



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:23 PM UTC

PDB ID : 2D3T / pdb_00002d3t
Title : Fatty Acid beta-oxidation multienzyme complex from Pseudomonas Fragi, Form V
Authors : Tsuchiya, D.; Shimizu, N.; Ishikawa, M.; Suzuki, Y.; Morikawa, K.
Deposited on : 2005-10-01
Resolution : 3.40 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

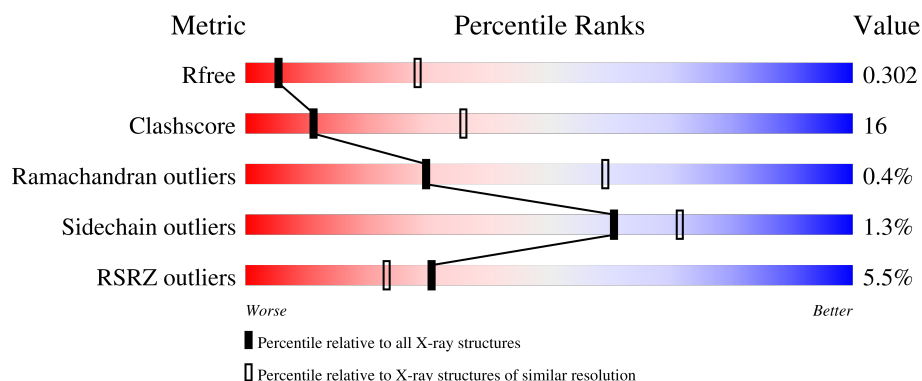
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	8% 62% 36% ..
1	B	715	6% 67% 32% .
2	C	390	3% 67% 31% .
2	D	390	3% 67% 32% .

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 16734 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.

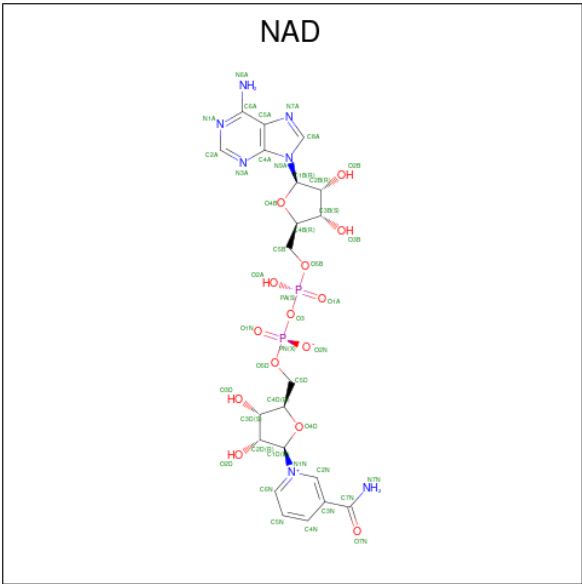
- Molecule 1 is a protein called Fatty oxidation complex alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	708	Total	C	N	O	S	0	0	0
			5368	3429	907	1005	27			
1	B	711	Total	C	N	O	S	0	0	0
			5390	3441	911	1011	27			

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

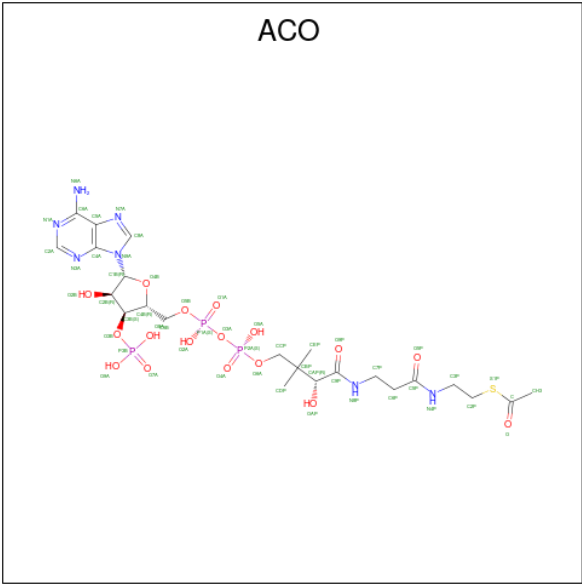
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	390	Total	C	N	O	S	0	0	0
			2893	1801	515	548	29			
2	D	390	Total	C	N	O	S	0	0	0
			2893	1801	515	548	29			

- 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
			44	21	7	14	2		
3	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

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



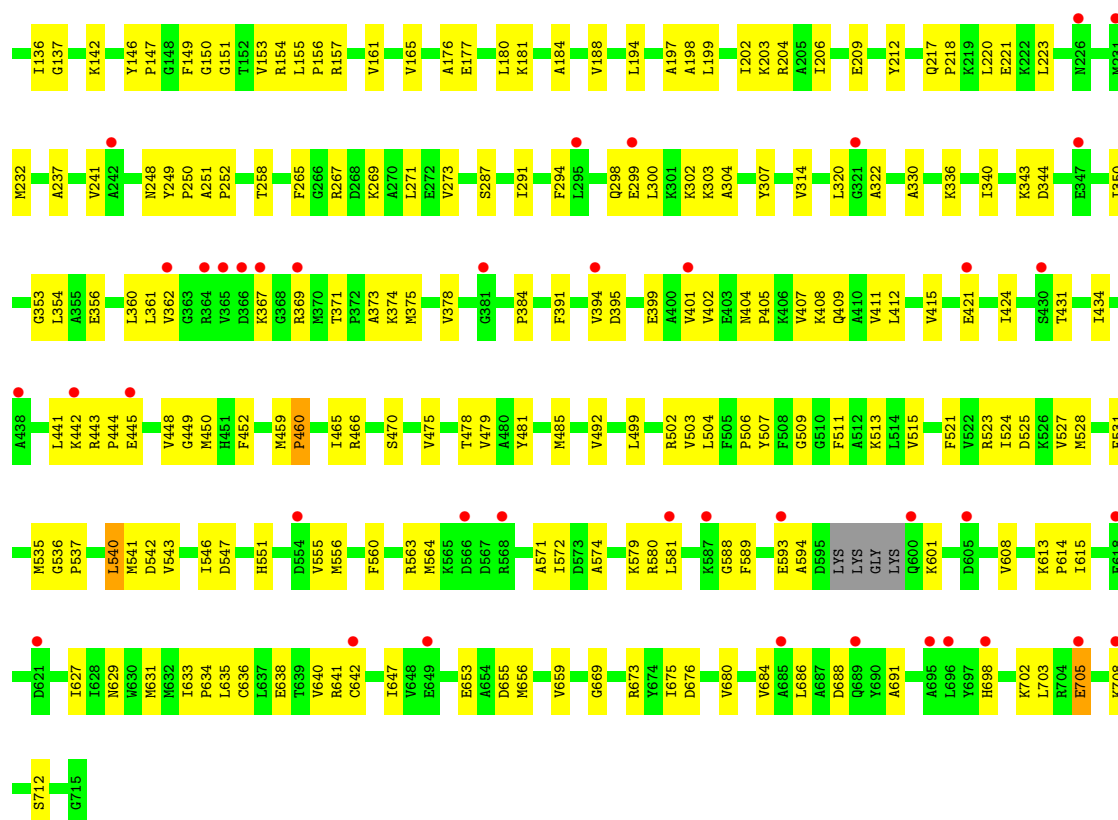
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	C	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
4	D	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		

3 Residue-property plots

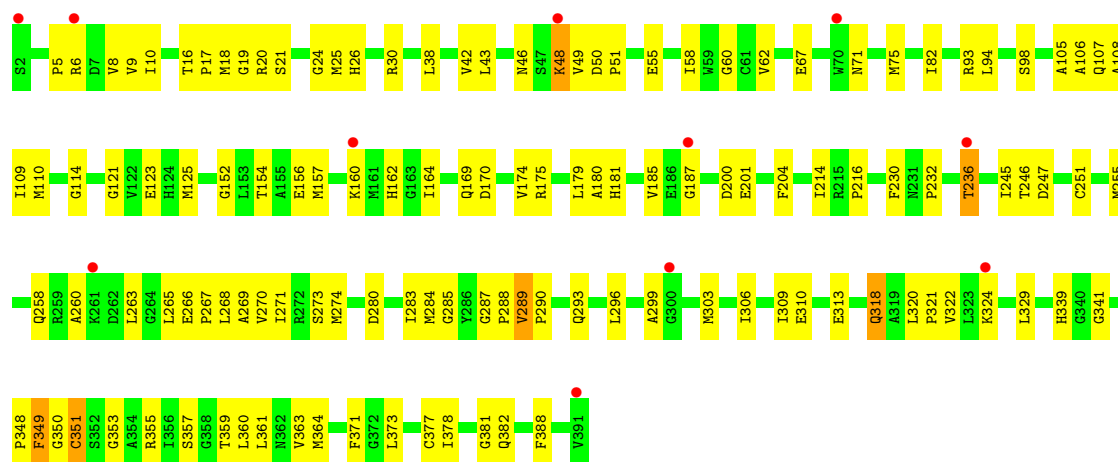
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

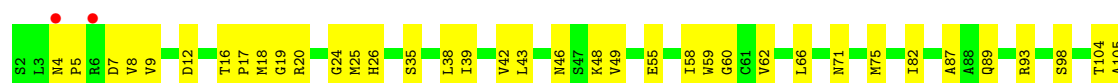


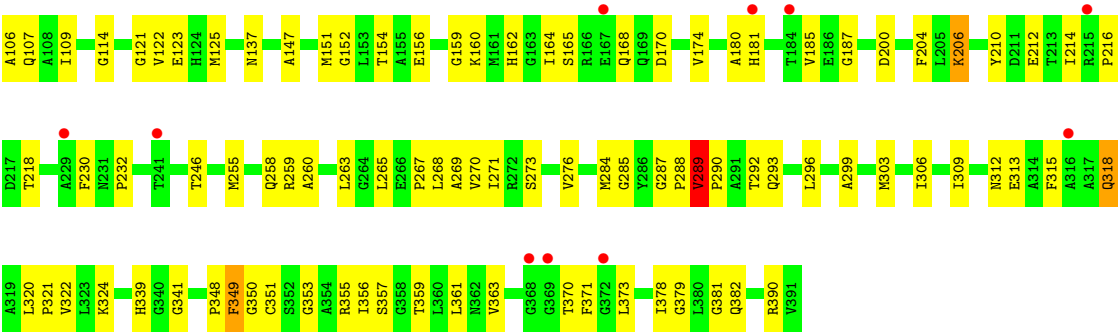


• Molecule 2: 3-ketoacyl-CoA thiolase



• Molecule 2: 3-ketoacyl-CoA thiolase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	95.23Å 137.55Å 198.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.40 15.00 – 3.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (15.00-3.40) 98.0 (15.00-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.29 (at 3.39Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.242 , 0.295 0.259 , 0.302	Depositor DCC
R_{free} test set	2509 reflections (7.00%)	wwPDB-VP
Wilson B-factor (Å ²)	44.0	Xtriage
Anisotropy	0.843	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 14.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	16734	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% 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: ACO, NAD

