Full wwPDB X-ray Structure Validation Report ⓘ

Oct 18, 2023 – 10:52 AM EDT

PDB ID	:	2D3T
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:

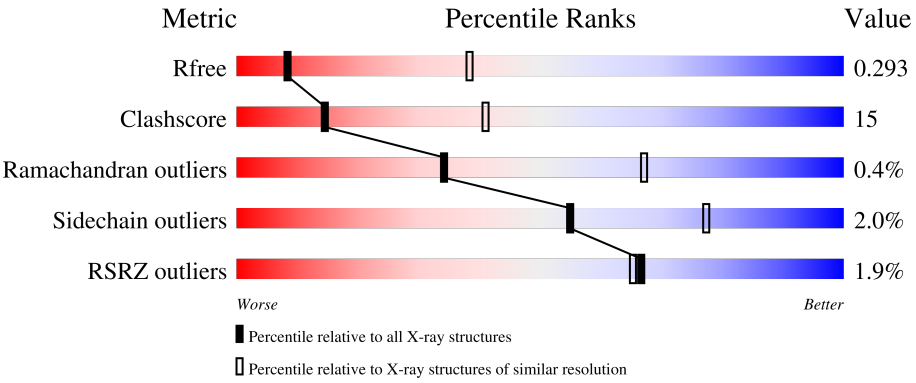
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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}	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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 <=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	3% 63% 35%
1	B	715	2% 68% 30%
2	C	390	% 69% 29%
2	D	390	% 68% 30%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	ACO	D	1004	-	-	-	X

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.

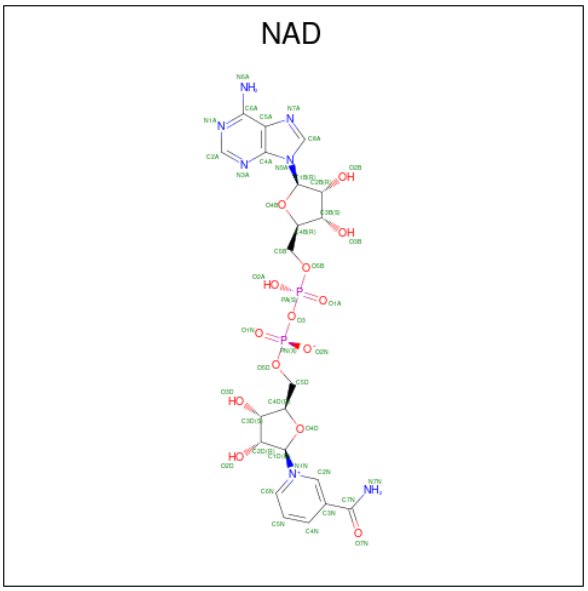
- Molecule 1 is a protein called Fatty oxidation complex alpha subunit.

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.

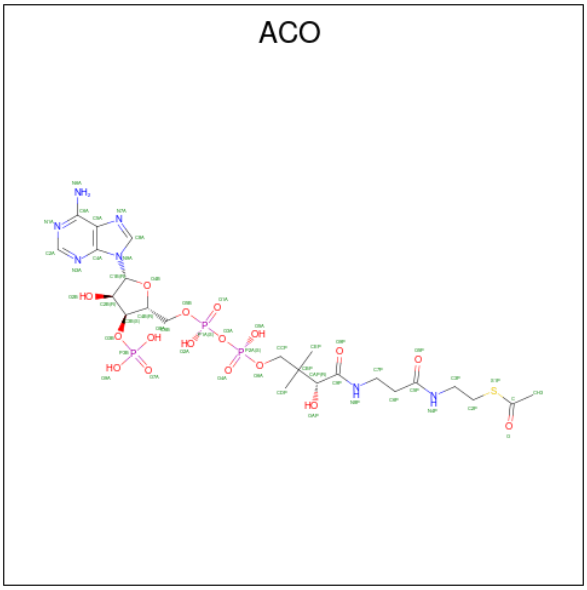
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	390	Total	C	N	O	S	0	0	0
			2893	1801	515	548	29			
2	D	390	Total	C	N	O	S	0	0	0
			2893	1801	515	548	29			

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



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 (three-letter code: ACO) (formula: $C_{23}H_{38}N_7O_{17}P_3S$).



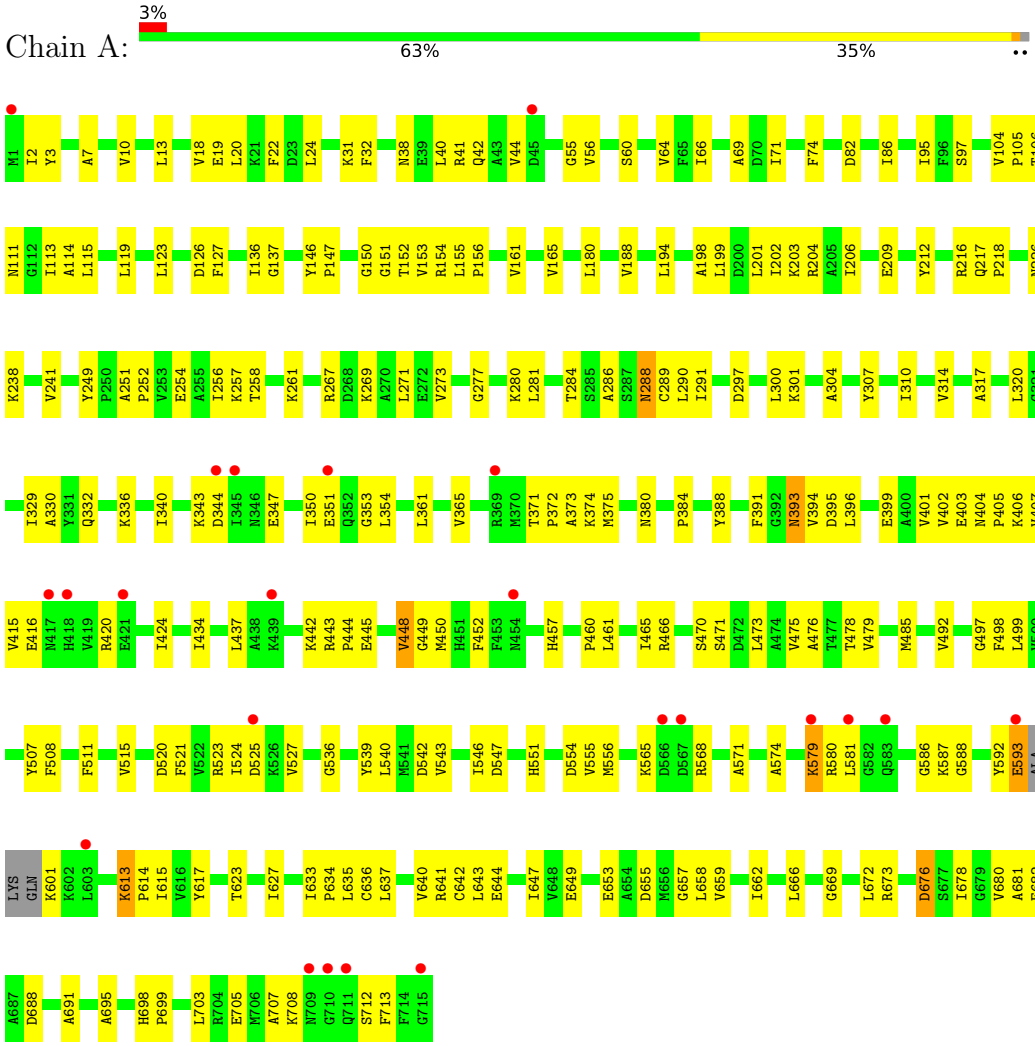
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	C	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
4	D	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		

