114:GLY:HA3	2:C:117:PHE:CE1	2.52	0.44
2:C:303:MET:HE2	2:C:309:ILE:HD11	1.99	0.44
1:A:547:ASP:HB3	1:A:581:LEU:HD22	1.98	0.44
1:B:105:PRO:HG3	1:B:212:TYR:CG	2.53	0.44
1:B:325:MET:O	1:B:329:ILE:HG13	2.17	0.44
1:A:107:VAL:HG22	1:A:127:PHE:HB2	1.98	0.44
1:A:113:ILE:CG2	1:A:115:LEU:HG	2.47	0.44
1:A:465:ILE:N	1:A:465:ILE:CD1	2.80	0.44
1:A:502:ARG:HA	1:A:556:MET:CE	2.46	0.44
1:B:157:ARG:HD2	1:B:219:LYS:HA	1.99	0.44
1:A:448:VAL:HG12	1:A:470:SER:HB3	1.99	0.44
1:A:655:ASP:O	1:A:659:VAL:HG23	2.18	0.44
1:B:364:ARG:HB3	1:B:370:MET:HB2	2.00	0.44
2:C:164:ILE:N	2:C:164:ILE:HD12	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:379:GLY:O	2:C:380:LEU:HB2	2.18	0.44
2:D:61:CYS:SG	2:D:68:GLN:HB3	2.57	0.44
2:D:99:MET:HB3	2:D:384:ILE:HD13	1.99	0.44
2:D:175:ARG:HG3	2:D:175:ARG:HH11	1.81	0.44
2:D:378:ILE:HG22	2:D:379:GLY:N	2.32	0.44
1:A:581:LEU:HB2	1:A:585:ASN:CB	2.45	0.44
1:B:611:VAL:O	1:B:614:PRO:HD2	2.17	0.44
1:B:643:LEU:HD23	1:B:643:LEU:C	2.43	0.44
2:D:361:LEU:HD23	2:D:364:MET:HE3	2.00	0.44
1:A:649:GLU:HB3	1:A:653:GLU:OE1	2.18	0.44
2:C:125:MET:HE3	2:C:246:THR:H	1.80	0.44
2:D:289:VAL:CG1	2:D:290:PRO:HD3	2.38	0.44
2:D:348:PRO:O	2:D:351:CYS:N	2.43	0.44
1:A:153:VAL:HG21	1:A:271:LEU:HD23	2.00	0.44
1:B:22:PHE:CE2	1:B:66:ILE:HD11	2.53	0.44
1:B:56:VAL:HG23	1:B:104:VAL:HG11	2.00	0.44
1:B:11:THR:O	1:B:18:VAL:HG23	2.17	0.44
2:C:155:ALA:HB2	2:C:315:PHE:CD2	2.53	0.44
2:C:310:GLU:HG3	2:C:360:LEU:HB2	2.00	0.44
2:D:51:PRO:HB3	2:D:82:ILE:HD13	2.00	0.44
1:A:629:ASN:HB3	1:A:633:ILE:HD11	2.00	0.44
1:B:676:ASP:OD2	1:B:712:SER:HB2	2.17	0.44
1:A:575:LEU:HD22	1:A:580:ARG:HD3	2.00	0.43
1:B:633:ILE:HD11	1:B:686:LEU:HD22	2.00	0.43
2:C:156:GLU:OE2	2:C:237:VAL:HG23	2.18	0.43
2:D:310:GLU:OE2	2:D:337:ASN:HA	2.17	0.43
1:A:424:ILE:HD12	1:A:424:ILE:H	1.83	0.43
2:C:302:ASN:C	2:C:304:ALA:H	2.26	0.43
2:D:218:THR:HG23	2:D:223:LEU:HD21	2.00	0.43
2:D:252:MET:CE	2:D:354:ALA:HB1	2.48	0.43
2:D:322:VAL:HG12	2:D:326:LEU:HD12	2.00	0.43
1:B:287:SER:C	1:B:289:CYS:H	2.27	0.43
2:C:59:TRP:O	2:C:90:THR:HA	2.19	0.43
2:C:64:GLN:HA	2:C:68:GLN:O	2.18	0.43
2:C:228:PRO:HB3	2:C:235:GLY:HA3	1.99	0.43
2:D:266:GLU:HA	2:D:267:PRO:HD3	1.88	0.43
1:A:100:GLU:OE1	1:A:154:ARG:NE	2.40	0.43
1:A:162:ASP:HB2	2:C:141:SER:OG	2.19	0.43
1:A:344:ASP:OD1	1:A:345:ILE:N	2.44	0.43
1:B:547:ASP:OD2	1:B:584:LYS:HD2	2.18	0.43
2:C:357:SER:O	2:C:361:LEU:HG	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201:LEU:C	1:B:201:LEU:HD23	2.44	0.43
1:B:235:GLU:HA	1:B:235:GLU:OE2	2.19	0.43
1:B:461:LEU:HB2	1:B:660:TYR:HB3	2.00	0.43
2:C:62:VAL:CG2	2:C:349:PHE:HB3	2.46	0.43
2:D:13:PHE:CE2	2:D:358:GLY:HA3	2.53	0.43
2:D:289:VAL:O	2:D:293:GLN:HG3	2.19	0.43
1:A:551:HIS:O	1:A:555:VAL:HG23	2.19	0.43
1:B:78:PHE:CD1	1:B:282:ALA:HB1	2.52	0.43
1:A:325:MET:HE2	1:A:428:ASN:HD21	1.84	0.43
1:B:73:GLU:HA	1:B:76:GLU:OE1	2.19	0.43
2:C:84:HIS:O	2:D:278:GLY:HA3	2.19	0.43
2:D:255:MET:HE3	2:D:259:ARG:CG	2.49	0.43
1:A:56:VAL:HG23	1:A:104:VAL:HG11	2.01	0.43
1:B:553:ARG:HH12	1:B:573:ASP:CG	2.25	0.43
2:C:72:ILE:O	2:C:72:ILE:HG12	2.19	0.43
2:C:348:PRO:O	2:C:351:CYS:N	2.45	0.43
1:A:350:ILE:CG2	1:A:384:PRO:HB3	2.45	0.43