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	0.29	0/5454	0.80	3/7357 (0.0%)
1	B	0.29	0/5476	0.80	2/7387 (0.0%)
2	C	0.32	0/2941	0.79	2/3967 (0.1%)
2	D	0.31	1/2941 (0.0%)	0.79	2/3967 (0.1%)
All	All	0.30	1/16812 (0.0%)	0.79	9/22678 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	289	VAL	CA-CB	5.05	1.57	1.54

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	249	TYR	CA-C-N	6.84	126.09	118.97
1	A	249	TYR	C-N-CA	6.84	126.09	118.97
1	B	184	ALA	N-CA-C	-5.60	105.70	112.54
2	D	268	LEU	N-CA-C	-5.42	107.31	114.31
1	A	184	ALA	N-CA-C	-5.41	105.95	112.54
2	D	66	LEU	CB-CA-C	-5.37	109.93	117.23
2	C	94	LEU	CB-CA-C	-5.17	110.60	116.54
1	B	589	PHE	N-CA-C	-5.11	105.79	112.23
2	C	268	LEU	N-CA-C	-5.10	107.72	114.04

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	5368	0	5494	191	0
1	B	5390	0	5511	167	0
2	C	2893	0	2903	102	0
2	D	2893	0	2903	103	0
3	A	44	0	26	0	0
3	B	44	0	26	0	0
4	C	51	0	34	0	0
4	D	51	0	34	2	0
All	All	16734	0	16931	550	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 16.