3 Residue-property plots (i)

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

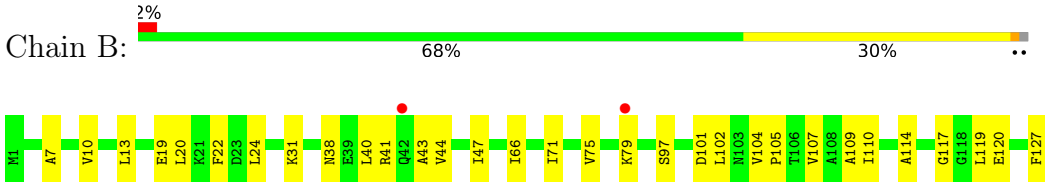
• Molecule 1: Fatty oxidation complex alpha subunit

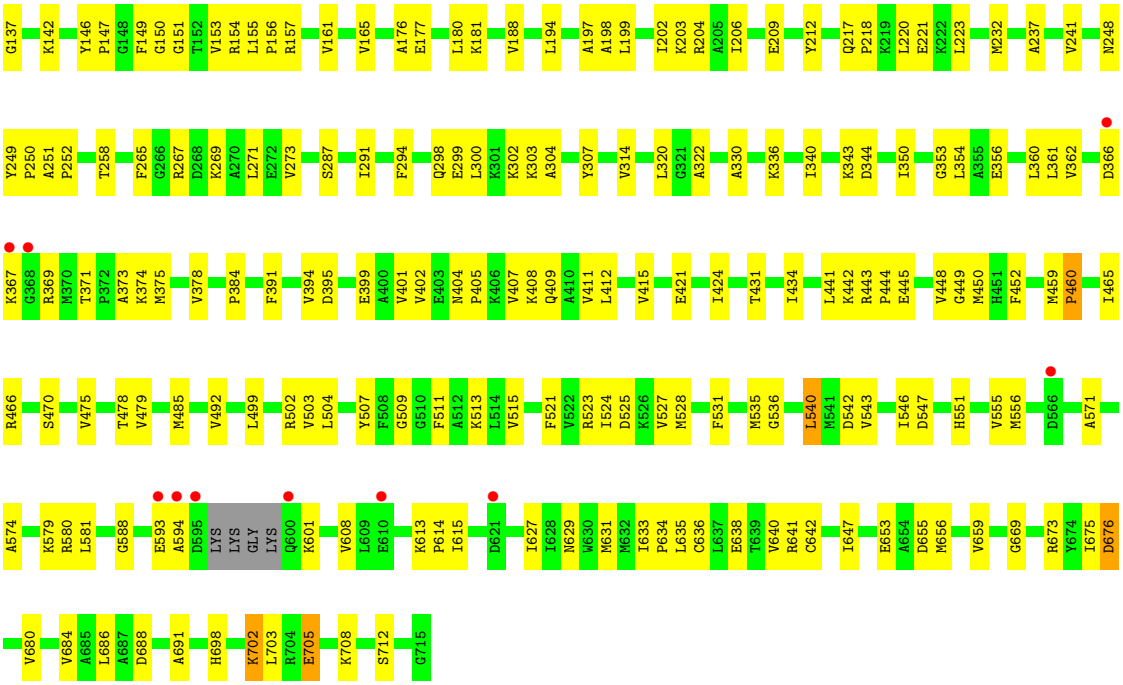
Chain A:



• Molecule 1: Fatty oxidation complex alpha subunit

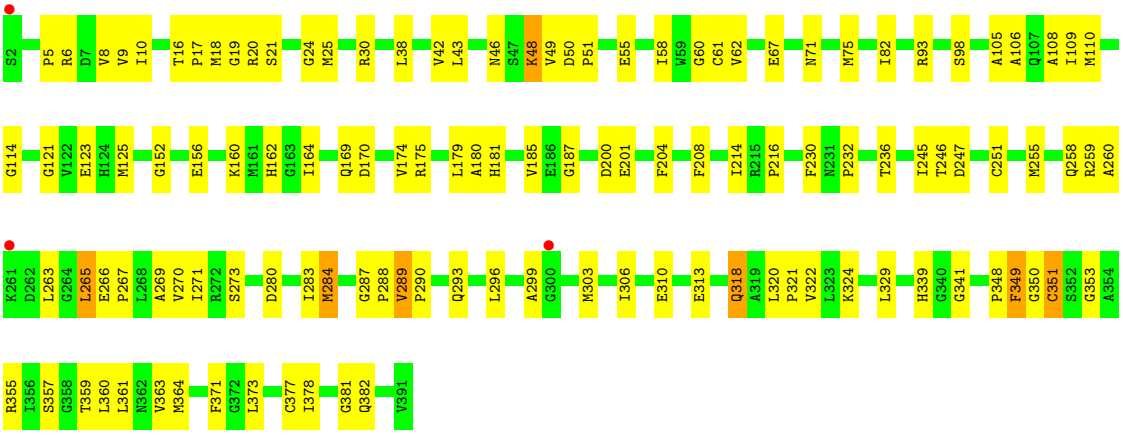
Chain B:





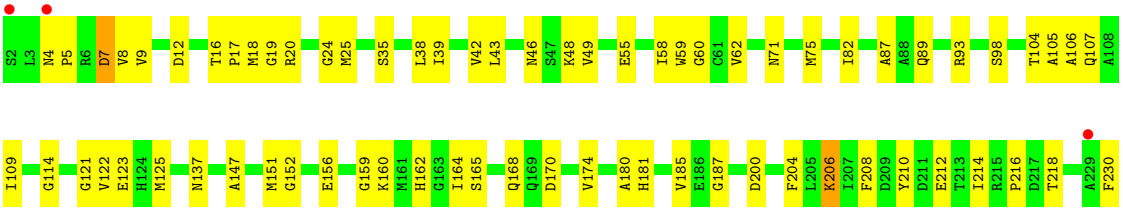
• Molecule 2: 3-ketoacyl-CoA thiolase

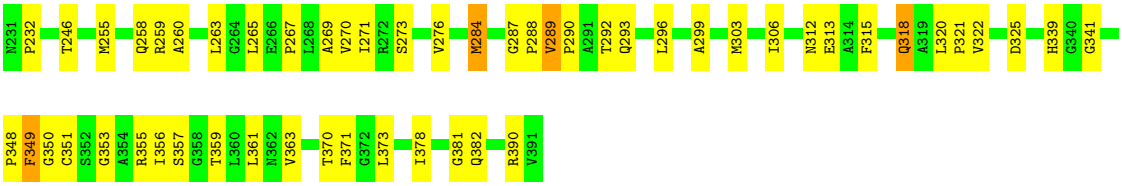
Chain C:



• Molecule 2: 3-ketoacyl-CoA thiolase

Chain D:




N231
P232
T246
M255
Q258
R259
A260
L263
G264
L265
E266
P267
L268
A269
V270
I271
R272
S273
V276
M284
G287
P288
V289
P290
A291
T292
Q293
L296
A299
M303
I306
N312
E313
A314
F315
Q318
A319
L320
P321
V322
D325
H339
G340
G341
P348
F349
G350
C351
S352
G353
A354
R355
I356
S357
G358
T359
L360
L361
N362
V363
T370
F371
G372
L373
I378
G381
Q382
R390
V391

4 Data and refinement statistics (i)

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 13.79 – 3.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (15.00-3.40) 99.7 (13.79-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.29 (at 3.39Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.242 , 0.295 0.247 , 0.293	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 , 13.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.85	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.25	0/5454	0.46	0/7357
1	B	0.25	0/5476	0.46	0/7387
2	C	0.25	0/2941	0.47	0/3967
2	D	0.26	0/2941	0.47	0/3967
All	All	0.25	0/16812	0.46	0/22678

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	179	0
1	B	5390	0	5511	156	0
2	C	2893	0	2903	96	0
2	D	2893	0	2903	97	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	517	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 15.

All (517) 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
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
2:D:303:MET:HE3	2:D:306:ILE:HD12	1.63	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: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
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
2:D:125:MET:HE2	2:D:348:PRO:HA	1.69	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
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:180:LEU:HD12	1:B:188:VAL:HG23	1.78	0.64
2:C:125:MET:HE2	2:C:348:PRO:HA	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
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: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:25:MET:HE1	2:D:208:PHE:HB2	1.82	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:43:LEU:HD11	2:C:82:ILE:HD11	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
2:C:313:GLU:CD	2:C:341:GLY:HA3	2.21	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: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
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
2:D:273:SER:HB3	2:D:299:ALA:HB2	1.86	0.58
2:C:98:SER:HB3	2:C:353:GLY:HA3	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:C:25:MET:HE1	2:C:208:PHE:HB2	1.86	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: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
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:655:ASP:O	1:A:659:VAL:HG23	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:D:151:MET:HE3	4:D:1004:ACO:H21	1.89	0.55
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
1:A:521:PHE:HA	1:A:524:ILE:HD12	1.87	0.55
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
1:B:101:ASP:CG	1:B:267:ARG:HH22	2.11	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
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
2:C:303:MET:HE3	2:C:306:ILE:HD12	1.91	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:507:TYR:CE1	1:B:631:MET:HB3	2.44	0.52
2:D:43:LEU:HD11	2:D:82:ILE:HD11	1.91	0.52
2:C:313:GLU:OE1	2:C:341:GLY:HA3	2.08	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
2:D:20:ARG:NH1	2:D:212:GLU:HB3	2.25	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:D:318:GLN:O	2:D:322:VAL:HG23	2.09	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: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: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:C:318:GLN:C	2:C:321:PRO:HD2	2.31	0.50
2:D:62:VAL:CG2	2:D:349:PHE:HB3	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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
2:D:125:MET:HE3	2:D:246:THR:H	1.77	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
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:255:MET:HE1	2:D:263:LEU:HD12	1.94	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
1:A:676:ASP:OD2	1:A:712:SER:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:125:MET:CE	2:C:246:THR:H	2.27	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
2:D:255:MET:HE3	2:D:259:ARG:HG3	1.95	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:502:ARG:HA	1:B:556:MET:HE1	1.96	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
2:D:318:GLN:C	2:D:321:PRO:HD2	2.34	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:593:GLU:H	1:A:593:GLU:CD	2.19	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
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
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: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
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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:445:GLU:CD	1:A:445:GLU:H	2.20	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
2:C:17:PRO:HB2	2:C:25:MET:CE	2.46	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
2:C:361:LEU:HA	2:C:364:MET:HE2	1.99	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
2:D:313:GLU:CD	2:D:341:GLY:HA3	2.37	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:269:ALA:CB	2:C:361:LEU:HD22	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:303:MET:HE1	2:C:373:LEU:HD22	2.00	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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:17:PRO:HB2	2:D:25:MET:CE	2.49	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
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:C:17:PRO:HB2	2:C:25:MET:HE1	2.01	0.42
2:D:19:GLY:H	2:D:246:THR:CG2	2.31	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:502:ARG:HA	1:A:556:MET:CE	2.49	0.42
1:B:120:GLU:CD	1:B:149:PHE:HB2	2.40	0.42
1:B:404:ASN:H	1:B:408:LYS:HE2	1.84	0.42
1:A:126:ASP:OD1	1:A:216:ARG:HB2	2.20	0.42
2:C:125:MET:HE3	2:C:246:THR:H	1.83	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: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
2:C:255:MET:HE1	2:C:263:LEU:HD12	2.01	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
1:A:7:ALA:HB2	1:A:24:LEU:HD13	2.02	0.41
1:A:672:LEU:HD22	1:A:713:PHE:CE2	2.56	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
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: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
1:B:445:GLU:CD	1:B:445:GLU:H	2.23	0.41
2:C:169:GLN:HE22	2:C:236:THR:HB	1.85	0.41
1:A:284:THR:C	1:A:286:ALA:H	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:C:201:GLU:CD	2:C:201:GLU:H	2.25	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:A:502:ARG:HG3	1:A:556:MET:HE1	2.02	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:255:MET:HE3	2:C:259:ARG:HG3	2.04	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 (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	704/715 (98%)	645 (92%)	57 (8%)	2 (0%)	41 72
1	B	707/715 (99%)	649 (92%)	57 (8%)	1 (0%)	51 82
2	C	388/390 (100%)	355 (92%)	30 (8%)	3 (1%)	19 51
2	D	388/390 (100%)	353 (91%)	32 (8%)	3 (1%)	19 51
All	All	2187/2210 (99%)	2002 (92%)	176 (8%)	9 (0%)	34 67

