Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 10:44 AM EDT

PDB ID	:	2FKN
Title	:	crystal structure of urocanase from bacillus subtilis
Authors	:	Yu, Y.-M.; Liang, Y.-H.; Su, X.-D.
Deposited on	:	2006-01-05
Resolution	:	2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

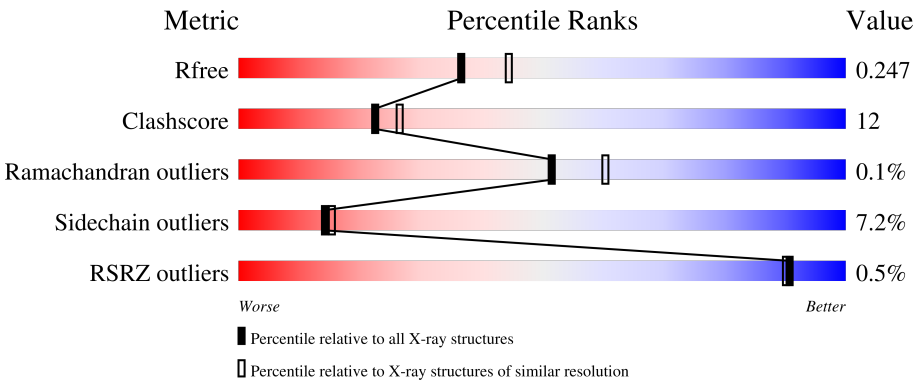
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	552	% 74% 21% • •
1	B	552	% 74% 22% • •
1	C	552	76% 20% • •
1	D	552	76% 19% • •

2 Entry composition (i)

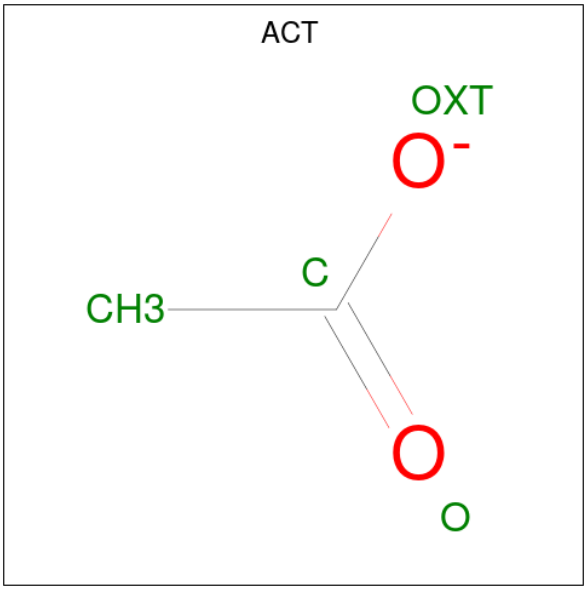
There are 4 unique types of molecules in this entry. The entry contains 17568 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Urocanate hydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	544	4195	2650	737	787	21	0	0	0
1	B	546	4213	2661	741	790	21	0	0	0
1	C	544	4195	2650	737	787	21	0	0	0
1	D	544	4195	2650	737	787	21	0	0	0

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	4	2	2	0	0
2	B	1	4	2	2	0	0

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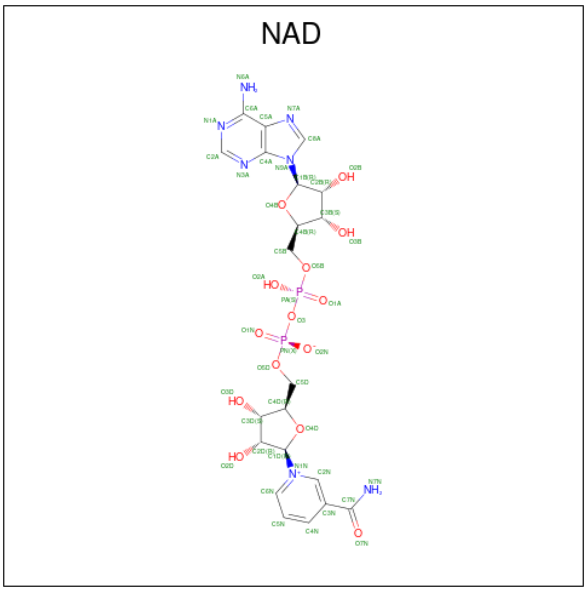
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
2	C	1	4	2	2		0	0
			Total	C	O			
2	D	1	4	2	2		0	0