All (550) 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	1.44	0.99
1:A:107:VAL:HG22	1:A:127:PHE:HB2	1.50	0.94
2:D:289:VAL:HG13	2:D:290:PRO:HD3	1.51	0.93
1:B:107:VAL:HG22	1:B:127:PHE:HB2	1.52	0.90
1:A:547:ASP:HB3	1:A:581:LEU:HD22	1.56	0.84
1:B:330:ALA:HA	1:B:340:ILE:HD13	1.60	0.83
1:A:330:ALA:HA	1:A:340:ILE:HD13	1.61	0.82
1:A:113:ILE:HD12	1:A:113:ILE:H	1.45	0.81
2:C:17:PRO:HB2	2:C:25:MET:HE1	1.62	0.81
1:A:525:ASP:HB2	1:A:536:GLY:HA3	1.63	0.80
1:A:64:VAL:HG12	1:A:113:ILE:HD13	1.62	0.80
1:A:371:THR:HB	1:A:374:LYS:HD3	1.63	0.79
2:C:306:ILE:HD13	2:C:373:LEU:HB2	1.65	0.79
1:A:109:ALA:HB1	1:A:194:LEU:HD21	1.66	0.78
2:D:17:PRO:HB2	2:D:25:MET:HE1	1.65	0.77
2:C:263:LEU:HB2	2:C:265:LEU:HD22	1.66	0.77
1:A:372:PRO:HB2	1:B:362:VAL:HG13	1.66	0.76
2:D:62:VAL:HG21	2:D:349:PHE:HB3	1.68	0.76
1:B:547:ASP:HB3	1:B:581:LEU:HD22	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:669:GLY:HA3	1:A:673:ARG:HD2	1.69	0.74
1:B:525:ASP:HB2	1:B:536:GLY:HA3	1.70	0.74
1:A:640:VAL:HG11	1:A:703:LEU:HD12	1.70	0.73
1:A:71:ILE:HD11	1:A:291:ILE:HG23	1.67	0.73
2:C:62:VAL:HG21	2:C:349:PHE:HB3	1.71	0.72
1:B:71:ILE:HD11	1:B:291:ILE:HG23	1.71	0.71
2:D:125:MET:HE2	2:D:348:PRO:HA	1.71	0.71
2:C:125:MET:HE3	2:C:246:THR:H	1.56	0.71
1:A:373:ALA:HA	1:B:362:VAL:HG21	1.73	0.70
2:D:348:PRO:HB2	2:D:351:CYS:HB3	1.72	0.70
2:C:125:MET:HE2	2:C:348:PRO:HA	1.73	0.70
2:D:159:GLY:HA2	2:D:164:ILE:HD13	1.74	0.69
1:B:314:VAL:HG13	1:B:395:ASP:HB2	1.73	0.69
1:B:153:VAL:HG21	1:B:271:LEU:HD23	1.74	0.69
1:A:613:LYS:HB3	1:A:614:PRO:HD3	1.75	0.68
1:A:254:GLU:HG3	1:A:281:LEU:HD21	1.74	0.68
2:D:55:GLU:HG3	2:D:114:GLY:HA2	1.76	0.68
2:C:123:GLU:HB2	2:C:350:GLY:H	1.59	0.68
1:A:364:ARG:HH21	1:A:370:MET:HE3	1.58	0.67
2:C:55:GLU:HG3	2:C:114:GLY:HA2	1.76	0.67
2:D:98:SER:HB3	2:D:353:GLY:HA3	1.77	0.67
2:D:265:LEU:H	2:D:265:LEU:HD23	1.60	0.67
2:D:287:GLY:O	2:D:290:PRO:HD2	1.95	0.67
2:C:287:GLY:O	2:C:290:PRO:HD2	1.95	0.66
1:A:465:ILE:HD12	1:A:465:ILE:H	1.59	0.66
2:D:306:ILE:HD13	2:D:373:LEU:HB2	1.76	0.66
1:A:251:ALA:HB3	1:A:252:PRO:HD3	1.78	0.66
2:D:378:ILE:HB	2:D:382:GLN:HB2	1.77	0.65
1:B:434:ILE:HD13	1:B:465:ILE:HG21	1.78	0.65
1:B:109:ALA:HB1	1:B:194:LEU:HD21	1.77	0.65
1:B:633:ILE:HB	1:B:634:PRO:HD3	1.79	0.65
2:D:263:LEU:HB2	2:D:265:LEU:HD22	1.77	0.65
1:B:251:ALA:HB3	1:B:252:PRO:HD3	1.78	0.64
2:C:313:GLU:CD	2:C:341:GLY:HA3	2.21	0.64
1:B:180:LEU:HD12	1:B:188:VAL:HG23	1.78	0.64
1:A:354:LEU:HD11	1:A:384:PRO:HG2	1.79	0.64
1:B:613:LYS:HB3	1:B:614:PRO:HD3	1.79	0.64
1:A:180:LEU:HD12	1:A:188:VAL:HG23	1.80	0.64
1:A:642:CYS:HA	1:A:647:ILE:HD13	1.79	0.64
2:C:289:VAL:HG23	2:C:293:GLN:HE21	1.63	0.64
1:A:361:LEU:HB3	1:A:375:MET:HG3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:633:ILE:HB	1:A:634:PRO:HD3	1.81	0.63
1:B:7:ALA:HA	1:B:24:LEU:HA	1.79	0.63
2:C:265:LEU:HD23	2:C:265:LEU:H	1.64	0.63
1:A:637:LEU:HB3	1:A:641:ARG:HH12	1.62	0.63
2:C:284:MET:HB3	2:C:381:GLY:H	1.64	0.63
2:C:255:MET:HE1	2:C:263:LEU:HD12	1.80	0.63
2:C:348:PRO:HB2	2:C:351:CYS:HB3	1.80	0.63
2:D:16:THR:HG23	2:D:38:LEU:HD22	1.79	0.63
1:B:503:VAL:HG12	1:B:635:LEU:HG	1.80	0.62
2:D:303:MET:HE1	2:D:373:LEU:HD22	1.80	0.62
1:B:155:LEU:HB3	1:B:156:PRO:HD3	1.80	0.62
1:B:367:LYS:HB3	1:B:369:ARG:HE	1.65	0.62
2:C:5:PRO:HB3	2:C:258:GLN:HB2	1.81	0.62
2:C:156:GLU:O	2:C:160:LYS:HG2	1.99	0.62
1:A:7:ALA:HA	1:A:24:LEU:HA	1.82	0.61
1:B:336:LYS:HG3	1:B:485:MET:HA	1.81	0.61
2:D:359:THR:O	2:D:363:VAL:HG23	2.00	0.61
1:A:155:LEU:HB3	1:A:156:PRO:HD3	1.82	0.61
1:B:535:MET:SD	1:B:543:VAL:HG21	2.41	0.61
2:D:123:GLU:HB2	2:D:350:GLY:H	1.64	0.61
2:C:48:LYS:H	2:C:48:LYS:HD2	1.65	0.61
1:B:640:VAL:HG11	1:B:703:LEU:HD12	1.83	0.60
2:D:48:LYS:H	2:D:48:LYS:HD2	1.64	0.60
2:C:43:LEU:HD11	2:C:82:ILE:HD11	1.83	0.60
1:A:232:MET:HB2	2:C:157:MET:HE1	1.83	0.60
1:A:288:ASN:HD22	1:A:289:CYS:N	1.98	0.60
1:A:350:ILE:HG21	1:A:384:PRO:HB3	1.83	0.60
1:B:705:GLU:HA	1:B:708:LYS:HE2	1.83	0.60
1:A:320:LEU:HD11	1:A:415:VAL:HG21	1.84	0.60
2:D:5:PRO:HB3	2:D:258:GLN:HB2	1.82	0.60
1:A:466:ARG:HD3	1:A:475:VAL:HG21	1.83	0.59
2:D:255:MET:HE1	2:D:263:LEU:HD12	1.85	0.59
2:D:320:LEU:HB2	2:D:321:PRO:HD3	1.85	0.59
1:A:705:GLU:HA	1:A:708:LYS:HE2	1.84	0.59
2:C:107:GLN:HG3	2:C:274:MET:HE1	1.83	0.59
1:A:226:ASN:ND2	1:A:227:ALA:H	2.01	0.59
1:A:307:TYR:HD2	1:A:476:ALA:HA	1.68	0.59
2:C:16:THR:HG23	2:C:38:LEU:HD22	1.84	0.59
1:B:101:ASP:CG	1:B:267:ARG:HH22	2.11	0.58
2:D:273:SER:HB3	2:D:299:ALA:HB2	1.86	0.58
1:A:130:MET:HE2	1:A:176:ALA:HA	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:98:SER:HB3	2:C:353:GLY:HA3	1.86	0.58
2:C:360:LEU:HG	2:C:364:MET:HE2	1.86	0.58
2:D:180:ALA:HA	2:D:339:HIS:O	2.04	0.58
2:D:315:PHE:O	2:D:318:GLN:HG3	2.03	0.58
1:A:393:ASN:H	1:A:393:ASN:HD22	1.52	0.58
1:B:594:ALA:H	1:B:601:LYS:HD3	1.68	0.58
1:B:673:ARG:HB2	1:B:673:ARG:HH11	1.69	0.58
1:A:465:ILE:HA	1:A:492:VAL:O	2.03	0.57
2:D:162:HIS:HB2	2:D:164:ILE:HD11	1.85	0.57
1:B:465:ILE:HA	1:B:492:VAL:O	2.04	0.57
2:D:9:VAL:HG13	2:D:267:PRO:HB3	1.87	0.57
1:B:350:ILE:HG21	1:B:384:PRO:HB3	1.86	0.57
2:C:320:LEU:HB2	2:C:321:PRO:HD3	1.87	0.57
1:A:375:MET:HE2	1:B:375:MET:HE2	1.87	0.57
1:A:404:ASN:H	1:A:408:LYS:HE2	1.70	0.57
1:B:300:LEU:HD11	1:B:656:MET:HG3	1.86	0.56
2:D:292:THR:O	2:D:296:LEU:HG	2.04	0.56
1:B:343:LYS:HD3	1:B:344:ASP:N	2.20	0.56
1:B:511:PHE:HB2	1:B:631:MET:HE1	1.88	0.56
2:C:8:VAL:HG11	2:C:271:ILE:HD12	1.86	0.56
2:C:273:SER:HB3	2:C:299:ALA:HB2	1.87	0.56
2:C:289:VAL:CG1	2:C:290:PRO:HD3	2.29	0.56
1:B:7:ALA:HB2	1:B:24:LEU:HD13	1.88	0.56
2:C:162:HIS:HB2	2:C:164:ILE:HD11	1.87	0.56
2:C:9:VAL:HG13	2:C:267:PRO:HB3	1.88	0.56
1:A:695:ALA:HA	1:A:698:HIS:HD2	1.70	0.56
1:B:593:GLU:HB2	1:B:601:LYS:NZ	2.21	0.56
1:B:655:ASP:O	1:B:659:VAL:HG23	2.06	0.56
1:A:502:ARG:HA	1:A:556:MET:HE2	1.88	0.56
1:A:655:ASP:O	1:A:659:VAL:HG23	2.05	0.56
1:A:680:VAL:HG21	1:A:712:SER:HA	1.87	0.55
1:B:399:GLU:HG2	1:B:401:VAL:HG23	1.87	0.55
2:C:324:LYS:HB2	2:C:329:LEU:HD12	1.89	0.55
1:B:198:ALA:O	1:B:202:ILE:HG12	2.05	0.55
2:C:60:GLY:H	2:C:121:GLY:HA2	1.72	0.55
1:A:434:ILE:HD13	1:A:465:ILE:HG21	1.88	0.55
1:B:411:VAL:O	1:B:415:VAL:HG23	2.07	0.55
2:C:318:GLN:C	2:C:321:PRO:HD2	2.31	0.55
1:A:161:VAL:O	1:A:165:VAL:HG23	2.07	0.55
1:A:399:GLU:HG2	1:A:401:VAL:HG23	1.87	0.55
1:B:442:LYS:HG3	1:B:443:ARG:HG3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:289:VAL:HG23	2:D:293:GLN:HE21	1.72	0.55
1:B:161:VAL:O	1:B:165:VAL:HG23	2.07	0.55
2:C:364:MET:HE1	2:C:388:PHE:HB2	1.89	0.55
2:D:125:MET:HE3	2:D:246:THR:H	1.72	0.55
1:A:521:PHE:HA	1:A:524:ILE:HD12	1.87	0.55
1:B:130:MET:HE2	1:B:176:ALA:HA	1.89	0.54
1:B:465:ILE:HD12	1:B:465:ILE:H	1.73	0.54
1:A:314:VAL:HG13	1:A:395:ASP:HB2	1.90	0.54
1:B:102:LEU:HG	1:B:104:VAL:HG12	1.88	0.54
2:C:98:SER:HB2	2:C:350:GLY:O	2.07	0.54
1:B:475:VAL:O	1:B:479:VAL:HG23	2.08	0.54
2:C:303:MET:HE2	2:C:309:ILE:HD11	1.89	0.54
1:A:258:THR:HG23	1:A:273:VAL:HG12	1.89	0.54
1:B:421:GLU:HA	1:B:443:ARG:NH2	2.23	0.54
1:B:636:CYS:O	1:B:640:VAL:HG23	2.08	0.54
1:A:388:TYR:HE2	1:A:415:VAL:HG22	1.73	0.53
2:D:98:SER:HB2	2:D:350:GLY:O	2.08	0.53
2:D:151:MET:HE3	4:D:1004:ACO:H21	1.90	0.53
1:B:119:LEU:HD12	1:B:137:GLY:N	2.24	0.53
1:B:322:ALA:HB1	1:B:353:GLY:HA3	1.89	0.53
2:D:339:HIS:CD2	2:D:363:VAL:HG22	2.43	0.53
1:A:411:VAL:O	1:A:415:VAL:HG23	2.09	0.53
1:A:461:LEU:HD22	1:A:657:GLY:O	2.09	0.53
2:D:98:SER:HB3	2:D:353:GLY:CA	2.38	0.53
1:B:502:ARG:HA	1:B:556:MET:HE2	1.90	0.53
2:C:378:ILE:HB	2:C:382:GLN:HB2	1.91	0.53
2:D:339:HIS:HD2	2:D:363:VAL:HG22	1.74	0.53
1:A:322:ALA:HB1	1:A:353:GLY:HA3	1.90	0.53
1:A:640:VAL:O	1:A:644:GLU:HG3	2.08	0.53
2:D:58:ILE:HD12	2:D:105:ALA:HB2	1.91	0.53
2:D:60:GLY:H	2:D:121:GLY:HA2	1.73	0.53
1:B:220:LEU:HD21	1:B:267:ARG:HH21	1.74	0.53
1:A:680:VAL:O	1:A:684:VAL:HG23	2.08	0.53
2:C:359:THR:O	2:C:363:VAL:HG23	2.09	0.53
1:B:507:TYR:CE1	1:B:631:MET:HB3	2.44	0.52
2:C:303:MET:HE1	2:C:373:LEU:HD22	1.90	0.52
2:D:43:LEU:HD11	2:D:82:ILE:HD11	1.91	0.52
2:C:284:MET:HE3	2:C:285:GLY:N	2.24	0.52
1:B:424:ILE:HD12	1:B:424:ILE:N	2.25	0.52
2:C:318:GLN:O	2:C:322:VAL:HG23	2.10	0.52
1:B:542:ASP:OD1	1:B:588:GLY:HA3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:20:ARG:NH1	2:D:212:GLU:HB3	2.25	0.52