2:D:63:ASN:HB3	2:D:128:VAL:CG1	2.48	0.43
2:D:269:ALA:HB2	2:D:361:LEU:HD22	2.01	0.43
1:B:708:LYS:C	1:B:710:GLY:N	2.77	0.42
1:B:712:SER:OG	1:B:715:GLY:HA3	2.19	0.42
1:A:130:MET:HG2	1:A:131:ALA:O	2.18	0.42
1:A:508:PHE:HZ	1:A:540:LEU:HD22	1.83	0.42
1:A:666:LEU:C	1:A:668:ARG:H	2.27	0.42
1:B:332:GLN:OE1	1:B:457:HIS:HA	2.19	0.42
1:B:373:ALA:O	1:B:376:ALA:HB3	2.19	0.42
1:B:540:LEU:HD23	1:B:544:VAL:HG23	2.01	0.42
2:D:162:HIS:CD2	2:D:321:PRO:HB3	2.55	0.42
2:D:200:ASP:OD2	2:D:204:PHE:HB2	2.19	0.42
1:B:504:LEU:HG	1:B:662:ILE:CD1	2.49	0.42
1:B:506:PRO:HG3	1:B:564:MET:CE	2.49	0.42
1:A:521:PHE:HA	1:A:524:ILE:HD12	2.01	0.42
1:A:540:LEU:HD23	1:A:544:VAL:HG23	2.01	0.42
1:A:668:ARG:HG2	1:A:668:ARG:NH1	2.34	0.42
1:B:162:ASP:HB2	2:D:141:SER:CB	2.49	0.42
1:B:539:TYR:CD1	1:B:602:LYS:HD3	2.54	0.42
1:B:658:LEU:C	1:B:662:ILE:HG22	2.45	0.42
2:C:278:GLY:O	2:D:85:THR:HA	2.18	0.42
2:D:230:PHE:O	2:D:232:PRO:HD3	2.19	0.42
1:B:130:MET:HG2	1:B:131:ALA:O	2.18	0.42
2:C:123:GLU:HG2	2:C:349:PHE:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:227:LYS:O	2:C:228:PRO:C	2.62	0.42
2:D:4:ASN:N	2:D:7:ASP:OD2	2.51	0.42
2:D:64:GLN:HA	2:D:68:GLN:O	2.19	0.42
2:D:287:GLY:N	2:D:288:PRO:CD	2.83	0.42
2:D:287:GLY:C	2:D:290:PRO:HD2	2.43	0.42
2:D:318:GLN:O	2:D:321:PRO:HD2	2.19	0.42
1:A:105:PRO:HG3	1:A:212:TYR:CG	2.54	0.42
1:B:258:THR:HG23	1:B:273:VAL:HG12	2.02	0.42
1:B:466:ARG:HG3	1:B:470:SER:HB2	2.00	0.42
1:B:697:TYR:O	1:B:699:PRO:HD3	2.19	0.42
1:A:102:LEU:C	1:A:104:VAL:H	2.28	0.42
1:B:102:LEU:C	1:B:104:VAL:H	2.28	0.42
1:B:453:PHE:HB2	1:B:459:MET:HG3	2.02	0.42
1:B:502:ARG:HH12	1:B:647:ILE:HG12	1.83	0.42
1:B:508:PHE:O	1:B:511:PHE:HB3	2.20	0.42
1:B:618:GLU:CD	1:B:618:GLU:N	2.77	0.42
1:A:119:LEU:HD12	1:A:137:GLY:N	2.34	0.42
1:B:30:ASN:ND2	1:B:62:LYS:HG3	2.35	0.42
2:C:87:ALA:HB1	2:D:93:ARG:NH2	2.32	0.42
2:D:13:PHE:CD2	2:D:358:GLY:HA3	2.55	0.42
1:A:55:GLY:HA2	1:A:104:VAL:CG1	2.47	0.42
1:A:318:ALA:HB3	1:A:397:VAL:HG22	2.01	0.42
1:A:336:LYS:HG3	1:A:485:MET:HA	2.02	0.42
1:A:370:MET:HE1	1:A:378:VAL:HG21	2.01	0.42
1:A:450:MET:HE3	1:A:478:THR:CG2	2.49	0.42
1:B:17:ILE:HG22	1:B:18:VAL:N	2.34	0.42
1:B:287:SER:O	1:B:291:ILE:HG13	2.20	0.42
1:B:673:ARG:HH11	1:B:673:ARG:CB	2.25	0.42
2:C:125:MET:CE	2:C:246:THR:H	2.32	0.42
2:D:294:LYS:HD3	2:D:298:ARG:NH2	2.34	0.42
2:D:354:ALA:O	2:D:358:GLY:N	2.51	0.42
1:A:436:LEU:HD23	1:A:436:LEU:C	2.45	0.42
1:A:479:VAL:HG13	1:A:489:PRO:CG	2.49	0.42
1:B:432:ILE:HG21	1:B:437:LEU:HD21	2.02	0.42
2:C:278:GLY:HA3	2:D:84:HIS:O	2.18	0.42
2:C:361:LEU:HD23	2:C:364:MET:HE3	2.01	0.42
2:D:49:VAL:O	2:D:49:VAL:HG23	2.19	0.42
1:A:525:ASP:HB3	1:A:537:PRO:HD2	2.02	0.41
1:A:642:CYS:O	1:A:647:ILE:HB	2.20	0.41
1:B:97:SER:HB3	1:B:267:ARG:NH1	2.35	0.41
1:B:211:ASP:OD1	1:B:214:ALA:N	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:682:GLU:OE1	1:B:682:GLU:N	2.51	0.41
1:B:704:ARG:HG2	1:B:704:ARG:NH1	2.35	0.41
2:C:265:LEU:N	2:C:265:LEU:CD2	2.83	0.41
1:B:90:LEU:O	1:B:94:LYS:HG3	2.20	0.41
1:B:119:LEU:HD12	1:B:137:GLY:N	2.34	0.41
2:C:56:ASP:OD1	2:D:93:ARG:NH2	2.53	0.41
2:D:15:ARG:NH2	2:D:193:ILE:HD11	2.35	0.41
2:D:72:ILE:O	2:D:72:ILE:HG12	2.19	0.41
2:D:201:GLU:H	2:D:201:GLU:CD	2.27	0.41