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	176	176	176	0	0
			Total	O		
4	B	122	122	122	0	0
			Total	O		
4	C	163	163	163	0	0

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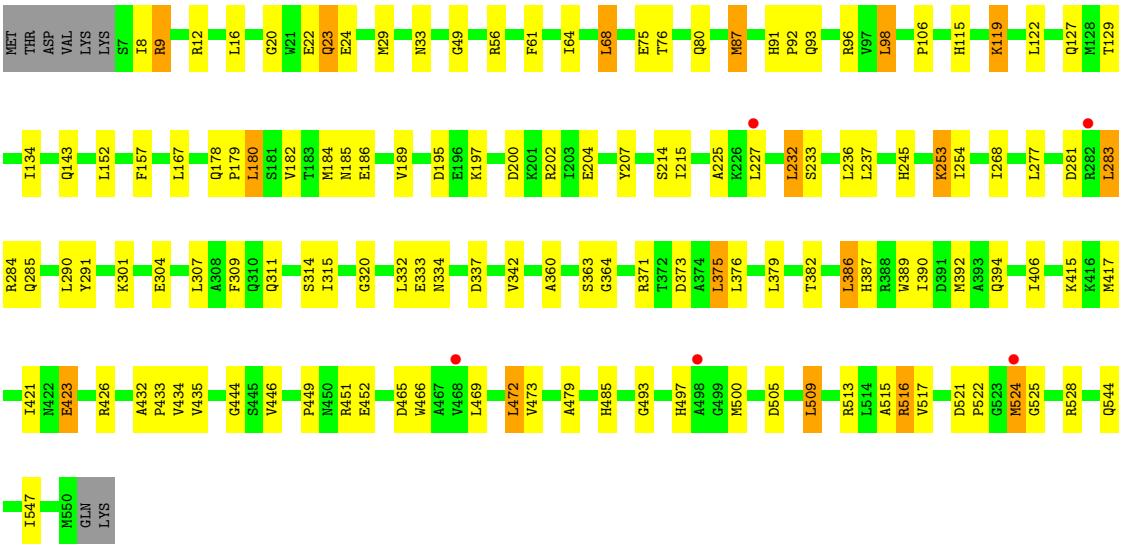
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	D	117	117	117	0	0

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.

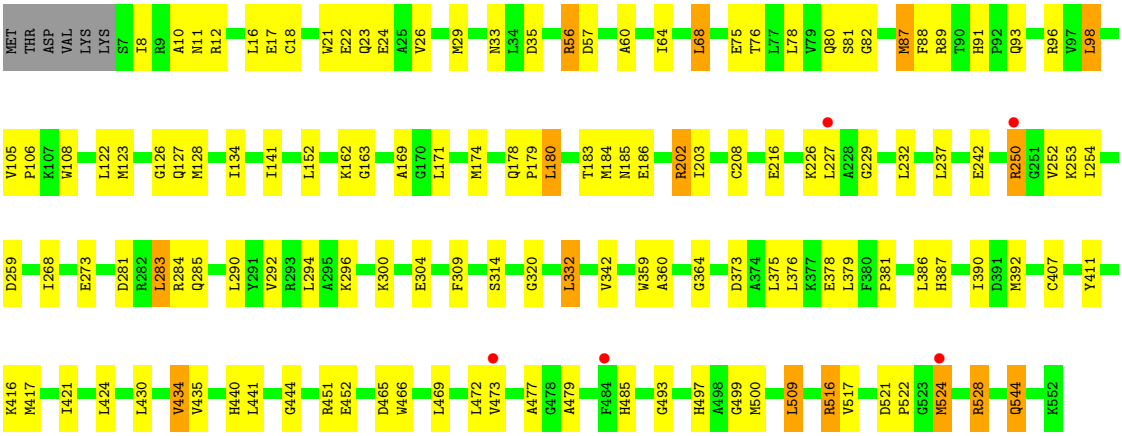
• Molecule 1: Urocanate hydratase

Chain A:



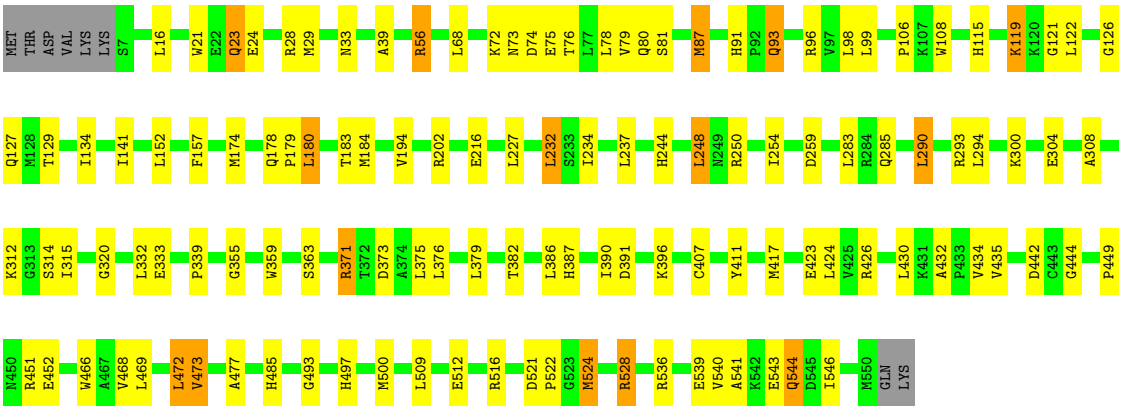
• Molecule 1: Urocanate hydratase

Chain B:



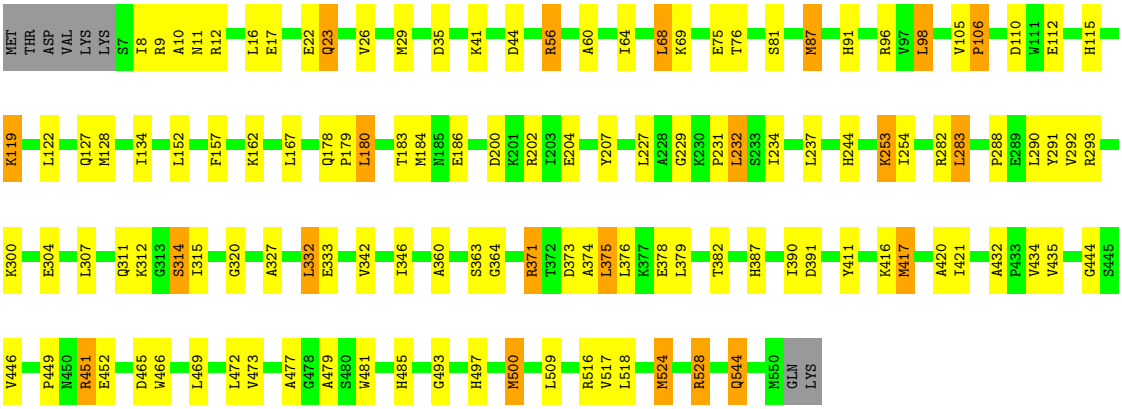
• Molecule 1: Urocanate hydratase

Chain C:



- Molecule 1: Urocanate hydratase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	99.79Å 131.27Å 164.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20 48.10 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.3 (50.00-2.20) 97.1 (48.10-2.20)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.77 (at 2.20Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.205 , 0.256 0.196 , 0.247	Depositor DCC
R_{free} test set	5358 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	26.2	Xtriage
Anisotropy	0.922	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 31.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	17568	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 9.83% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ACT, 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	0.34	0/4283	0.62	0/5797
1	B	0.32	0/4301	0.62	0/5820
1	C	0.33	0/4283	0.63	0/5797
1	D	0.32	0/4283	0.61	0/5797
All	All	0.33	0/17150	0.62	0/23211

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4195	0	4157	107	0
1	B	4213	0	4178	99	0
1	C	4195	0	4157	104	0
1	D	4195	0	4157	102	0
2	A	4	0	3	0	0
2	B	4	0	3	1	0
2	C	4	0	3	1	0
2	D	4	0	3	0	0
3	A	44	0	26	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	44	0	26	1	0
3	C	44	0	26	1	0
3	D	44	0	26	0	0
4	A	176	0	0	2	0
4	B	122	0	0	2	0
4	C	163	0	0	8	0
4	D	117	0	0	4	0
All	All	17568	0	16765	390	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 12.