1:A:537:PRO:HG2	1:A:631:MET:HE2	1.91	0.52
2:C:260:ALA:HA	2:C:265:LEU:HD21	1.92	0.52
1:B:571:ALA:HA	1:B:615:ILE:HG13	1.91	0.52
1:A:636:CYS:O	1:A:640:VAL:HG23	2.10	0.52
2:C:313:GLU:OE1	2:C:341:GLY:HA3	2.08	0.52
2:D:318:GLN:O	2:D:322:VAL:HG23	2.09	0.52
2:D:318:GLN:C	2:D:321:PRO:HD2	2.34	0.52
1:A:380:ASN:HB3	1:B:354:LEU:HD13	1.92	0.52
1:A:249:TYR:OH	1:A:666:LEU:HB2	2.10	0.51
2:C:180:ALA:HA	2:C:339:HIS:O	2.10	0.51
1:A:499:LEU:O	1:A:503:VAL:HG23	2.09	0.51
1:B:536:GLY:O	1:B:540:LEU:HB2	2.10	0.51
1:A:38:ASN:O	1:A:41:ARG:HB3	2.10	0.51
1:A:424:ILE:HD12	1:A:424:ILE:N	2.24	0.51
1:A:593:GLU:H	1:A:593:GLU:CD	2.19	0.51
1:B:202:ILE:HG22	1:B:206:ILE:HD11	1.93	0.51
1:B:105:PRO:HG3	1:B:212:TYR:CD2	2.45	0.51
2:C:8:VAL:HG21	2:C:106:ALA:HB1	1.93	0.51
1:B:265:PHE:HB3	1:B:269:LYS:HB2	1.91	0.51
1:A:249:TYR:O	1:A:252:PRO:HD2	2.10	0.51
1:A:568:ARG:HD2	1:A:617:TYR:HE1	1.76	0.51
1:B:680:VAL:O	1:B:684:VAL:HG23	2.11	0.51
2:C:200:ASP:OD2	2:C:204:PHE:HB2	2.10	0.51
1:B:10:VAL:HG22	1:B:20:LEU:HG	1.93	0.51
1:A:204:ARG:O	1:A:209:GLU:HB3	2.11	0.51
1:A:150:GLY:HA3	1:A:154:ARG:NH1	2.26	0.50
2:C:10:ILE:HD11	2:C:271:ILE:HG13	1.93	0.50
2:C:361:LEU:HA	2:C:364:MET:HE3	1.93	0.50
2:D:8:VAL:HG11	2:D:271:ILE:HD12	1.92	0.50
2:D:306:ILE:HA	2:D:371:PHE:HB2	1.92	0.50
1:A:336:LYS:HG3	1:A:485:MET:HA	1.94	0.50
1:A:449:GLY:HA3	1:A:465:ILE:HB	1.93	0.50
1:A:699:PRO:HB3	1:A:703:LEU:HD22	1.94	0.50
1:B:523:ARG:O	1:B:527:VAL:HG23	2.11	0.50
1:B:551:HIS:O	1:B:555:VAL:HG23	2.11	0.50
2:C:38:LEU:O	2:C:42:VAL:HG23	2.12	0.50
2:C:105:ALA:O	2:C:109:ILE:HG13	2.11	0.50
2:D:62:VAL:CG2	2:D:349:PHE:HB3	2.40	0.50
1:B:546:ILE:HD12	1:B:546:ILE:H	1.76	0.50
2:D:16:THR:HG22	2:D:38:LEU:HD13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:48:LYS:HD2	2:D:48:LYS:N	2.25	0.50
2:D:164:ILE:HD12	2:D:164:ILE:N	2.26	0.50
1:A:343:LYS:HD3	1:A:344:ASP:N	2.27	0.50
1:A:551:HIS:O	1:A:555:VAL:HG23	2.10	0.50
1:B:304:ALA:HA	1:B:307:TYR:HD1	1.76	0.50
1:A:571:ALA:HA	1:A:615:ILE:HG13	1.93	0.50
1:B:114:ALA:HB3	1:B:136:ILE:HG22	1.92	0.50
1:B:492:VAL:HG13	1:B:647:ILE:CG2	2.42	0.50
2:D:12:ASP:CB	2:D:46:ASN:HD21	2.24	0.50
1:A:217:GLN:HB3	1:A:218:PRO:HD3	1.93	0.49
1:A:405:PRO:HA	1:A:437:LEU:HD21	1.93	0.49
1:B:465:ILE:HD12	1:B:465:ILE:N	2.27	0.49
2:C:30:ARG:HD3	2:D:137:ASN:ND2	2.26	0.49
2:C:125:MET:HE3	2:C:246:THR:N	2.25	0.49
2:C:21:SER:OG	2:C:245:ILE:HG22	2.12	0.49
1:A:105:PRO:HG3	1:A:212:TYR:CD2	2.48	0.49
1:A:445:GLU:CD	1:A:445:GLU:H	2.20	0.49
1:A:466:ARG:HG3	1:A:470:SER:HB2	1.95	0.49
1:B:204:ARG:O	1:B:209:GLU:HB3	2.13	0.49
1:B:269:LYS:O	1:B:273:VAL:HG23	2.12	0.49
2:C:21:SER:HA	2:C:247:ASP:OD2	2.12	0.49
1:A:40:LEU:HD23	1:A:44:VAL:HG23	1.94	0.49
1:B:367:LYS:HB3	1:B:369:ARG:NE	2.28	0.49
1:B:580:ARG:NH2	1:B:608:VAL:HG22	2.27	0.49
1:B:150:GLY:HA3	1:B:154:ARG:NH1	2.27	0.49
1:B:563:ARG:HH12	1:B:564:MET:HE2	1.77	0.49
2:C:42:VAL:HG21	2:C:251:CYS:HB3	1.94	0.49
1:B:330:ALA:HA	1:B:340:ILE:HG21	1.94	0.49
2:D:313:GLU:CD	2:D:341:GLY:HA3	2.37	0.49
2:D:25:MET:HE2	2:D:26:HIS:CE1	2.47	0.49
1:A:31:LYS:HB2	1:A:69:ALA:HA	1.95	0.49
1:A:119:LEU:HD12	1:A:137:GLY:N	2.27	0.49
1:A:288:ASN:HD22	1:A:289:CYS:H	1.59	0.49
1:B:147:PRO:HB3	1:B:151:GLY:HA3	1.95	0.49
2:C:93:ARG:HH12	2:D:87:ALA:HB1	1.77	0.49
2:C:164:ILE:N	2:C:164:ILE:HD12	2.27	0.49
2:D:123:GLU:HG2	2:D:349:PHE:HB2	1.95	0.49
1:A:542:ASP:OD1	1:A:588:GLY:HA3	2.13	0.48
2:D:8:VAL:O	2:D:270:VAL:HG13	2.14	0.48
1:A:97:SER:HB3	1:A:267:ARG:NH1	2.28	0.48
1:A:393:ASN:HD22	1:A:393:ASN:N	2.10	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:676:ASP:OD2	1:A:712:SER:HB2	2.13	0.48
1:B:638:GLU:HA	1:B:641:ARG:HH11	1.77	0.48
1:A:269:LYS:O	1:A:273:VAL:HG23	2.13	0.48
1:A:416:GLU:OE1	1:A:442:LYS:HG2	2.13	0.48
1:A:330:ALA:HA	1:A:340:ILE:HG21	1.95	0.48
1:A:40:LEU:O	1:A:44:VAL:HG23	2.13	0.48
1:A:146:TYR:HB2	1:A:147:PRO:HD2	1.96	0.48
1:B:199:LEU:HD11	1:B:203:LYS:HE3	1.94	0.48
1:A:202:ILE:O	1:A:206:ILE:HG13	2.14	0.48
1:A:288:ASN:HA	1:A:291:ILE:HD12	1.96	0.48
1:A:508:PHE:HZ	1:A:540:LEU:HD22	1.77	0.48
1:B:97:SER:HB3	1:B:267:ARG:NH1	2.29	0.48
1:B:371:THR:HG22	1:B:373:ALA:H	1.79	0.48
2:D:259:ARG:NH2	2:D:263:LEU:HD21	2.28	0.48
2:D:260:ALA:HA	2:D:265:LEU:HD21	1.96	0.48
1:A:22:PHE:CD2	1:A:66:ILE:HD11	2.49	0.47
1:A:202:ILE:HG22	1:A:206:ILE:HD11	1.96	0.47
1:A:504:LEU:O	1:A:507:TYR:HB3	2.14	0.47
2:C:280:ASP:HB2	2:C:283:ILE:HG12	1.96	0.47
2:D:206:LYS:HB2	2:D:206:LYS:NZ	2.28	0.47
1:A:127:PHE:CD2	1:A:201:LEU:HD21	2.49	0.47
1:B:354:LEU:HD21	1:B:384:PRO:HG3	1.95	0.47
1:B:521:PHE:HA	1:B:524:ILE:HD12	1.94	0.47
1:A:443:ARG:N	1:A:444:PRO:HD3	2.29	0.47
1:B:110:ILE:HB	1:B:130:MET:HG3	1.95	0.47
1:B:594:ALA:N	1:B:601:LYS:HD3	2.29	0.47
2:D:93:ARG:NH1	2:D:276:VAL:HG11	2.30	0.47
2:D:289:VAL:CG1	2:D:290:PRO:HD3	2.35	0.47
1:B:299:GLU:O	1:B:303:LYS:HG2	2.15	0.47
1:A:198:ALA:O	1:A:202:ILE:HG12	2.15	0.47
2:D:18:MET:HB3	2:D:246:THR:HG21	1.96	0.47
1:B:504:LEU:O	1:B:507:TYR:HB3	2.15	0.47
2:D:214:ILE:O	2:D:216:PRO:HD3	2.15	0.47
1:A:113:ILE:HG22	1:A:115:LEU:HG	1.97	0.47
1:A:147:PRO:HB3	1:A:151:GLY:HA3	1.96	0.47
1:A:475:VAL:O	1:A:479:VAL:HG23	2.13	0.47
1:B:120:GLU:CD	1:B:149:PHE:HB2	2.40	0.47
2:C:214:ILE:O	2:C:216:PRO:HD3	2.15	0.47
2:D:105:ALA:O	2:D:109:ILE:HG13	2.14	0.47
1:B:248:ASN:O	1:B:250:PRO:HD3	2.14	0.47
1:A:678:ILE:HG21	1:A:686:LEU:HD11	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:LEU:HD11	1:B:19:GLU:HB2	1.98	0.46
1:B:202:ILE:O	1:B:206:ILE:HG13	2.16	0.46
1:A:60:SER:HB3	1:A:111:ASN:OD1	2.16	0.46
1:A:691:ALA:HB1	1:A:698:HIS:CE1	2.50	0.46
2:C:108:ALA:HA	2:D:107:GLN:OE1	2.16	0.46
2:C:288:PRO:HB2	2:C:322:VAL:HG11	1.97	0.46
2:D:59:TRP:HE1	2:D:122:VAL:CG1	2.28	0.46
2:D:165:SER:HG	2:D:168:GLN:HG3	1.80	0.46
1:A:150:GLY:HA3	1:A:154:ARG:HH12	1.80	0.46
1:B:691:ALA:HB1	1:B:698:HIS:NE2	2.30	0.46
2:C:125:MET:CE	2:C:246:THR:H	2.27	0.46
2:D:218:THR:HG23	4:D:1004:ACO:H61A	1.80	0.46
1:A:13:LEU:HD11	1:A:19:GLU:HB2	1.98	0.46
1:A:393:ASN:HA	1:A:420:ARG:NH1	2.30	0.46
1:B:669:GLY:HA3	1:B:673:ARG:HD2	1.97	0.46
1:B:673:ARG:HB2	1:B:673:ARG:NH1	2.30	0.46
2:C:296:LEU:HD21	2:C:306:ILE:HD11	1.96	0.46
1:A:32:PHE:CE1	1:A:66:ILE:HG21	2.50	0.46
1:A:373:ALA:HB2	1:B:362:VAL:HG11	1.97	0.46
2:C:8:VAL:O	2:C:270:VAL:HG13	2.16	0.46
2:C:18:MET:HB3	2:C:246:THR:HG21	1.98	0.46
1:A:649:GLU:HB3	1:A:653:GLU:OE1	2.16	0.46
1:B:499:LEU:O	1:B:503:VAL:HG23	2.16	0.46
2:C:152:GLY:HA3	2:C:230:PHE:CE2	2.51	0.46
1:A:391:PHE:HA	1:A:394:VAL:HG23	1.98	0.46
1:A:406:LYS:HE2	1:A:406:LYS:HA	1.97	0.46
1:B:445:GLU:CD	1:B:445:GLU:H	2.23	0.46
2:D:8:VAL:HG21	2:D:106:ALA:HB1	1.97	0.46
1:A:2:ILE:HD12	1:A:18:VAL:HG21	1.97	0.45
1:A:119:LEU:HD23	1:A:123:LEU:HG	1.97	0.45
1:A:284:THR:C	1:A:286:ALA:H	2.24	0.45
1:B:537:PRO:HG2	1:B:631:MET:HE2	1.99	0.45
2:D:59:TRP:HE1	2:D:122:VAL:HG12	1.81	0.45
2:D:200:ASP:OD2	2:D:204:PHE:HB2	2.15	0.45
1:A:407:VAL:O	1:A:411:VAL:HG23	2.15	0.45
1:B:75:VAL:HG12	1:B:79:LYS:HE3	1.98	0.45
1:B:560:PHE:HB2	1:B:564:MET:HE3	1.98	0.45
2:C:30:ARG:NH1	2:C:67:GLU:HG2	2.32	0.45
2:D:58:ILE:HD13	2:D:104:THR:HB	1.98	0.45
1:A:647:ILE:N	1:A:647:ILE:HD12	2.31	0.45
2:D:284:MET:HB3	2:D:381:GLY:H	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:VAL:HG21	1:A:256:ILE:HD11	1.99	0.45
1:B:157:ARG:HG2	1:B:223:LEU:HD23	1.98	0.45
1:B:434:ILE:HD12	1:B:434:ILE:N	2.31	0.45
2:C:201:GLU:CD	2:C:201:GLU:H	2.25	0.45
2:D:19:GLY:O	2:D:246:THR:HG23	2.16	0.45
1:A:523:ARG:O	1:A:527:VAL:HG23	2.16	0.45
1:B:594:ALA:O	1:B:601:LYS:HB3	2.16	0.45
2:D:35:SER:O	2:D:39:ILE:HG13	2.17	0.45
1:A:465:ILE:HG12	1:A:498:PHE:CE2	2.52	0.45
1:A:681:ALA:HA	1:A:707:ALA:HB1	1.99	0.45
1:B:258:THR:HG23	1:B:273:VAL:HG12	1.99	0.45
1:B:459:MET:HA	1:B:460:PRO:HD3	1.77	0.45
2:C:46:ASN:O	2:C:49:VAL:HG22	2.15	0.45
2:D:20:ARG:O	2:D:24:GLY:HA3	2.17	0.45
1:A:613:LYS:HE2	1:A:613:LYS:HA	1.98	0.45
1:A:347:GLU:O	1:A:351:GLU:HG2	2.17	0.45
1:B:320:LEU:HD11	1:B:415:VAL:HG21	1.98	0.45
1:B:546:ILE:HD12	1:B:546:ILE:N	2.32	0.45
2:C:98:SER:HB3	2:C:353:GLY:CA	2.47	0.45
2:D:156:GLU:O	2:D:160:LYS:HG2	2.17	0.45
1:B:580:ARG:CZ	1:B:608:VAL:HG22	2.48	0.44
1:B:391:PHE:HA	1:B:394:VAL:HG23	1.99	0.44