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 (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	557/562 (99%)	545 (98%)	12 (2%)	52 75
1	B	559/562 (100%)	552 (99%)	7 (1%)	69 84
2	C	307/307 (100%)	299 (97%)	8 (3%)	46 72
2	D	307/307 (100%)	300 (98%)	7 (2%)	50 74
All	All	1730/1738 (100%)	1696 (98%)	34 (2%)	55 77

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	PHE
1	A	288	ASN

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Mol	Chain	Res	Type
1	A	393	ASN
1	A	554	ASP
1	A	565	LYS
1	A	579	LYS
1	A	593	GLU
1	A	601	LYS
1	A	613	LYS
1	A	643	LEU
1	A	676	ASP
1	A	682	GLU
1	B	31	LYS
1	B	366	ASP
1	B	540	LEU
1	B	676	ASP
1	B	686	LEU
1	B	702	LYS
1	B	705	GLU
2	C	48	LYS
2	C	61	CYS
2	C	265	LEU
2	C	284	MET
2	C	289	VAL
2	C	318	GLN
2	C	351	CYS
2	C	355	ARG
2	D	7	ASP
2	D	206	LYS
2	D	284	MET
2	D	289	VAL
2	D	318	GLN
2	D	325	ASP
2	D	355	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) 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	296	ASN
1	A	298	GLN

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Mol	Chain	Res	Type
1	A	393	ASN
1	A	409	GLN
1	A	488	ASN
1	A	493	ASN
1	A	629	ASN
1	A	698	HIS
1	B	38	ASN
1	B	42	GLN
1	B	163	ASN
1	B	260	GLN
1	B	296	ASN
1	B	298	GLN
1	B	409	GLN
2	C	4	ASN
2	C	46	ASN
2	C	197	GLN
2	C	231	ASN
2	C	293	GLN
2	C	318	GLN
2	D	4	ASN
2	D	46	ASN
2	D	162	HIS
2	D	197	GLN
2	D	293	GLN
2	D	339	HIS
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 monosaccharides in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAD	A	1001	-	42,48,48	1.52	5 (11%)	50,73,73	1.57	7 (14%)
3	NAD	B	1002	-	42,48,48	1.51	5 (11%)	50,73,73	1.61	5 (10%)
4	ACO	C	1003	-	45,53,53	0.78	1 (2%)	56,79,79	0.90	3 (5%)
4	ACO	D	1004	-	45,53,53	0.79	1 (2%)	56,79,79	0.85	2 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAD	A	1001	-	-	6/26/62/62	0/5/5/5
3	NAD	B	1002	-	-	6/26/62/62	0/5/5/5
4	ACO	C	1003	-	-	7/47/67/67	0/3/3/3
4	ACO	D	1004	-	-	7/47/67/67	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	NAD	C3N-C7N	5.80	1.59	1.50
3	B	1002	NAD	C3N-C7N	5.65	1.59	1.50
3	B	1002	NAD	C6N-N1N	3.74	1.44	1.35
3	A	1001	NAD	C2N-N1N	3.63	1.39	1.35
3	A	1001	NAD	C6N-N1N	3.62	1.44	1.35
3	B	1002	NAD	C2N-N1N	3.61	1.39	1.35
3	B	1002	NAD	C4N-C3N	3.43	1.45	1.39
3	A	1001	NAD	C4N-C3N	3.37	1.45	1.39
4	D	1004	ACO	C2A-N3A	2.28	1.35	1.32
4	C	1003	ACO	C2A-N3A	2.19	1.35	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1002	NAD	C2A-N3A	2.16	1.35	1.32
3	A	1001	NAD	C2A-N3A	2.11	1.35	1.32

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1002	NAD	C6N-C5N-C4N	5.89	127.99	119.44
3	B	1002	NAD	C5N-C4N-C3N	-5.77	113.52	120.34
3	A	1001	NAD	C5N-C4N-C3N	-5.64	113.67	120.34
3	A	1001	NAD	C6N-C5N-C4N	5.52	127.47	119.44
3	B	1002	NAD	C5N-C6N-N1N	-4.05	114.60	120.40
3	A	1001	NAD	C5N-C6N-N1N	-3.80	114.96	120.40
4	C	1003	ACO	C2P-S1P-C	3.61	120.68	101.68
4	D	1004	ACO	C2P-S1P-C	3.55	120.35	101.68
4	C	1003	ACO	P2A-O3A-P1A	-3.51	120.79	132.83
4	D	1004	ACO	P2A-O3A-P1A	-3.40	121.17	132.83
3	A	1001	NAD	PN-O3-PA	-3.29	121.55	132.83
3	B	1002	NAD	PN-O3-PA	-3.20	121.85	132.83
3	A	1001	NAD	C2N-C3N-C4N	3.02	121.68	118.26
3	B	1002	NAD	C2N-C3N-C4N	2.98	121.64	118.26
3	A	1001	NAD	O4D-C1D-C2D	-2.23	103.67	106.93
3	A	1001	NAD	C5A-C6A-N6A	2.02	123.43	120.35
4	C	1003	ACO	C5A-C6A-N6A	2.01	123.41	120.35