2:D:268:LEU:O	2:D:269:ALA:HB2	2.20	0.41
1:A:287:SER:O	1:A:291:ILE:HG13	2.21	0.41
1:A:508:PHE:O	1:A:511:PHE:HB3	2.20	0.41
2:C:162:HIS:O	2:C:164:ILE:HD12	2.20	0.41
2:D:155:ALA:HB2	2:D:315:PHE:CD2	2.55	0.41
2:D:164:ILE:HD11	2:D:321:PRO:HG3	2.03	0.41
1:A:3:TYR:HB3	1:A:10:VAL:HB	2.01	0.41
1:A:248:ASN:O	1:A:250:PRO:HD3	2.20	0.41
1:B:233:ALA:HB2	2:D:145:ALA:CB	2.51	0.41
1:B:581:LEU:HB2	1:B:585:ASN:CB	2.45	0.41
2:C:5:PRO:HA	2:C:258:GLN:HB2	2.02	0.41
2:C:334:GLU:O	2:C:334:GLU:HG2	2.20	0.41
2:D:288:PRO:HD3	2:D:377:CYS:HB3	2.01	0.41
1:A:320:LEU:HD13	1:A:411:VAL:CG1	2.51	0.41
1:A:669:GLY:HA3	1:A:673:ARG:HD2	2.02	0.41
2:C:10:ILE:HD11	2:C:271:ILE:HG13	2.03	0.41
2:C:268:LEU:O	2:C:269:ALA:HB2	2.20	0.41
1:A:154:ARG:HD3	1:A:219:LYS:HD2	2.02	0.41
1:A:349:GLY:O	1:A:352:GLN:HB2	2.19	0.41
1:A:704:ARG:HG2	1:A:704:ARG:HH11	1.86	0.41
1:B:97:SER:O	1:B:100:GLU:HB3	2.20	0.41
1:B:344:ASP:OD1	1:B:345:ILE:N	2.50	0.41
1:A:130:MET:HE3	1:A:176:ALA:CA	2.47	0.41
1:A:535:MET:SD	1:A:543:VAL:HG21	2.60	0.41
1:B:311:ALA:HB2	1:B:476:ALA:HB1	2.03	0.41
1:B:617:TYR:CB	1:B:618:GLU:OE2	2.68	0.41
2:C:104:THR:HG23	2:D:104:THR:HG23	2.03	0.41
1:A:201:LEU:HD23	1:A:201:LEU:C	2.46	0.41
1:A:438:ALA:HB2	1:A:447:PHE:HD2	1.84	0.41
2:C:166:ARG:HG2	2:C:166:ARG:NH1	2.36	0.41
2:D:303:MET:CE	2:D:309:ILE:HD11	2.51	0.41
1:A:147:PRO:HB2	1:A:152:THR:HG23	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:MET:HG3	5:A:1001:NAD:O4D	2.20	0.41
1:A:393:ASN:H	1:A:393:ASN:HD22	1.68	0.41
1:A:535:MET:SD	1:A:539:TYR:CE2	3.13	0.41
1:B:100:GLU:OE1	1:B:154:ARG:NE	2.44	0.41
2:C:233:LYS:H	2:C:233:LYS:HG2	1.69	0.41
2:D:9:VAL:CG1	2:D:267:PRO:HB3	2.48	0.41
2:D:310:GLU:CG	2:D:360:LEU:HB2	2.51	0.41
1:A:232:MET:HE3	1:A:236:THR:CG2	2.51	0.41
1:A:365:VAL:HG22	1:A:370:MET:HG2	2.01	0.41
1:A:639:THR:HG21	1:A:671:ALA:HB3	2.01	0.41
1:B:465:ILE:N	1:B:465:ILE:CD1	2.83	0.41
1:B:679:GLY:O	1:B:680:VAL:C	2.63	0.41
1:A:393:ASN:HD22	1:A:393:ASN:C	2.27	0.40
2:C:15:ARG:NH2	2:C:193:ILE:HD11	2.36	0.40
1:A:287:SER:C	1:A:289:CYS:N	2.79	0.40
1:A:466:ARG:HG3	1:A:470:SER:HB2	2.04	0.40
1:A:473:LEU:HD23	1:A:473:LEU:O	2.20	0.40
2:D:5:PRO:HA	2:D:258:GLN:HB2	2.02	0.40
2:D:164:ILE:HD12	2:D:164:ILE:N	2.36	0.40
2:D:204:PHE:N	2:D:204:PHE:CD1	2.88	0.40
1:A:434:ILE:HD12	1:A:434:ILE:N	2.37	0.40
1:B:128:ARG:HG3	1:B:128:ARG:NH1	2.36	0.40
2:D:303:MET:HE2	2:D:309:ILE:HD11	2.03	0.40
1:A:258:THR:HG23	1:A:273:VAL:HG12	2.03	0.40
1:A:288:ASN:N	1:A:288:ASN:ND2	2.66	0.40
1:A:397:VAL:HB	1:A:425:LEU:HD23	2.02	0.40
1:B:194:LEU:C	1:B:194:LEU:CD2	2.94	0.40
1:B:499:LEU:C	1:B:499:LEU:HD13	2.47	0.40
2:C:255:MET:HE3	2:C:259:ARG:HB3	2.03	0.40
1:A:17:ILE:HG22	1:A:18:VAL:N	2.36	0.40
1:A:18:VAL:HG12	1:A:55:GLY:O	2.21	0.40
1:B:622:VAL:HG23	1:B:626:ASP:CB	2.51	0.40
2:C:360:LEU:CG	2:C:364:MET:HE2	2.44	0.40
2:D:164:ILE:HG22	2:D:169:GLN:HG3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	703/715 (98%)	632 (90%)	66 (9%)	5 (1%)	18	51
1	B	706/715 (99%)	628 (89%)	73 (10%)	5 (1%)	18	51
2	C	388/390 (100%)	343 (88%)	37 (10%)	8 (2%)	5	31
2	D	388/390 (100%)	346 (89%)	35 (9%)	7 (2%)	6	33
All	All	2185/2210 (99%)	1949 (89%)	211 (10%)	25 (1%)	11	41