1:B:443:ARG:N	1:B:444:PRO:HD3	2.31	0.44
2:C:10:ILE:HD12	2:C:10:ILE:N	2.31	0.44
1:A:257:LYS:O	1:A:261:LYS:HG3	2.18	0.44
1:B:703:LEU:HD23	1:B:703:LEU:O	2.17	0.44
1:A:497:GLY:O	1:A:501:ASN:HB2	2.18	0.44
2:C:20:ARG:O	2:C:24:GLY:HA3	2.16	0.44
2:C:58:ILE:HD12	2:C:105:ALA:HB2	1.98	0.44
2:C:306:ILE:HA	2:C:371:PHE:HB2	1.99	0.44
1:A:546:ILE:HD12	1:A:546:ILE:N	2.32	0.44
1:A:574:ALA:HB2	1:A:615:ILE:HD11	1.99	0.44
1:B:401:VAL:HG12	1:B:402:VAL:N	2.32	0.44
1:B:431:THR:HB	1:B:555:VAL:HG21	1.99	0.44
2:D:170:ASP:O	2:D:174:VAL:HG23	2.18	0.44
2:D:4:ASN:HB2	2:D:7:ASP:OD1	2.17	0.44
2:D:38:LEU:O	2:D:42:VAL:HG23	2.16	0.44
1:A:361:LEU:O	1:A:365:VAL:HG23	2.18	0.44
1:B:177:GLU:HG2	1:B:181:LYS:HE3	2.00	0.44
2:C:19:GLY:O	2:C:246:THR:HG23	2.18	0.44
2:C:154:THR:OG1	2:C:284:MET:HE2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:269:ALA:CB	2:C:361:LEU:HD22	2.48	0.44
1:B:142:LYS:HB3	1:B:294:PHE:CE2	2.53	0.44
1:B:371:THR:HB	1:B:374:LYS:HG3	2.00	0.44
1:B:642:CYS:O	1:B:647:ILE:HB	2.17	0.44
2:C:71:ASN:O	2:C:75:MET:HG2	2.18	0.44
1:B:197:ALA:HA	2:C:204:PHE:CE2	2.53	0.44
1:B:361:LEU:HB3	1:B:375:MET:HG3	1.99	0.44
1:B:702:LYS:HD2	1:B:702:LYS:O	2.18	0.43
1:A:10:VAL:HG22	1:A:20:LEU:HG	1.99	0.43
1:B:40:LEU:O	1:B:44:VAL:HG23	2.18	0.43
2:D:151:MET:HE1	2:D:379:GLY:CA	2.48	0.43
1:A:623:THR:O	1:A:627:ILE:HG13	2.18	0.43
1:B:676:ASP:OD2	1:B:712:SER:HB2	2.19	0.43
2:C:93:ARG:NH1	2:D:87:ALA:HB1	2.33	0.43
2:C:288:PRO:HD3	2:C:377:CYS:HB3	2.00	0.43
2:D:152:GLY:HA3	2:D:230:PHE:CE2	2.53	0.43
1:B:217:GLN:HG3	1:B:221:GLU:OE1	2.19	0.43
1:B:407:VAL:O	1:B:411:VAL:HG23	2.18	0.43
1:B:503:VAL:C	1:B:506:PRO:HD2	2.44	0.43
2:D:125:MET:CE	2:D:246:THR:H	2.31	0.43
1:A:520:ASP:O	1:A:524:ILE:HG13	2.18	0.43
1:B:43:ALA:O	1:B:47:ILE:HG13	2.17	0.43
2:C:164:ILE:HD11	2:C:321:PRO:HG3	2.00	0.43
2:C:265:LEU:H	2:C:265:LEU:CD2	2.29	0.43
1:A:147:PRO:HB2	1:A:152:THR:HG23	2.00	0.43
1:A:226:ASN:HD22	1:A:227:ALA:H	1.66	0.43
1:B:117:GLY:HA2	1:B:120:GLU:OE1	2.19	0.43
1:B:405:PRO:O	1:B:409:GLN:HG3	2.18	0.43
1:B:528:MET:O	1:B:531:PHE:HB3	2.18	0.43
2:C:19:GLY:H	2:C:246:THR:CG2	2.31	0.43
2:C:93:ARG:CZ	2:D:89:GLN:HB3	2.48	0.43
1:A:226:ASN:ND2	1:A:227:ALA:N	2.66	0.43
1:B:146:TYR:HB2	1:B:147:PRO:HD2	2.01	0.43
1:B:374:LYS:O	1:B:378:VAL:HG23	2.19	0.43
1:B:412:LEU:HB3	1:B:441:LEU:HD21	2.01	0.43
1:B:511:PHE:O	1:B:515:VAL:HG23	2.19	0.43
1:B:574:ALA:HB2	1:B:615:ILE:HD11	2.00	0.43
2:C:181:HIS:O	2:C:185:VAL:HG23	2.18	0.43
1:A:40:LEU:HD23	1:A:40:LEU:O	2.19	0.43
1:A:113:ILE:H	1:A:113:ILE:CD1	2.22	0.43
1:A:310:ILE:O	1:A:473:LEU:HG	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:580:ARG:NH1	1:A:587:LYS:HB3	2.33	0.43
1:B:249:TYR:O	1:B:252:PRO:HD2	2.19	0.43
1:B:343:LYS:HB2	1:B:391:PHE:HZ	1.84	0.43
2:C:266:GLU:HA	2:C:267:PRO:HD3	1.92	0.43
2:C:310:GLU:HG3	2:C:360:LEU:HB2	2.01	0.43
1:A:317:ALA:O	1:A:340:ILE:HA	2.18	0.43
1:B:267:ARG:O	1:B:271:LEU:HG	2.19	0.43
1:B:523:ARG:NH2	1:B:627:ILE:HD11	2.34	0.43
2:C:175:ARG:NH1	2:C:179:LEU:HD11	2.33	0.43
2:C:339:HIS:CE1	2:C:363:VAL:HG22	2.54	0.43
2:D:20:ARG:CZ	2:D:212:GLU:HB3	2.49	0.43
2:D:269:ALA:CB	2:D:361:LEU:HD22	2.49	0.43
1:A:153:VAL:HG21	1:A:271:LEU:HD23	2.01	0.43
1:A:297:ASP:OD2	1:A:301:LYS:HE3	2.19	0.43
1:A:332:GLN:OE1	1:A:457:HIS:HA	2.19	0.43
1:A:448:VAL:HG21	1:A:478:THR:OG1	2.19	0.43
1:A:618:GLU:CD	1:A:618:GLU:H	2.27	0.43
1:A:658:LEU:O	1:A:662:ILE:HG22	2.18	0.43
1:A:688:ASP:HA	1:A:691:ALA:HB2	2.01	0.43
1:B:466:ARG:HD3	1:B:475:VAL:HG21	2.00	0.43
2:D:122:VAL:HG22	2:D:123:GLU:N	2.34	0.43
2:D:165:SER:OG	2:D:168:GLN:HG3	2.19	0.43
2:D:303:MET:HE2	2:D:309:ILE:HD11	2.00	0.43
1:A:3:TYR:HE1	1:A:42:GLN:HE21	1.66	0.42
1:A:40:LEU:HD22	1:A:95:ILE:HG22	2.01	0.42
1:A:55:GLY:HA2	1:A:104:VAL:HG22	2.01	0.42
1:A:234:PHE:O	1:A:238:LYS:HG3	2.19	0.42
1:A:434:ILE:N	1:A:434:ILE:HD12	2.34	0.42
1:B:629:ASN:HB3	1:B:633:ILE:HD11	2.00	0.42
2:D:19:GLY:H	2:D:246:THR:CG2	2.31	0.42
1:B:541:MET:HE2	1:B:572:ILE:HG12	2.00	0.42
2:C:25:MET:HE2	2:C:26:HIS:CE1	2.53	0.42
1:A:56:VAL:HB	1:A:106:THR:HG22	2.01	0.42
1:B:287:SER:O	1:B:291:ILE:HG13	2.20	0.42
1:B:492:VAL:HG13	1:B:647:ILE:HG23	2.00	0.42
2:D:17:PRO:HB3	2:D:210:TYR:O	2.19	0.42
2:D:71:ASN:O	2:D:75:MET:HG2	2.19	0.42
2:D:284:MET:HE3	2:D:285:GLY:N	2.34	0.42
1:A:325:MET:O	1:A:329:ILE:HG13	2.20	0.42
1:B:450:MET:HG2	1:B:452:PHE:CE1	2.55	0.42
2:D:181:HIS:O	2:D:185:VAL:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:LYS:HB2	1:A:280:LYS:NZ	2.34	0.42
1:A:515:VAL:HG11	1:A:571:ALA:HB2	2.02	0.42
2:D:46:ASN:O	2:D:49:VAL:HG22	2.20	0.42
1:A:401:VAL:HG12	1:A:402:VAL:N	2.35	0.42
1:A:442:LYS:HG3	1:A:443:ARG:HG3	2.01	0.42
1:A:502:ARG:HA	1:A:556:MET:CE	2.49	0.42
1:B:404:ASN:H	1:B:408:LYS:HE2	1.84	0.42
1:B:450:MET:HE1	1:B:481:TYR:CD2	2.55	0.42
1:A:126:ASP:OD1	1:A:216:ARG:HB2	2.20	0.42
1:A:364:ARG:NH2	1:A:370:MET:HE3	2.29	0.42
2:C:287:GLY:N	2:C:288:PRO:CD	2.82	0.42
2:D:287:GLY:N	2:D:288:PRO:CD	2.83	0.42
2:D:370:THR:HA	2:D:390:ARG:HB2	2.00	0.42
1:B:130:MET:CE	1:B:176:ALA:HA	2.49	0.42
1:A:300:LEU:HD21	1:A:653:GLU:HG2	2.02	0.42
1:A:402:VAL:HG12	1:A:403:GLU:N	2.35	0.42
1:A:502:ARG:HD3	1:A:642:CYS:SG	2.60	0.42
1:A:632:MET:HE1	1:A:664:PHE:CE1	2.55	0.42
2:D:287:GLY:C	2:D:290:PRO:HD2	2.44	0.42
1:A:40:LEU:HD22	1:A:95:ILE:CG2	2.50	0.41
1:B:525:ASP:CB	1:B:536:GLY:HA3	2.45	0.41
1:A:450:MET:HE3	1:A:478:THR:CG2	2.50	0.41
1:A:586:GLY:HA2	1:A:592:TYR:HB2	2.02	0.41
1:B:466:ARG:HG3	1:B:470:SER:HB2	2.02	0.41
1:A:539:TYR:O	1:A:543:VAL:HG23	2.20	0.41
1:B:232:MET:HG2	2:D:147:ALA:HB3	2.02	0.41
1:A:288:ASN:ND2	1:A:288:ASN:N	2.67	0.41
2:C:48:LYS:HD2	2:C:48:LYS:N	2.33	0.41
2:C:287:GLY:C	2:C:290:PRO:HD2	2.45	0.41
2:D:348:PRO:O	2:D:349:PHE:C	2.63	0.41
1:A:7:ALA:HB2	1:A:24:LEU:HD13	2.02	0.41
1:A:499:LEU:HD13	1:A:499:LEU:C	2.45	0.41
1:A:672:LEU:HD22	1:A:713:PHE:CE2	2.56	0.41
1:B:151:GLY:C	1:B:153:VAL:H	2.28	0.41
1:A:199:LEU:HD11	1:A:203:LYS:HE3	2.02	0.41
1:A:350:ILE:CG2	1:A:384:PRO:HB3	2.47	0.41
1:A:450:MET:HG2	1:A:452:PHE:CE1	2.55	0.41
1:B:298:GLN:O	1:B:302:LYS:HG3	2.20	0.41
1:B:300:LEU:CD2	1:B:653:GLU:HG2	2.50	0.41
1:B:579:LYS:HD2	1:B:579:LYS:N	2.35	0.41
2:D:312:ASN:HB2	2:D:356:ILE:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:ASP:O	1:A:86:ILE:HG13	2.21	0.41
1:A:146:TYR:OH	1:A:277:GLY:HA3	2.21	0.41
1:A:579:LYS:HE2	1:A:579:LYS:HA	2.02	0.41
1:B:217:GLN:HB3	1:B:218:PRO:HD3	2.03	0.41
1:B:499:LEU:HD13	1:B:499:LEU:C	2.46	0.41
1:B:636:CYS:HB3	1:B:675:ILE:HD11	2.03	0.41
1:B:350:ILE:CG2	1:B:384:PRO:HB3	2.49	0.41
2:C:169:GLN:HE22	2:C:236:THR:HB	1.85	0.41
1:A:286:ALA:O	1:A:290:LEU:HG	2.21	0.41
1:A:396:LEU:HA	1:A:424:ILE:O	2.21	0.41
1:A:452:PHE:HZ	1:A:485:MET:HE1	1.85	0.41
1:A:511:PHE:O	1:A:515:VAL:HG23	2.21	0.41
1:B:204:ARG:HH11	1:B:204:ARG:HG2	1.86	0.41
1:B:448:VAL:HG21	1:B:478:THR:OG1	2.21	0.41
1:B:509:GLY:O	1:B:513:LYS:HG3	2.20	0.41
2:C:106:ALA:O	2:C:110:MET:HG3	2.21	0.41
2:C:170:ASP:O	2:C:174:VAL:HG23	2.20	0.41
2:D:356:ILE:HG13	2:D:357:SER:N	2.36	0.41
1:B:22:PHE:CD2	1:B:66:ILE:HD11	2.57	0.41
1:B:356:GLU:O	1:B:360:LEU:HG	2.21	0.41
2:D:154:THR:OG1	2:D:284:MET:HE2	2.21	0.41
1:A:288:ASN:HD22	1:A:288:ASN:N	2.19	0.40
1:A:301:LYS:O	1:A:304:ALA:HB3	2.20	0.40
1:A:471:SER:O	1:A:475:VAL:HG23	2.20	0.40
1:A:492:VAL:HG13	1:A:647:ILE:CG2	2.51	0.40
1:B:449:GLY:HA3	1:B:465:ILE:HB	2.03	0.40
1:B:688:ASP:HA	1:B:691:ALA:HB2	2.03	0.40
2:C:284:MET:HB2	2:C:378:ILE:O	2.21	0.40
2:D:315:PHE:H	2:D:318:GLN:CG	2.34	0.40
1:A:503:VAL:CG1	1:A:635:LEU:HG	2.52	0.40
1:A:641:ARG:C	1:A:643:LEU:H	2.29	0.40
1:B:237:ALA:O	1:B:241:VAL:HG23	2.22	0.40
2:C:50:ASP:HA	2:C:51:PRO:HD3	1.98	0.40
2:D:259:ARG:HH21	2:D:263:LEU:HD21	1.87	0.40
1:A:114:ALA:HB3	1:A:136:ILE:HG22	2.04	0.40
1:B:38:ASN:O	1:B:41:ARG:HB3	2.22	0.40
1:B:40:LEU:HD23	1:B:44:VAL:HG23	2.04	0.40
2:C:6:ARG:HA	2:C:6:ARG:HE	1.87	0.40
2:C:357:SER:O	2:C:361:LEU:HG	2.22	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	704/715 (98%)	645 (92%)	57 (8%)	2 (0%)	36	65
1	B	707/715 (99%)	649 (92%)	57 (8%)	1 (0%)	48	78
2	C	388/390 (100%)	355 (92%)	30 (8%)	3 (1%)	16	44
2	D	388/390 (100%)	353 (91%)	32 (8%)	3 (1%)	16	44
All	All	2187/2210 (99%)	2002 (92%)	176 (8%)	9 (0%)	30	59