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

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Mol	Chain	Res	Type	Atoms
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
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

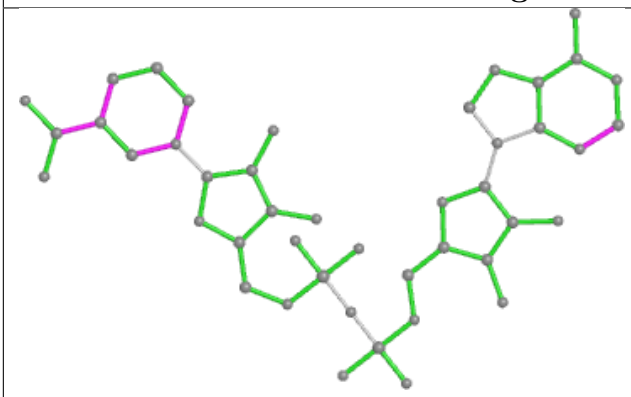
There are no ring outliers.

1 monomer is involved in 2 short contacts:

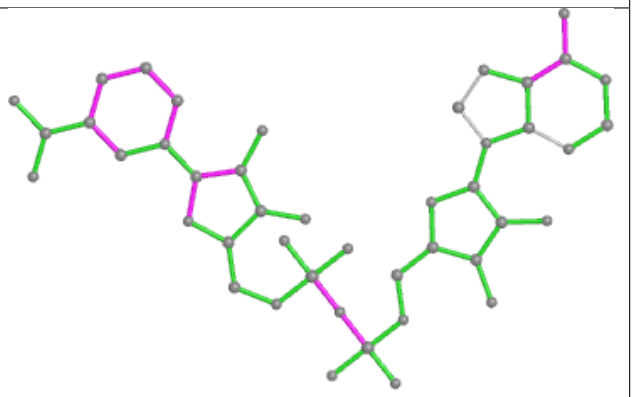
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1004	ACO	2	0

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 then 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.