All (390) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:376:LEU:HD23	1:C:417:MET:HE3	1.27	1.16
1:B:469:LEU:O	1:B:473:VAL:HG23	1.59	1.03
1:B:75:GLU:HB3	1:B:87:MET:HE3	1.38	1.01
1:A:376:LEU:HD23	1:A:417:MET:HE3	1.42	1.00
1:D:253:LYS:H	1:D:253:LYS:HD3	1.23	1.00
1:B:373:ASP:HA	1:B:390:ILE:HD11	1.42	0.98
1:C:469:LEU:O	1:C:473:VAL:HG23	1.67	0.95
1:D:253:LYS:HD3	1:D:253:LYS:N	1.88	0.89
1:C:23:GLN:H	1:C:23:GLN:HE21	0.93	0.88
1:B:174:MET:SD	2:B:553:ACT:H3	2.18	0.84
1:D:373:ASP:CA	1:D:390:ILE:HD11	2.08	0.83
1:B:376:LEU:HA	1:B:417:MET:HE1	1.60	0.83
1:C:23:GLN:HE21	1:C:23:GLN:N	1.77	0.82
1:B:376:LEU:HD12	1:B:390:ILE:HD12	1.62	0.82
1:D:469:LEU:O	1:D:473:VAL:HG23	1.79	0.81
1:D:12:ARG:HD2	1:D:364:GLY:HA3	1.62	0.81
1:A:200:ASP:O	1:A:204:GLU:HG3	1.82	0.79
1:B:376:LEU:HD22	1:B:386:LEU:HD11	1.64	0.78
1:C:23:GLN:H	1:C:23:GLN:NE2	1.77	0.78
1:C:254:ILE:O	1:C:314:SER:HB3	1.84	0.77
1:A:469:LEU:O	1:A:473:VAL:HG23	1.85	0.77
1:B:76:THR:HG21	1:B:98:LEU:HD22	1.67	0.76
1:C:376:LEU:CD2	1:C:417:MET:HE3	2.14	0.75
1:A:376:LEU:HD12	1:A:390:ILE:HD12	1.68	0.75
1:A:76:THR:HG21	1:A:98:LEU:HD22	1.67	0.74
1:B:75:GLU:CB	1:B:87:MET:HE3	2.18	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:GLN:HG3	4:A:5606:HOH:O	1.89	0.73
1:B:373:ASP:CA	1:B:390:ILE:HD11	2.19	0.73
1:C:466:TRP:HB3	1:C:524:MET:HE1	1.71	0.72
1:D:444:GLY:O	1:D:524:MET:SD	2.46	0.72
1:D:373:ASP:HA	1:D:390:ILE:HD11	1.70	0.72
1:C:16:LEU:HG	1:C:24:GLU:HG3	1.72	0.72
1:A:376:LEU:CD2	1:A:417:MET:HE3	2.19	0.72
1:B:254:ILE:O	1:B:314:SER:HB3	1.89	0.72
1:C:376:LEU:HD12	1:C:390:ILE:HD12	1.73	0.71
1:C:382:THR:HG22	1:C:382:THR:O	1.90	0.71
1:D:76:THR:HG21	1:D:98:LEU:HD22	1.73	0.70
1:D:379:LEU:HD12	1:D:417:MET:CE	2.20	0.70
1:A:373:ASP:CA	1:A:390:ILE:HD11	2.21	0.70
1:D:200:ASP:O	1:D:204:GLU:HG3	1.90	0.70
1:B:87:MET:HE2	1:B:88:PHE:N	2.07	0.70
1:A:373:ASP:HA	1:A:390:ILE:HD11	1.74	0.69
1:A:253:LYS:H	1:A:253:LYS:HD3	1.58	0.69
1:A:379:LEU:HD12	1:A:417:MET:HE2	1.74	0.69
1:C:373:ASP:CA	1:C:390:ILE:HD11	2.22	0.69
1:C:472:LEU:HB3	1:D:98:LEU:HG	1.75	0.69
1:B:466:TRP:HB3	1:B:524:MET:HE1	1.75	0.67
1:D:524:MET:HE2	1:D:524:MET:O	1.95	0.67
1:A:373:ASP:CB	1:A:390:ILE:HD11	2.24	0.67
1:D:115:HIS:O	1:D:119:LYS:HG2	1.94	0.67
1:D:373:ASP:CB	1:D:390:ILE:HD11	2.24	0.67
1:B:184:MET:CE	1:B:392:MET:HB3	2.24	0.67
1:A:254:ILE:O	1:A:314:SER:HB3	1.94	0.67