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	232	PRO
2	C	232	PRO
2	C	349	PHE
2	D	349	PHE
2	C	187	GLY
2	D	187	GLY
1	A	448	VAL
1	A	460	PRO
1	B	460	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	557/562 (99%)	549 (99%)	8 (1%)	59	70
1	B	559/562 (100%)	556 (100%)	3 (0%)	81	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	307/307 (100%)	301 (98%)	6 (2%)	48	65
2	D	307/307 (100%)	302 (98%)	5 (2%)	55	68
All	All	1730/1738 (100%)	1708 (99%)	22 (1%)	61	71

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	PHE
1	A	280	LYS
1	A	288	ASN
1	A	393	ASN
1	A	579	LYS
1	A	613	LYS
1	A	643	LEU
1	A	682	GLU
1	B	540	LEU
1	B	686	LEU
1	B	705	GLU
2	C	48	LYS
2	C	236	THR
2	C	289	VAL
2	C	318	GLN
2	C	351	CYS
2	C	355	ARG
2	D	206	LYS
2	D	289	VAL
2	D	318	GLN
2	D	324	LYS
2	D	355	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	A	42	GLN
1	A	226	ASN
1	A	288	ASN
1	A	298	GLN
1	A	393	ASN
1	A	409	GLN

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Mol	Chain	Res	Type
1	A	493	ASN
1	A	629	ASN
1	A	698	HIS
1	B	38	ASN
1	B	42	GLN
1	B	260	GLN
1	B	296	ASN
1	B	298	GLN
1	B	409	GLN
1	B	493	ASN
1	B	600	GLN
1	B	711	GLN
2	C	4	ASN
2	C	46	ASN
2	C	113	ASN
2	C	197	GLN
2	C	231	ASN
2	C	244	GLN
2	C	293	GLN
2	C	312	ASN
2	C	318	GLN
2	D	4	ASN
2	D	46	ASN
2	D	64	GLN
2	D	71	ASN
2	D	162	HIS
2	D	197	GLN
2	D	202	ASN
2	D	293	GLN
2	D	312	ASN
2	D	337	ASN
2	D	362	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ACO	C	1003	-	51,53,53	0.82	0	73,79,79	0.68	1 (1%)
3	NAD	A	1001	-	46,48,48	1.53	5 (10%)	64,73,73	1.37	4 (6%)
3	NAD	B	1002	-	46,48,48	1.53	4 (8%)	64,73,73	1.42	4 (6%)
4	ACO	D	1004	-	51,53,53	0.78	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
4	ACO	C	1003	-	-	7/51/67/67	0/3/3/3
3	NAD	A	1001	-	-	6/30/62/62	0/5/5/5
3	NAD	B	1002	-	-	6/30/62/62	0/5/5/5
4	ACO	D	1004	-	-	7/51/67/67	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	NAD	C3N-C7N	5.84	1.59	1.50
3	B	1002	NAD	C3N-C7N	5.68	1.59	1.50
3	B	1002	NAD	C6N-N1N	4.04	1.44	1.35
3	A	1001	NAD	C2N-N1N	4.00	1.39	1.35
3	B	1002	NAD	C2N-N1N	3.98	1.39	1.35
3	A	1001	NAD	C6N-N1N	3.91	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1002	NAD	C4N-C3N	3.80	1.45	1.39
3	A	1001	NAD	C4N-C3N	3.73	1.45	1.39
3	A	1001	NAD	C5N-C4N	2.08	1.42	1.38

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1002	NAD	C5N-C4N-C3N	-6.96	113.52	120.36
3	A	1001	NAD	C5N-C4N-C3N	-6.82	113.67	120.36
3	B	1002	NAD	C6N-C5N-C4N	5.93	127.99	119.45
3	A	1001	NAD	C6N-C5N-C4N	5.57	127.47	119.45
3	B	1002	NAD	C5N-C6N-N1N	-4.24	114.60	120.38
4	C	1003	ACO	C2P-S1P-C	4.00	120.68	101.42
3	A	1001	NAD	C5N-C6N-N1N	-3.98	114.96	120.38
4	D	1004	ACO	C2P-S1P-C	3.93	120.35	101.42
3	A	1001	NAD	C2N-C3N-C4N	2.94	121.68	118.26
3	B	1002	NAD	C2N-C3N-C4N	2.91	121.64	118.26