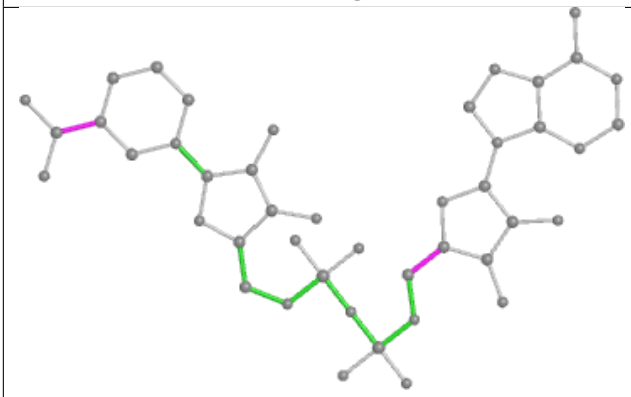
Ligand NAD A 1001



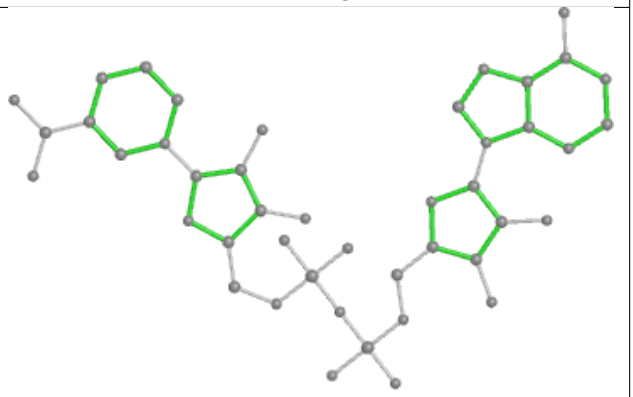
Bond lengths



Bond angles

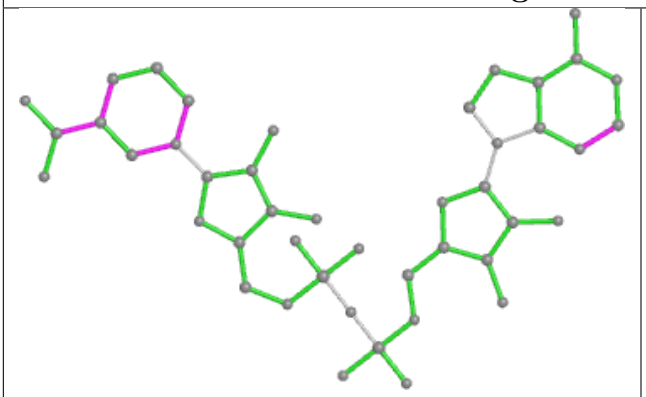


Torsions

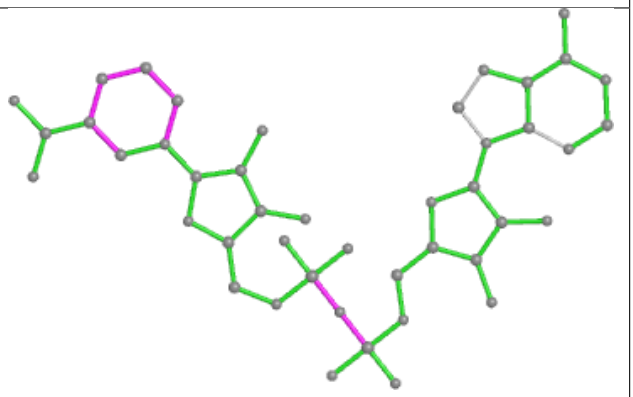


Rings

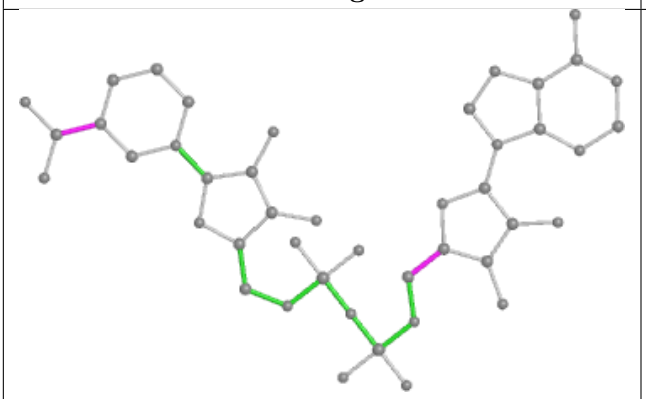
Ligand NAD B 1002



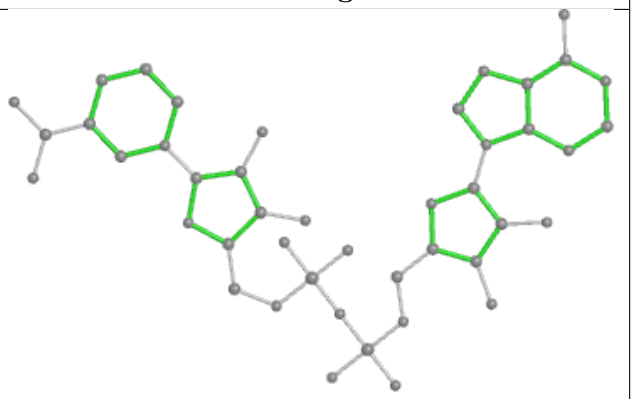
Bond lengths



Bond angles

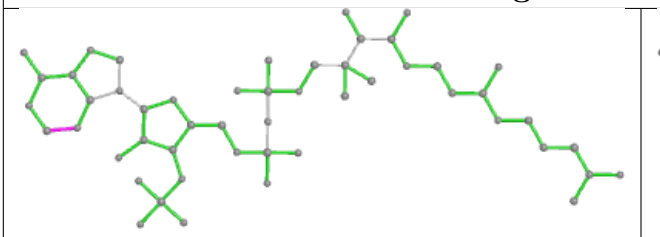


Torsions

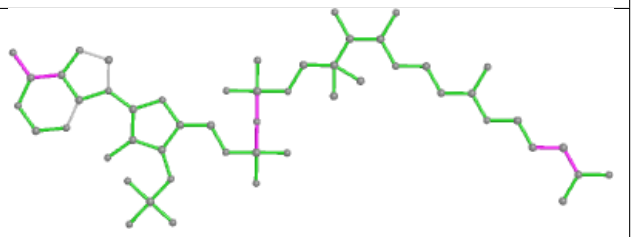


Rings

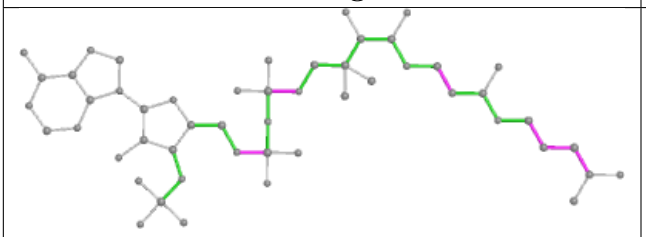
Ligand ACO C 1003



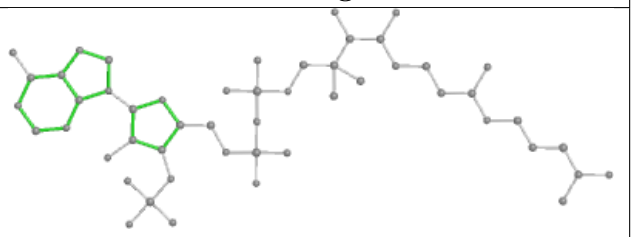
Bond lengths



Bond angles

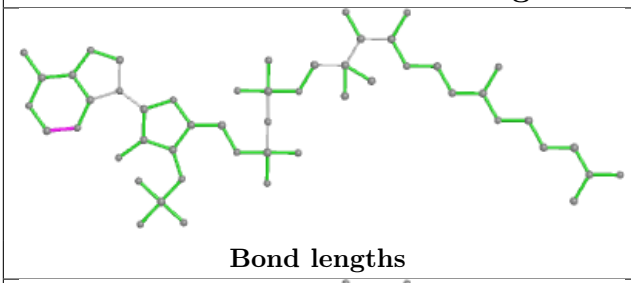


Torsions

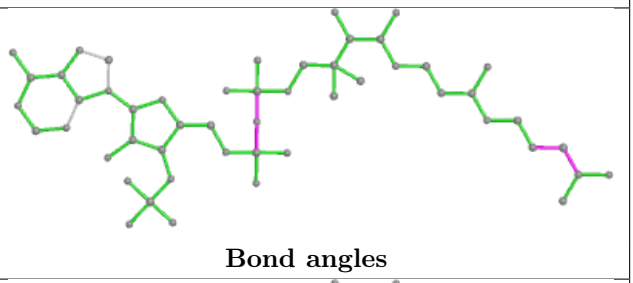


Rings

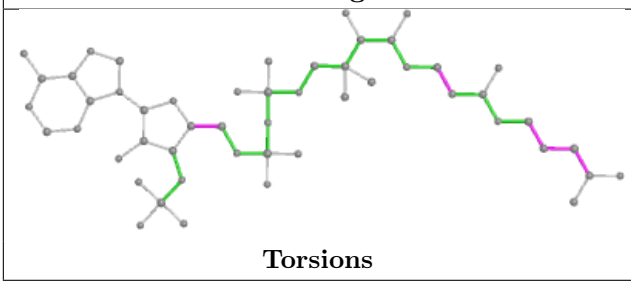
Ligand ACO D 1004



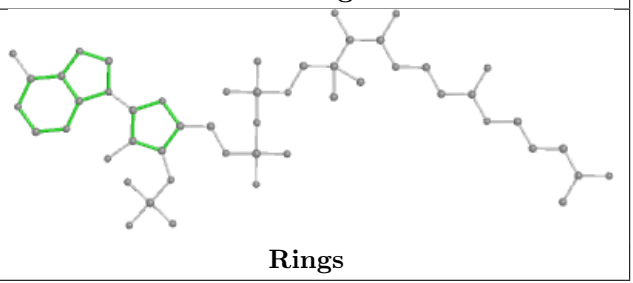
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	0.18	24 (3%)	45	44	1, 34, 104, 149	0
1	B	711/715 (99%)	-0.08	12 (1%)	70	68	1, 18, 79, 148	0
2	C	390/390 (100%)	-0.29	3 (0%)	86	85	1, 4, 49, 126	0
2	D	390/390 (100%)	-0.15	3 (0%)	86	85	1, 11, 68, 109	0
All	All	2199/2210 (99%)	-0.05	42 (1%)	66	65	1, 17, 85, 149	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	2	SER	4.8