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	324	ILE
2	C	332	MET
2	C	349	PHE
2	D	332	MET
2	D	349	PHE
1	A	15	SER
1	A	324	ILE
1	B	15	SER
2	C	303	MET
2	D	303	MET
1	B	709	ASN
2	C	186	GLU
2	C	333	ASN
2	D	333	ASN
1	A	287	SER
2	C	264	GLY
2	D	186	GLU
1	B	667	PHE
2	C	54	VAL
2	D	54	VAL
2	D	264	GLY
1	A	368	GLY

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Mol	Chain	Res	Type
1	B	616	VAL
1	A	616	VAL
2	C	232	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	532/562 (95%)	521 (98%)	11 (2%)	47	64
1	B	539/562 (96%)	526 (98%)	13 (2%)	43	62
2	C	302/307 (98%)	294 (97%)	8 (3%)	40	60
2	D	301/307 (98%)	293 (97%)	8 (3%)	39	59
All	All	1674/1738 (96%)	1634 (98%)	40 (2%)	43	62

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	113	ILE
1	A	142	LYS
1	A	178	ASP
1	A	280	LYS
1	A	288	ASN
1	A	289	CYS
1	A	366	ASP
1	A	393	ASN
1	A	504	LEU
1	A	546	ILE
1	A	618	GLU
1	B	113	ILE
1	B	142	LYS
1	B	178	ASP
1	B	280	LYS
1	B	288	ASN
1	B	289	CYS
1	B	366	ASP

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Mol	Chain	Res	Type
1	B	393	ASN
1	B	424	ILE
1	B	504	LEU
1	B	546	ILE
1	B	673	ARG
1	B	692	GLU
2	C	158	LEU
2	C	245	ILE
2	C	265	LEU
2	C	289	VAL
2	C	318	GLN
2	C	324	LYS
2	C	351	CYS
2	C	355	ARG
2	D	115	ASP
2	D	158	LEU
2	D	252	MET
2	D	265	LEU
2	D	289	VAL
2	D	318	GLN
2	D	351	CYS
2	D	355	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	A	288	ASN
1	A	296	ASN
1	A	298	GLN
1	A	393	ASN
1	A	409	GLN
1	A	428	ASN
1	A	551	HIS
1	A	629	ASN
1	A	698	HIS
1	B	30	ASN
1	B	38	ASN
1	B	42	GLN
1	B	288	ASN
1	B	296	ASN
1	B	298	GLN

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Mol	Chain	Res	Type
1	B	393	ASN
1	B	409	GLN
1	B	428	ASN
1	B	451	HIS
1	B	629	ASN
2	C	4	ASN
2	C	46	ASN
2	C	89	GLN
2	C	162	HIS
2	C	181	HIS
2	C	197	GLN
2	C	293	GLN
2	C	362	ASN
2	D	4	ASN
2	D	46	ASN
2	D	89	GLN
2	D	132	HIS
2	D	162	HIS
2	D	197	GLN
2	D	231	ASN
2	D	293	GLN
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](#)

Of 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 for Mogul analysis.

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
5	NAD	B	2001	-	46,48,48	1.50	5 (10%)	64,73,73	1.34	4 (6%)
4	ACO	A	1002	-	51,53,53	0.80	1 (1%)	73,79,79	0.66	1 (1%)
5	NAD	A	1001	-	46,48,48	1.49	4 (8%)	64,73,73	1.35	4 (6%)
4	ACO	C	3001	-	51,53,53	0.96	3 (5%)	73,79,79	0.69	1 (1%)
4	ACO	D	4001	-	51,53,53	0.71	0	73,79,79	0.65	1 (1%)