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1001	NAD	C2N-C3N-C7N-O7N
3	A	1001	NAD	C2N-C3N-C7N-N7N
3	B	1002	NAD	C2N-C3N-C7N-O7N
3	B	1002	NAD	C2N-C3N-C7N-N7N
4	C	1003	ACO	C5P-C6P-C7P-N8P
4	C	1003	ACO	S1P-C2P-C3P-N4P
4	C	1003	ACO	C3P-C2P-S1P-C
4	C	1003	ACO	O-C-S1P-C2P
4	C	1003	ACO	CH3-C-S1P-C2P
4	D	1004	ACO	C3B-C4B-C5B-O5B
4	D	1004	ACO	O4B-C4B-C5B-O5B
4	D	1004	ACO	C5P-C6P-C7P-N8P
4	D	1004	ACO	S1P-C2P-C3P-N4P
4	D	1004	ACO	C3P-C2P-S1P-C
4	D	1004	ACO	O-C-S1P-C2P
4	D	1004	ACO	CH3-C-S1P-C2P
3	A	1001	NAD	C4N-C3N-C7N-O7N
3	A	1001	NAD	C4N-C3N-C7N-N7N
3	B	1002	NAD	C4N-C3N-C7N-O7N
3	B	1002	NAD	C4N-C3N-C7N-N7N

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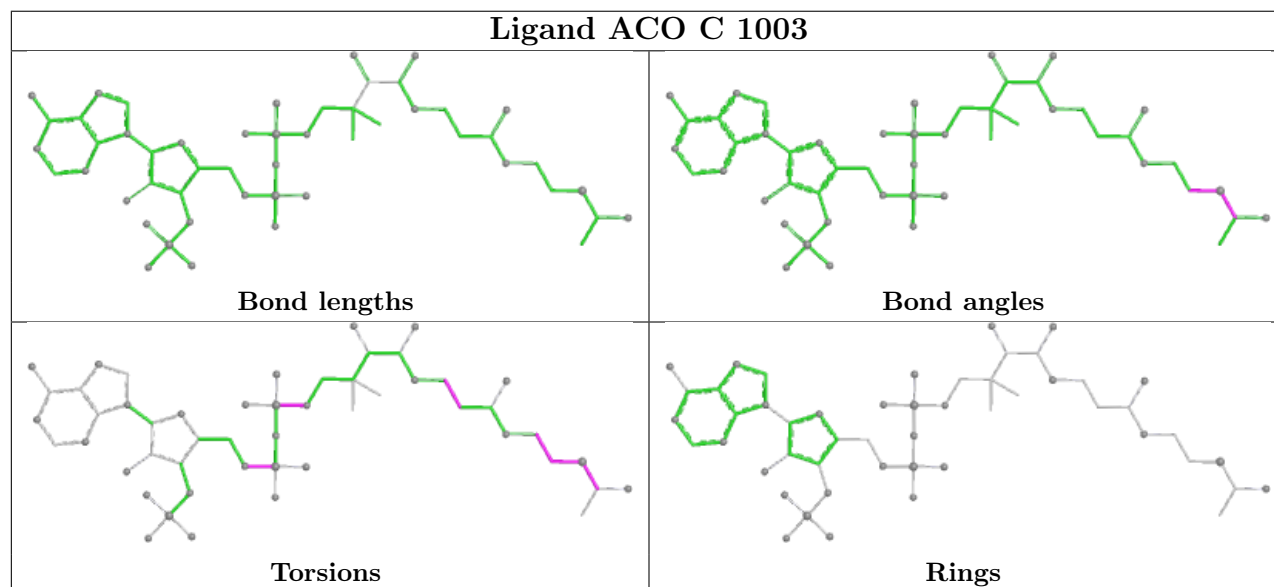
Mol	Chain	Res	Type	Atoms
3	A	1001	NAD	O4B-C4B-C5B-O5B
3	A	1001	NAD	C3B-C4B-C5B-O5B
3	B	1002	NAD	O4B-C4B-C5B-O5B
3	B	1002	NAD	C3B-C4B-C5B-O5B
4	C	1003	ACO	C5B-O5B-P1A-O1A
4	C	1003	ACO	CCP-O6A-P2A-O4A

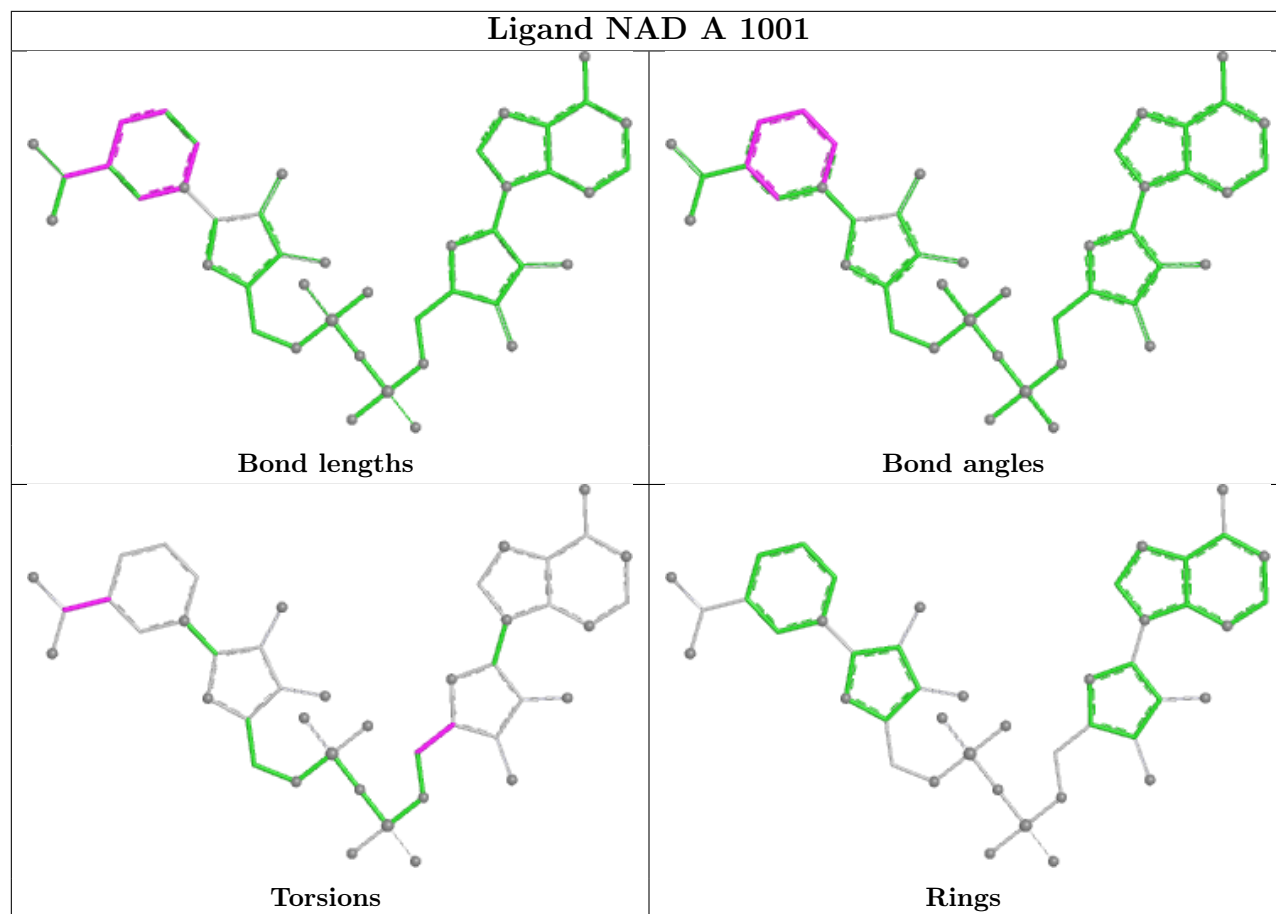
There are no ring outliers.

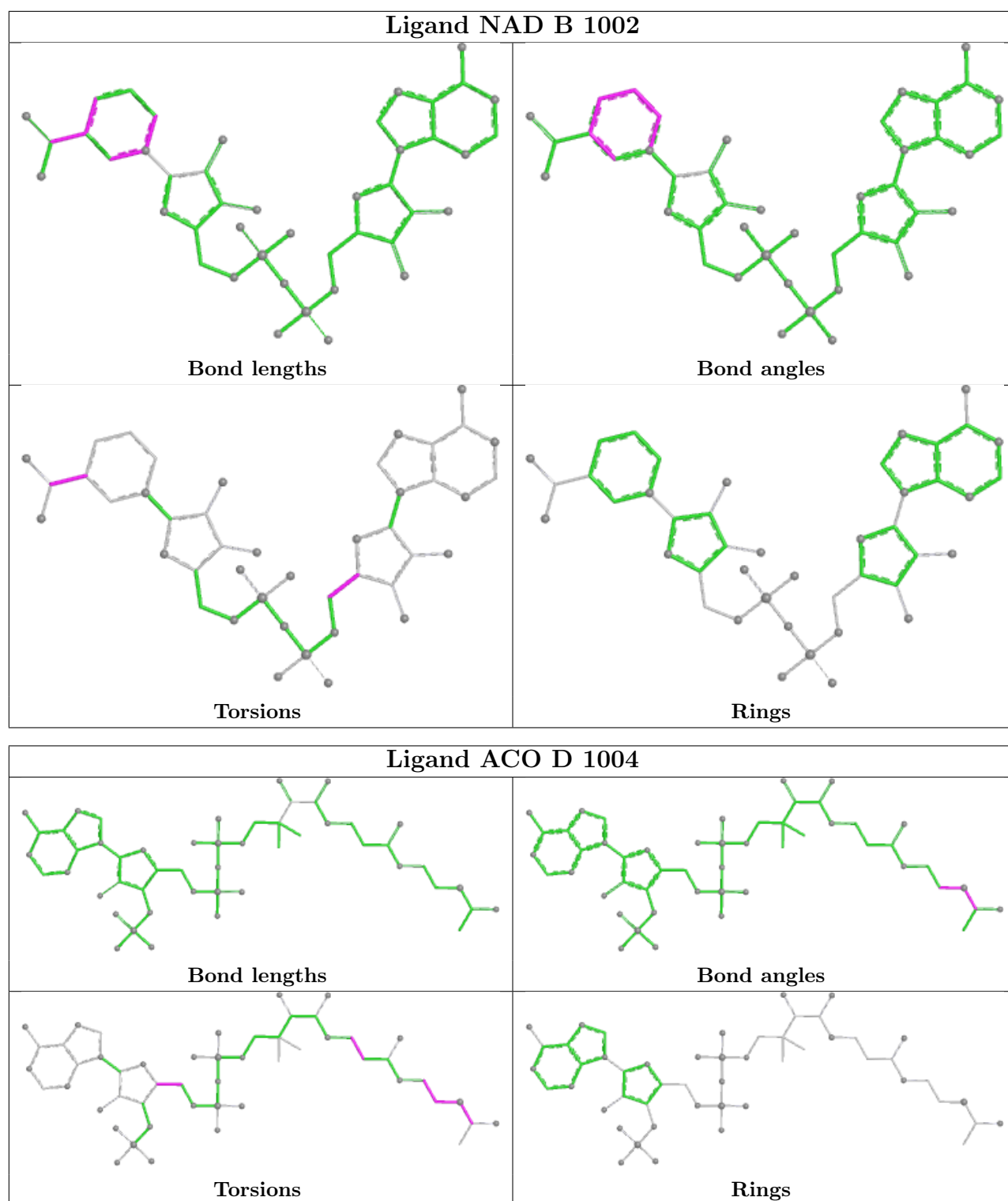
1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1004	ACO	2	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	708/715 (99%)	0.65	54 (7%) 20 17	1, 34, 104, 149	0
1	B	711/715 (99%)	0.39	43 (6%) 27 21	1, 18, 79, 148	0
2	C	390/390 (100%)	0.21	11 (2%) 55 41	1, 4, 49, 126	0
2	D	390/390 (100%)	0.34	12 (3%) 51 38	1, 11, 68, 109	0
All	All	2199/2210 (99%)	0.43	120 (5%) 30 23	1, 17, 85, 149	0