1	B	367	LYS	4.6
1	A	566	ASP	3.9
1	A	567	ASP	3.7
1	A	417	ASN	3.7
1	A	593	GLU	3.6
1	A	715	GLY	3.2
1	A	710	GLY	3.2
1	B	566	ASP	3.1
2	D	2	SER	3.1
1	A	345	ILE	3.0
1	A	579	LYS	2.9
1	B	593	GLU	2.9
1	A	709	ASN	2.8
1	B	595	ASP	2.8
1	B	366	ASP	2.7
1	A	421	GLU	2.7
1	B	600	GLN	2.5
1	A	454	ASN	2.5
1	A	439	LYS	2.4
1	B	610	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
2	C	300	GLY	2.4
1	A	711	GLN	2.3
1	A	344	ASP	2.3
1	B	594	ALA	2.3
2	D	229	ALA	2.3
2	C	261	LYS	2.3
1	A	324	ILE	2.3
1	B	621	ASP	2.2
1	A	1	MET	2.2
1	B	368	GLY	2.2
1	A	603	LEU	2.2
1	A	525	ASP	2.1
2	D	4	ASN	2.1
1	A	581	LEU	2.1
1	A	583	GLN	2.1
1	B	79	LYS	2.1
1	A	45	ASP	2.1
1	A	418	HIS	2.1
1	B	42	GLN	2.0
1	A	351	GLU	2.0
1	A	369	ARG	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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	D	1004	51/51	0.69	0.42	184,184,184,184	0
4	ACO	C	1003	51/51	0.75	0.36	134,134,134,134	0

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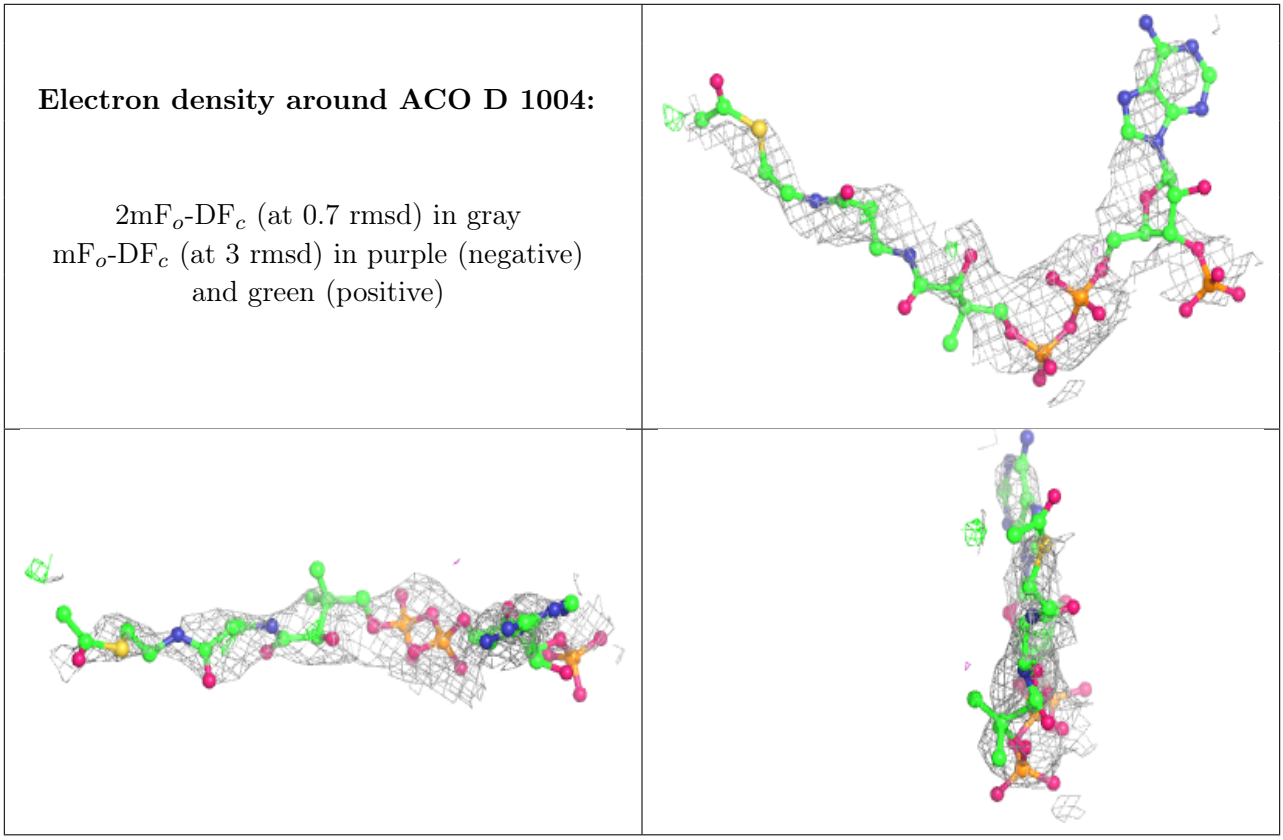
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAD	A	1001	44/44	0.78	0.36	57,57,57,57	0
3	NAD	B	1002	44/44	0.81	0.34	56,56,56,56	0

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.