1:D:421:ILE:HG21	1:D:434:VAL:HG21	1.77	0.67
1:B:376:LEU:CD1	1:B:390:ILE:HD12	2.25	0.67
1:D:11:ASN:ND2	1:D:17:GLU:OE2	2.27	0.66
1:A:254:ILE:HD12	1:A:309:PHE:CZ	2.29	0.66
1:C:56:ARG:HD3	1:C:81:SER:O	1.95	0.66
1:B:22:GLU:HG2	1:B:96:ARG:HG3	1.77	0.66
1:C:75:GLU:HG2	1:C:87:MET:HE1	1.77	0.66
1:C:373:ASP:CB	1:C:390:ILE:HD11	2.26	0.65
1:D:466:TRP:HE3	1:D:524:MET:HE3	1.60	0.65
1:D:110:ASP:OD1	1:D:112:GLU:HG2	1.96	0.65
1:C:444:GLY:O	1:C:524:MET:SD	2.55	0.65
1:D:179:PRO:HG2	1:D:207:TYR:O	1.96	0.65
1:D:23:GLN:HG3	4:D:8643:HOH:O	1.97	0.64
1:B:16:LEU:HG	1:B:24:GLU:HG3	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:MET:SD	1:B:435:VAL:HG21	2.38	0.64
1:A:253:LYS:HD3	1:A:253:LYS:N	2.13	0.64
1:A:382:THR:O	1:A:382:THR:HG22	1.97	0.64
1:D:254:ILE:O	1:D:314:SER:HB3	1.98	0.64
1:A:376:LEU:HD23	1:A:417:MET:CE	2.23	0.64
1:D:253:LYS:H	1:D:253:LYS:CD	1.95	0.63
1:B:411:TYR:CE2	1:B:544:GLN:HG2	2.33	0.63
1:C:293:ARG:NE	4:C:7662:HOH:O	2.28	0.63
1:D:41:LYS:HE2	1:D:44:ASP:OD2	1.99	0.62
1:D:387:HIS:O	1:D:390:ILE:HG22	1.99	0.62
1:B:376:LEU:HD11	1:B:407:CYS:SG	2.39	0.62
1:C:91:HIS:HB3	1:C:93:GLN:OE1	1.99	0.62
1:D:421:ILE:HG21	1:D:434:VAL:CG2	2.29	0.62
1:D:524:MET:HE1	1:D:528:ARG:HB2	1.81	0.62
1:C:371:ARG:HD2	1:C:371:ARG:O	1.99	0.62
1:A:93:GLN:HG2	1:A:509:LEU:HD21	1.81	0.62
1:A:75:GLU:HG2	1:A:87:MET:HE3	1.82	0.62
1:D:75:GLU:CG	1:D:87:MET:HE1	2.30	0.62
1:D:22:GLU:HG2	1:D:96:ARG:HG3	1.80	0.61
1:A:387:HIS:O	1:A:390:ILE:HG22	1.99	0.61
1:D:320:GLY:HA3	1:D:451:ARG:HD2	1.81	0.61
1:D:379:LEU:HD12	1:D:417:MET:HE1	1.82	0.61
1:D:10:ALA:O	1:D:12:ARG:NH1	2.32	0.61
1:A:307:LEU:O	1:A:311:GLN:HG3	2.00	0.61
1:C:423:GLU:HG2	1:C:426:ARG:HH21	1.65	0.61
1:D:244:HIS:HE1	4:D:8652:HOH:O	1.83	0.61
1:D:379:LEU:HD12	1:D:417:MET:HE2	1.83	0.61
1:A:12:ARG:HD2	1:A:364:GLY:HA3	1.83	0.61
1:A:253:LYS:H	1:A:253:LYS:CD	2.11	0.61
1:C:75:GLU:CG	1:C:87:MET:HE1	2.29	0.61
1:B:93:GLN:HG2	1:B:509:LEU:HD21	1.83	0.60
1:D:376:LEU:HD12	1:D:390:ILE:HD12	1.83	0.60
1:D:60:ALA:O	1:D:64:ILE:HG13	2.02	0.59
1:A:106:PRO:HB2	1:B:493:GLY:HA2	1.84	0.59
1:B:180:LEU:HD22	1:B:184:MET:HG3	1.85	0.59
1:C:536:ARG:O	1:C:540:VAL:HG23	2.02	0.59
1:A:379:LEU:HD12	1:A:417:MET:CE	2.33	0.59
1:C:285:GLN:HG3	4:C:7634:HOH:O	2.02	0.59
1:C:373:ASP:HA	1:C:390:ILE:HD11	1.85	0.59
1:A:493:GLY:HA2	1:B:106:PRO:HB2	1.84	0.58