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
5	NAD	B	2001	-	-	5/30/62/62	0/5/5/5
4	ACO	A	1002	-	-	10/51/67/67	0/3/3/3
5	NAD	A	1001	-	-	8/30/62/62	0/5/5/5
4	ACO	C	3001	-	-	7/51/67/67	0/3/3/3
4	ACO	D	4001	-	-	13/51/67/67	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1001	NAD	C3N-C7N	5.40	1.58	1.50
5	B	2001	NAD	C3N-C7N	5.14	1.58	1.50
5	B	2001	NAD	C2N-N1N	4.74	1.40	1.35
5	A	1001	NAD	C2N-N1N	4.69	1.40	1.35
5	B	2001	NAD	C4N-C3N	3.58	1.44	1.39
5	B	2001	NAD	C6N-N1N	3.56	1.43	1.35
5	A	1001	NAD	C4N-C3N	3.54	1.44	1.39
5	A	1001	NAD	C6N-N1N	3.46	1.43	1.35
4	C	3001	ACO	P2A-O3A	3.16	1.62	1.59
5	B	2001	NAD	C5N-C4N	2.17	1.42	1.38
4	C	3001	ACO	P1A-O3A	2.15	1.61	1.59
4	C	3001	ACO	C4A-N3A	2.04	1.38	1.34
4	A	1002	ACO	C4A-N3A	2.01	1.38	1.34

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1001	NAD	C5N-C4N-C3N	-6.90	113.58	120.36
5	B	2001	NAD	C5N-C4N-C3N	-6.68	113.80	120.36
5	A	1001	NAD	C6N-C5N-C4N	5.51	127.39	119.45
5	B	2001	NAD	C6N-C5N-C4N	5.46	127.32	119.45
4	A	1002	ACO	C2P-S1P-C	3.89	120.15	101.42
5	B	2001	NAD	C5N-C6N-N1N	-3.84	115.15	120.38
4	D	4001	ACO	C2P-S1P-C	3.80	119.72	101.42
4	C	3001	ACO	C2P-S1P-C	3.75	119.46	101.42
5	A	1001	NAD	C5N-C6N-N1N	-3.61	115.46	120.38
5	A	1001	NAD	C2N-C3N-C4N	3.09	121.85	118.26
5	B	2001	NAD	C2N-C3N-C4N	2.94	121.67	118.26

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1002	ACO	C5B-O5B-P1A-O2A
4	A	1002	ACO	C5B-O5B-P1A-O3A
4	A	1002	ACO	C3P-C2P-S1P-C
4	A	1002	ACO	O-C-S1P-C2P
4	A	1002	ACO	CH3-C-S1P-C2P
4	C	3001	ACO	C5B-O5B-P1A-O1A
4	C	3001	ACO	C5B-O5B-P1A-O3A
4	C	3001	ACO	S1P-C2P-C3P-N4P
4	C	3001	ACO	C3P-C2P-S1P-C
4	C	3001	ACO	O-C-S1P-C2P
4	C	3001	ACO	CH3-C-S1P-C2P
4	D	4001	ACO	C5B-O5B-P1A-O1A
4	D	4001	ACO	C5B-O5B-P1A-O3A
4	D	4001	ACO	N8P-C9P-CAP-OAP
4	D	4001	ACO	S1P-C2P-C3P-N4P
4	D	4001	ACO	C3P-C2P-S1P-C
4	D	4001	ACO	O-C-S1P-C2P
4	D	4001	ACO	CH3-C-S1P-C2P
5	A	1001	NAD	C2N-C3N-C7N-O7N
5	A	1001	NAD	C2N-C3N-C7N-N7N
5	B	2001	NAD	C2N-C3N-C7N-O7N
5	B	2001	NAD	C2N-C3N-C7N-N7N
5	A	1001	NAD	C4N-C3N-C7N-O7N
5	A	1001	NAD	C4N-C3N-C7N-N7N
5	B	2001	NAD	C4N-C3N-C7N-O7N