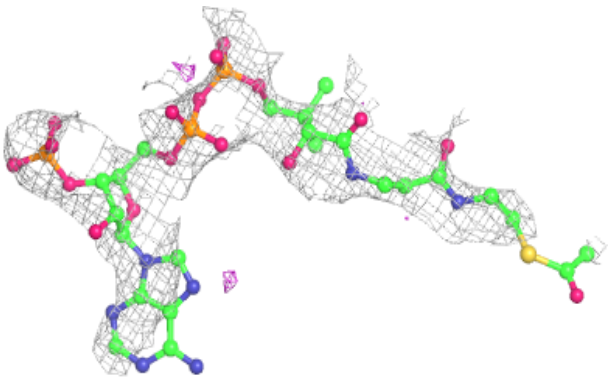
Electron density around ACO D 1004:

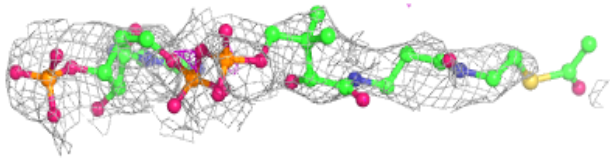
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

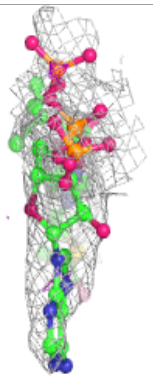


Electron density around ACO C 1003:

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

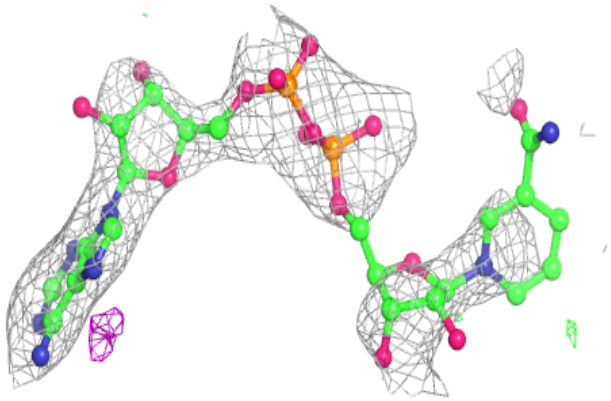


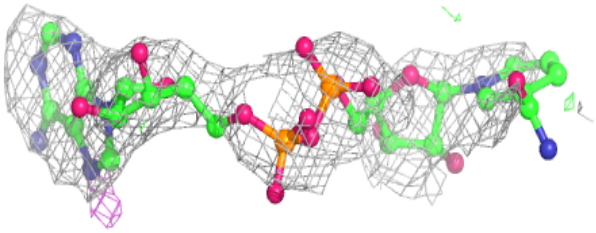


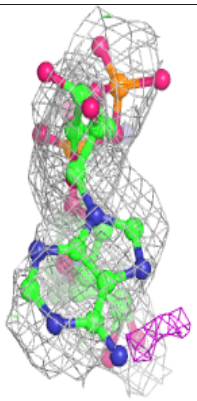


Electron density around NAD A 1001:

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

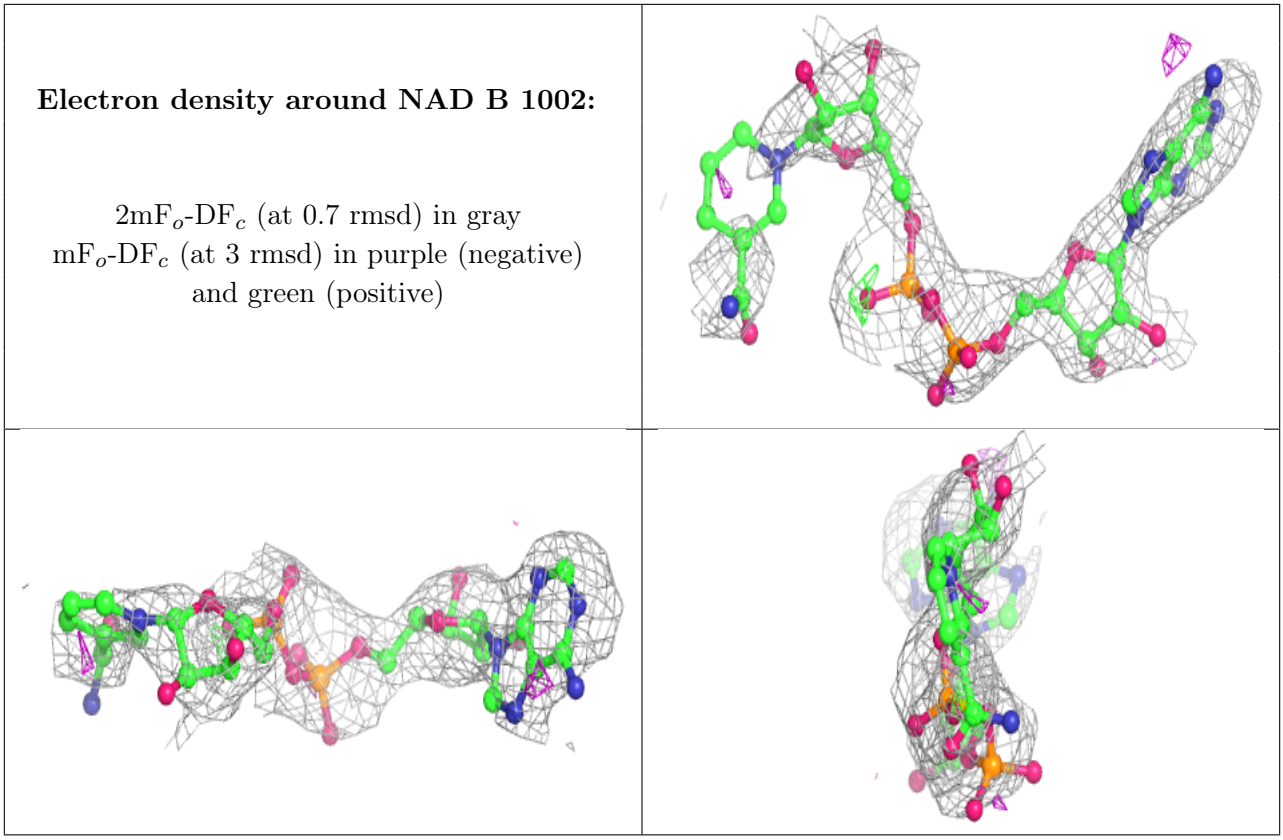






Electron density around NAD B 1002:

$2mF_o$-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.