All (120) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	525	ASP	5.4
2	C	6	ARG	3.9
1	A	344	ASP	3.7
1	A	402	VAL	3.7
1	A	401	VAL	3.7
1	A	566	ASP	3.6
2	D	369	GLY	3.6
1	B	618	GLU	3.6
1	B	605	ASP	3.6
1	A	454	ASN	3.6
1	A	581	LEU	3.6
2	D	229	ALA	3.5
1	B	76	GLU	3.5
2	D	6	ARG	3.4
1	A	366	ASP	3.2
1	A	445	GLU	3.2
2	C	2	SER	3.1
1	B	698	HIS	3.1
1	A	45	ASP	3.1
1	A	345	ILE	3.1
1	B	593	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
2	C	236	THR	3.0
1	B	600	GLN	3.0
1	A	333	SER	3.0
2	C	160	LYS	3.0
1	B	11	THR	3.0
1	A	3	TYR	2.9
1	A	307	TYR	2.9
2	C	48	LYS	2.9
1	A	614	PRO	2.8
1	A	420	ARG	2.8
2	D	167	GLU	2.8
2	C	261	LYS	2.8
1	A	326	GLY	2.8
1	B	401	VAL	2.8
1	A	54	LYS	2.8
1	B	231	MET	2.7
2	C	324	LYS	2.7
1	B	362	VAL	2.7
1	A	587	LYS	2.7
1	A	547	ASP	2.7
1	B	695	ALA	2.7
1	A	417	ASN	2.7
1	A	569	ARG	2.7
1	B	708	LYS	2.7
1	B	689	GLN	2.6
1	B	445	GLU	2.6
1	A	554	ASP	2.6
1	B	321	GLY	2.6
1	A	615	ILE	2.6
1	A	677	SER	2.6
1	A	567	ASP	2.6
1	B	566	ASP	2.6
1	A	698	HIS	2.5
1	A	369	ARG	2.5
1	B	705	GLU	2.5
1	B	394	VAL	2.5
2	D	368	GLY	2.5
1	A	570	SER	2.5
1	B	696	LEU	2.5
2	D	181	HIS	2.5
1	B	366	ASP	2.4
1	B	68	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
2	D	372	GLY	2.4
1	B	685	ALA	2.4
1	B	367	LYS	2.4
1	A	680	VAL	2.4
1	B	621	ASP	2.4
1	B	438	ALA	2.4
1	A	447	PHE	2.4
1	A	577	GLU	2.4
1	B	369	ARG	2.4
1	B	299	GLU	2.4
1	A	231	MET	2.3
1	A	612	LEU	2.3
1	B	649	GLU	2.3
1	B	642	CYS	2.3
1	B	581	LEU	2.3
2	C	300	GLY	2.3
2	D	184	THR	2.3
2	D	316	ALA	2.3
1	B	226	ASN	2.3
1	A	199	LEU	2.3
1	A	441	LEU	2.3
1	A	642	CYS	2.3
1	B	347	GLU	2.3
1	A	588	GLY	2.3
1	A	579	LYS	2.3
1	B	430	SER	2.2
2	D	215	ARG	2.2
1	B	421	GLU	2.2
1	A	400	ALA	2.2
1	B	568	ARG	2.2
1	A	605	ASP	2.2
2	C	187	GLY	2.2
1	B	442	LYS	2.2
2	C	70	TRP	2.2
1	A	590	TYR	2.2
1	A	543	VAL	2.2
1	A	610	GLU	2.2
1	A	438	ALA	2.2
1	B	587	LYS	2.1
1	A	38	ASN	2.1
1	A	446	ASN	2.1
2	D	241	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	710	GLY	2.1
2	D	4	ASN	2.1
1	A	361	LEU	2.1
1	A	602	LYS	2.1
1	B	295	LEU	2.1
1	B	364	ARG	2.1
1	B	554	ASP	2.1
1	B	242	ALA	2.1
1	B	365	VAL	2.0
1	A	393	ASN	2.0
1	A	696	LEU	2.0
1	B	381	GLY	2.0
1	A	593	GLU	2.0
1	A	553	ARG	2.0
2	C	391	VAL	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](#)

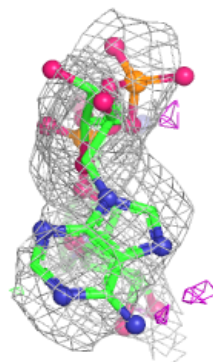
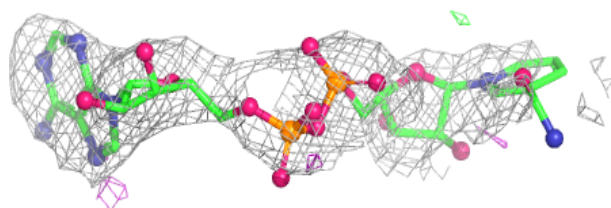
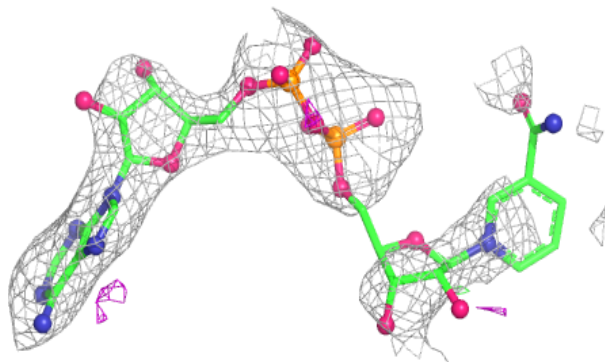
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
3	NAD	A	1001	44/44	0.71	0.17	57,57,57,57	0
4	ACO	C	1003	51/51	0.72	0.24	134,134,134,134	0
4	ACO	D	1004	51/51	0.73	0.25	184,184,184,184	0
3	NAD	B	1002	44/44	0.79	0.18	56,56,56,56	0

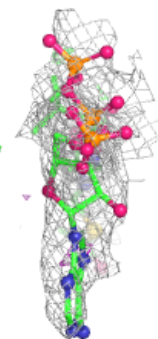
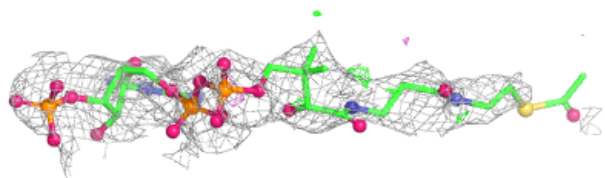
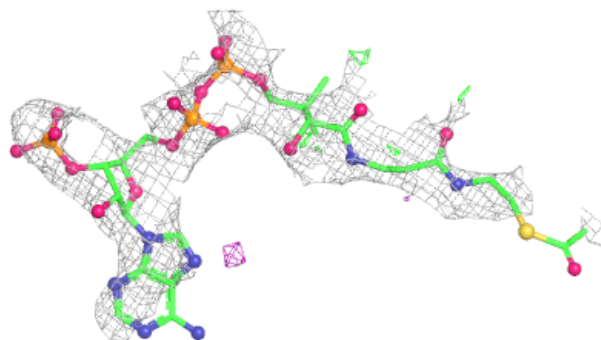
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 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)

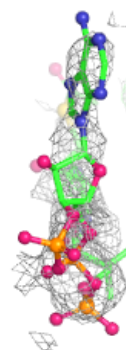
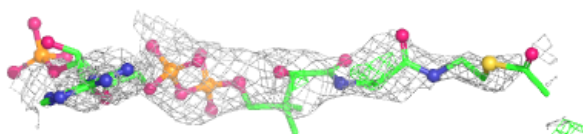
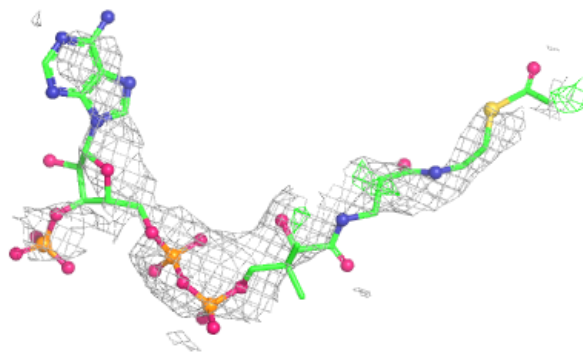
**Electron density around ACO C 1003:**

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

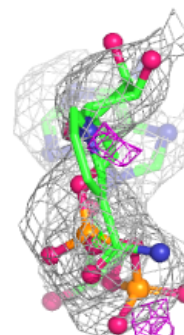
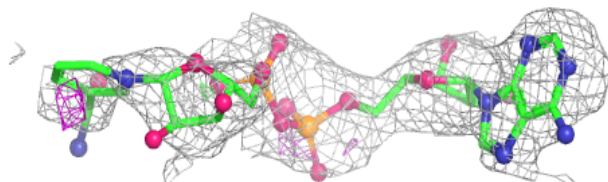
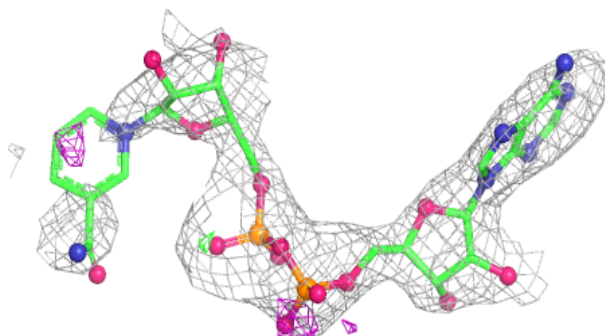


Electron density around ACO D 1004:

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

**Electron density around NAD B 1002:**

$2mF_o-DF_c$ (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.