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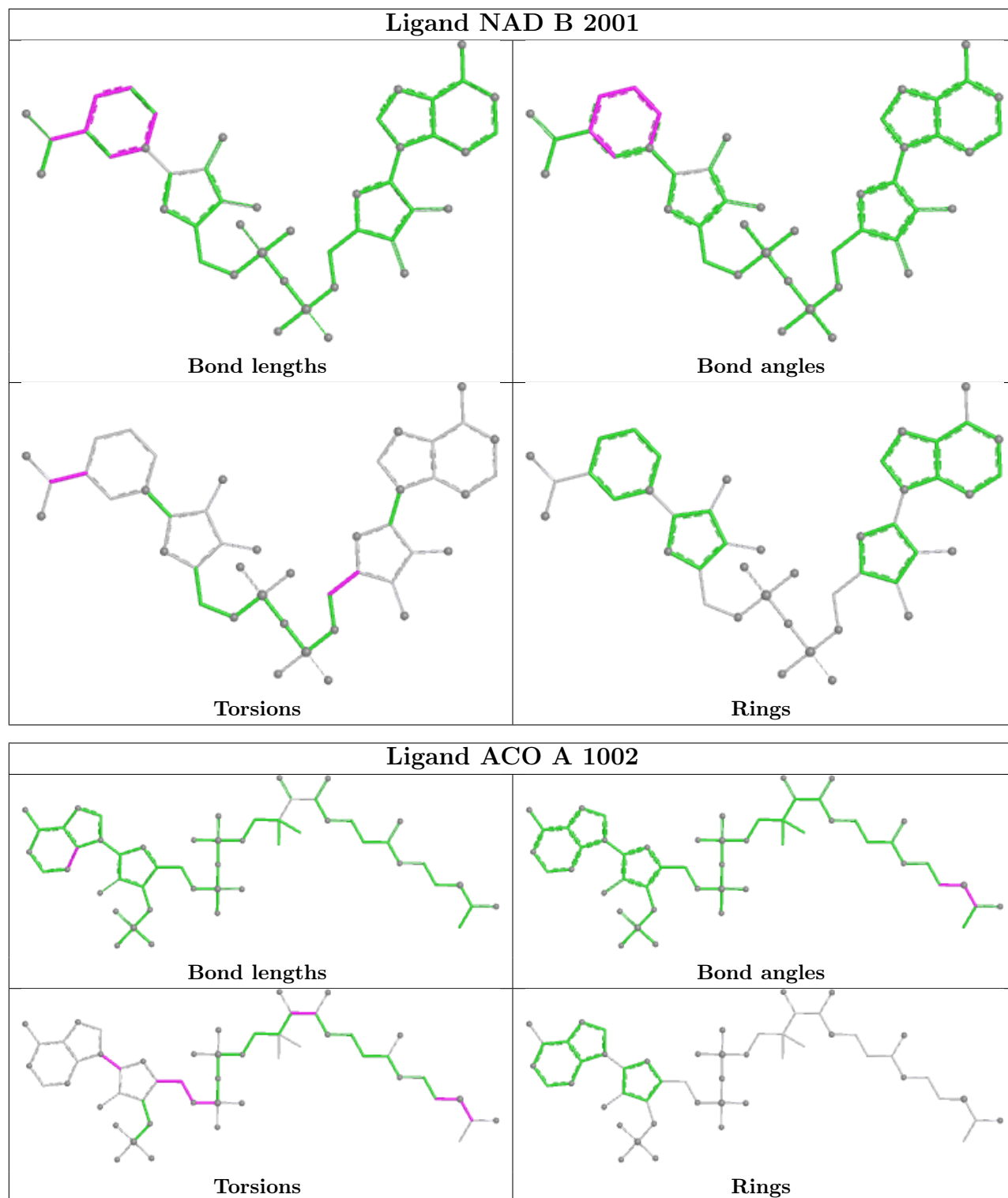
Mol	Chain	Res	Type	Atoms
5	B	2001	NAD	C4N-C3N-C7N-N7N
4	A	1002	ACO	C3B-C4B-C5B-O5B
4	D	4001	ACO	O4B-C4B-C5B-O5B
4	D	4001	ACO	C3B-C4B-C5B-O5B
4	A	1002	ACO	O4B-C4B-C5B-O5B
4	A	1002	ACO	C4B-C5B-O5B-P1A
4	A	1002	ACO	C2B-C1B-N9A-C8A
4	D	4001	ACO	O9P-C9P-CAP-OAP
4	C	3001	ACO	C5B-O5B-P1A-O2A
4	D	4001	ACO	CCP-O6A-P2A-O4A
5	A	1001	NAD	O4D-C1D-N1N-C2N
5	A	1001	NAD	O4D-C1D-N1N-C6N
5	A	1001	NAD	O4B-C4B-C5B-O5B
4	D	4001	ACO	C2P-C3P-N4P-C5P
5	B	2001	NAD	O4B-C4B-C5B-O5B
4	D	4001	ACO	C3B-O3B-P3B-O8A
5	A	1001	NAD	C3B-C4B-C5B-O5B
4	A	1002	ACO	N8P-C9P-CAP-OAP

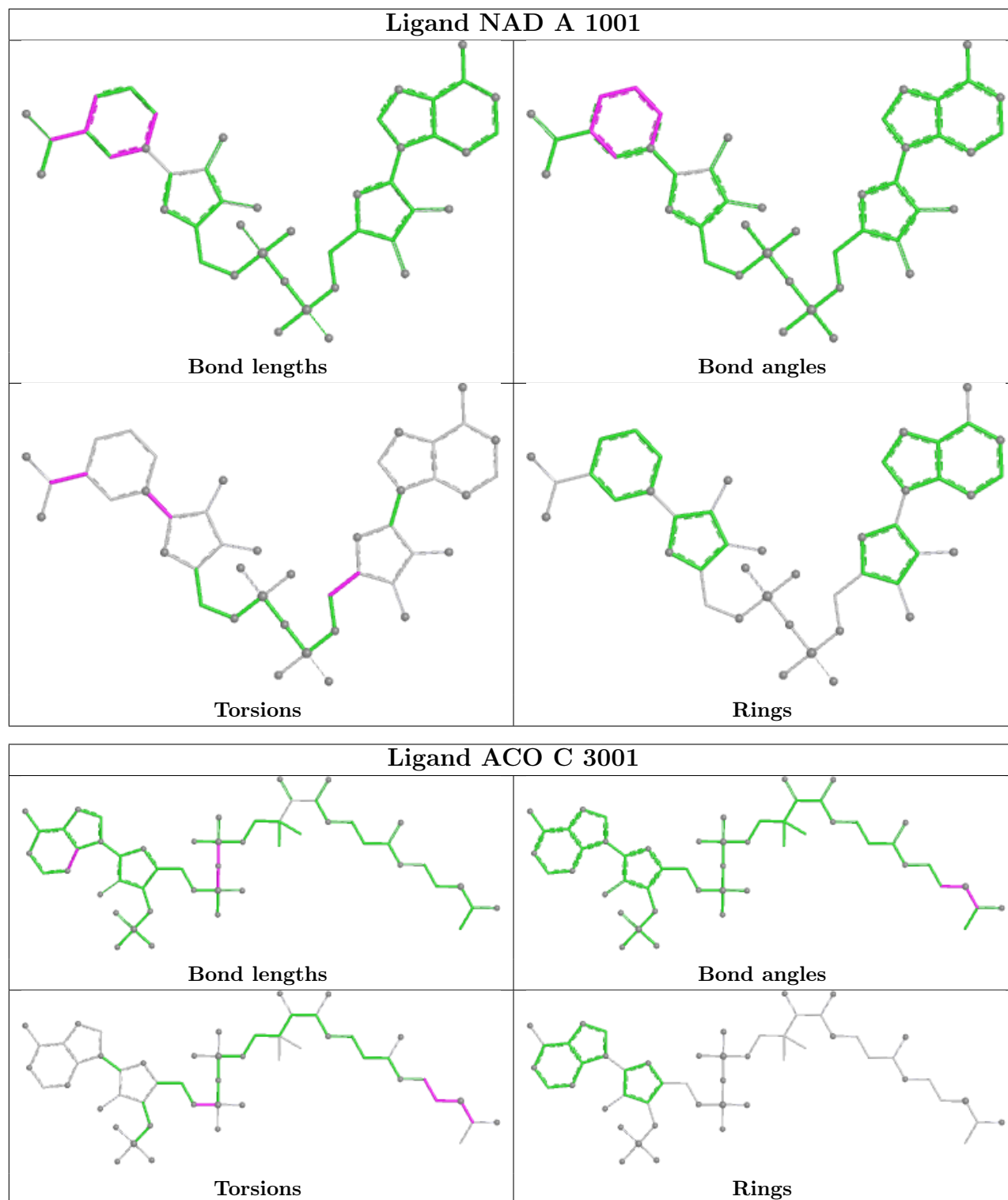
There are no ring outliers.

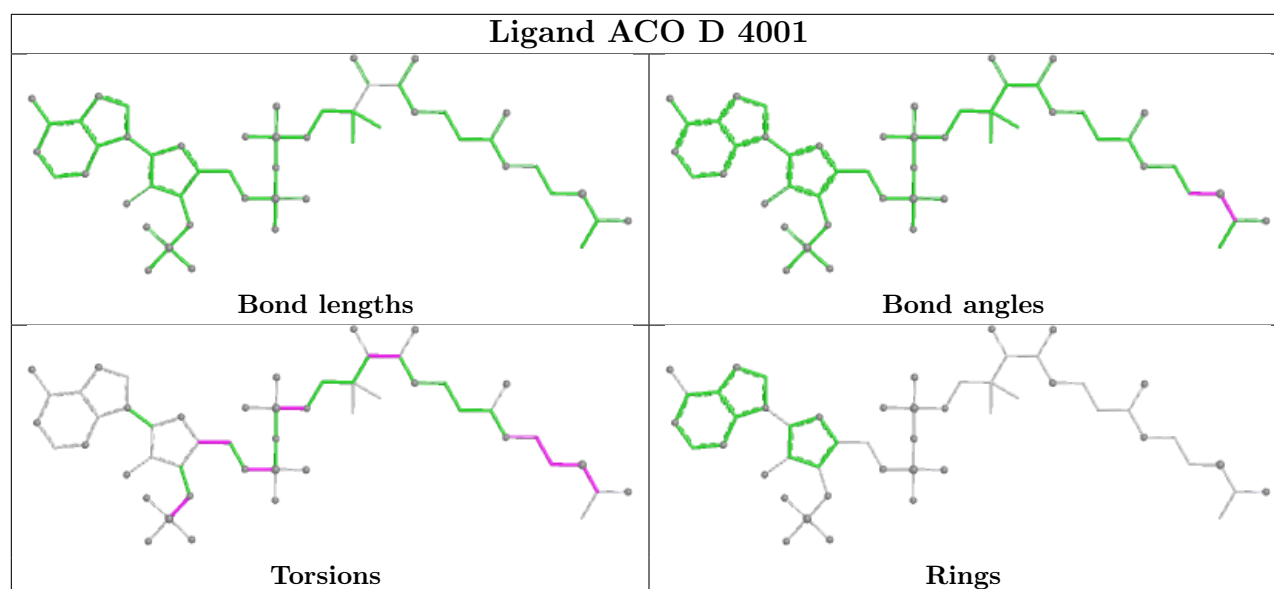
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	2001	NAD	1	0
4	A	1002	ACO	2	0
5	A	1001	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 [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	707/715 (98%)	-0.34	0 100 100	1, 21, 67, 97	0
1	B	710/715 (99%)	-0.36	0 100 100	1, 22, 65, 99	0
2	C	390/390 (100%)	-0.44	0 100 100	1, 8, 45, 83	0
2	D	390/390 (100%)	-0.44	0 100 100	1, 11, 45, 97	0
All	All	2197/2210 (99%)	-0.38	0 100 100	1, 17, 61, 99	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	ACO	A	1002	51/51	0.67	0.26	160,160,160,160	0
4	ACO	C	3001	51/51	0.77	0.18	159,159,159,159	0
5	NAD	B	2001	44/44	0.84	0.15	123,123,123,123	0
4	ACO	D	4001	51/51	0.85	0.15	133,133,133,133	0

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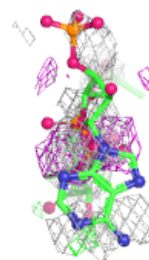
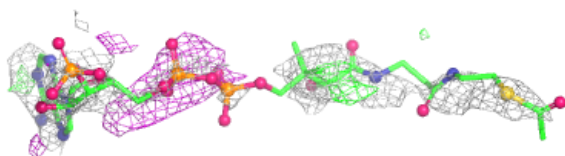
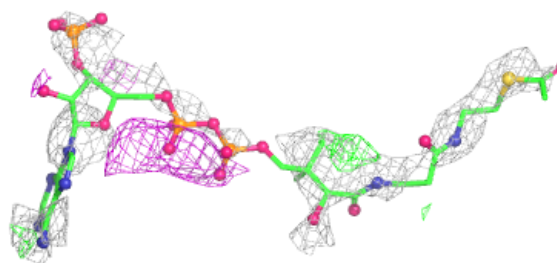
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NAD	A	1001	44/44	0.88	0.13	98,98,98,98	0
3	ZN	A	716	1/1	1.00	0.03	5,5,5,5	0

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.

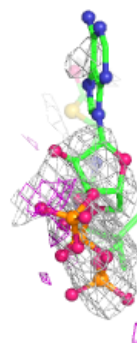
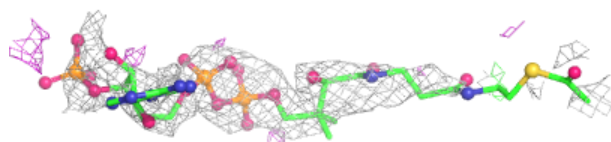
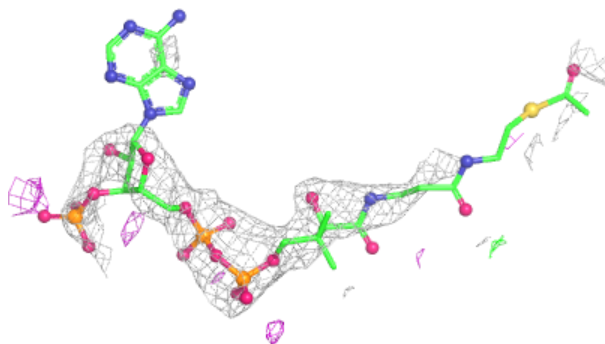
Electron density around ACO A 1002:

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

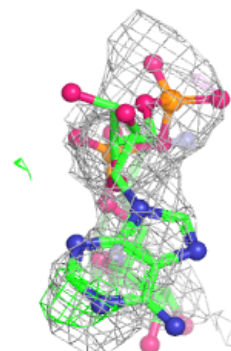
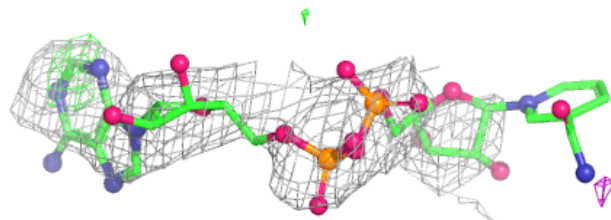
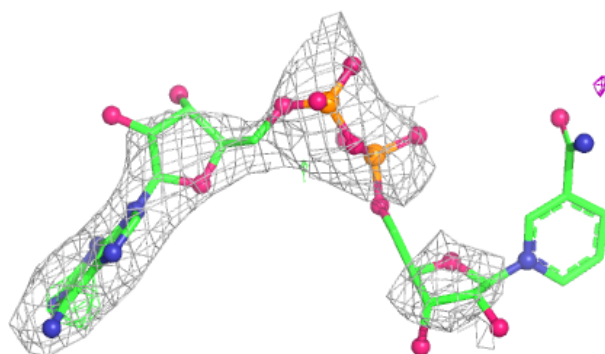


Electron density around ACO C 3001:

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

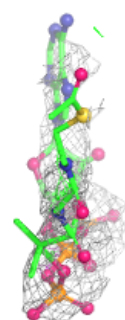
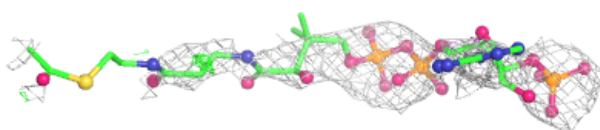
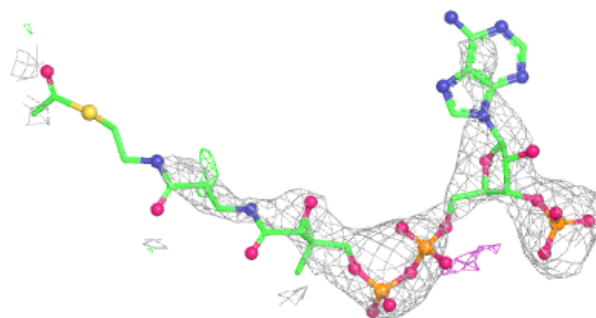
**Electron density around NAD B 2001:**

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

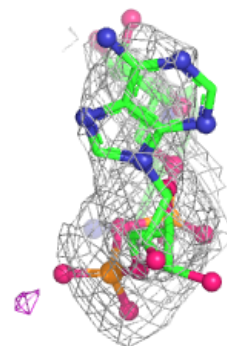
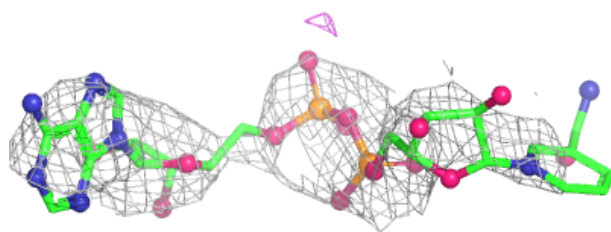
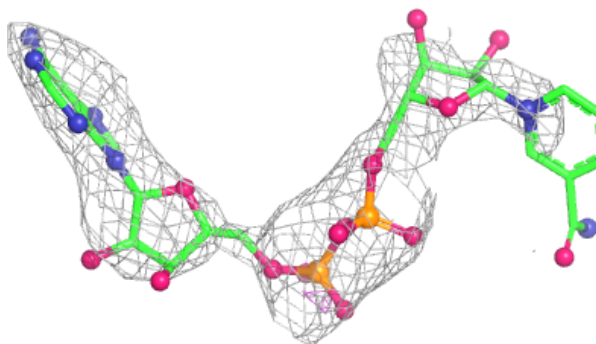


Electron density around ACO D 4001:

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

**Electron density around NAD 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.