1:B:134:ILE:HG13	1:B:134:ILE:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:411:TYR:HE2	1:B:544:GLN:HG2	1.67	0.58
1:C:106:PRO:HB2	1:D:493:GLY:HA2	1.86	0.58
1:D:134:ILE:O	1:D:134:ILE:HG13	2.02	0.58
1:D:371:ARG:HD2	1:D:371:ARG:O	2.03	0.58
1:B:479:ALA:HB2	1:B:517:VAL:HG21	1.86	0.58
1:C:115:HIS:O	1:C:119:LYS:HE2	2.02	0.58
1:C:73:ASN:ND2	4:C:7647:HOH:O	2.29	0.58
1:A:180:LEU:HD22	1:A:184:MET:HG3	1.85	0.57
1:B:516:ARG:HE	1:B:516:ARG:HA	1.69	0.57
1:C:379:LEU:HD12	1:C:417:MET:CE	2.34	0.57
1:A:342:VAL:HG21	1:A:452:GLU:HA	1.87	0.57
1:B:29:MET:CE	1:B:435:VAL:HG21	2.35	0.57
1:C:539:GLU:O	1:C:543:GLU:HG3	2.05	0.57
1:A:93:GLN:OE1	1:B:91:HIS:CD2	2.58	0.57
1:A:75:GLU:CG	1:A:87:MET:HE3	2.34	0.56
1:A:91:HIS:HB3	1:A:92:PRO:HD2	1.87	0.56
1:C:216:GLU:OE2	1:C:250:ARG:NH1	2.38	0.56
1:A:182:VAL:HG11	1:A:189:VAL:HB	1.87	0.56
1:D:374:ALA:O	1:D:378:GLU:HG3	2.06	0.56
1:A:376:LEU:CD1	1:A:390:ILE:HD12	2.34	0.56
1:C:387:HIS:O	1:C:390:ILE:HG22	2.06	0.55
1:D:56:ARG:HD3	1:D:81:SER:O	2.07	0.55
1:A:184:MET:CE	1:A:392:MET:HB3	2.35	0.55
1:C:493:GLY:HA2	1:D:106:PRO:HB2	1.88	0.55
1:A:22:GLU:HG2	1:A:96:ARG:HG3	1.88	0.55
1:C:512:GLU:O	1:C:516:ARG:HG2	2.06	0.55
1:C:152:LEU:O	1:C:152:LEU:HD23	2.07	0.55
1:D:186:GLU:HA	1:D:231:PRO:HB3	1.89	0.55
1:A:509:LEU:HD22	1:A:513:ARG:HD2	1.88	0.55
1:A:516:ARG:NH2	4:A:5700:HOH:O	2.37	0.55
1:C:73:ASN:ND2	1:C:73:ASN:H	2.05	0.54
1:B:250:ARG:HG3	1:B:252:VAL:HG23	1.88	0.54
1:B:524:MET:CE	1:B:528:ARG:HB2	2.37	0.54
1:A:184:MET:HE1	1:A:392:MET:HB3	1.89	0.54
1:B:12:ARG:HD2	1:B:364:GLY:HA3	1.88	0.54
1:D:485:HIS:HB2	1:D:497:HIS:CE1	2.42	0.54
1:A:115:HIS:O	1:A:119:LYS:HG2	2.07	0.54
1:A:421:ILE:HG21	1:A:434:VAL:HG21	1.90	0.54
1:C:24:GLU:OE1	1:C:28:ARG:NE	2.41	0.53
1:C:75:GLU:HB3	1:C:87:MET:CE	2.38	0.53
1:C:184:MET:HE3	1:C:396:LYS:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:ARG:HD3	1:B:81:SER:O	2.08	0.53
1:D:375:LEU:HD22	1:D:417:MET:HE1	1.89	0.53
1:A:254:ILE:HD12	1:A:309:PHE:CE1	2.43	0.53
1:A:16:LEU:N	1:A:16:LEU:HD12	2.23	0.53
1:A:376:LEU:HD12	1:A:390:ILE:CD1	2.38	0.53
1:B:300:LYS:O	1:B:304:GLU:HG3	2.09	0.53
1:D:162:LYS:HE3	1:D:229:GLY:O	2.07	0.53
1:A:423:GLU:HG2	1:A:426:ARG:HH21	1.74	0.53
1:C:423:GLU:HG2	1:C:426:ARG:NH2	2.23	0.53
1:B:283:LEU:HD11	1:B:294:LEU:HD12	1.89	0.53
1:B:421:ILE:HG21	1:B:434:VAL:HG21	1.90	0.53
1:A:466:TRP:HE3	1:A:524:MET:HE3	1.74	0.52
1:C:300:LYS:O	1:C:304:GLU:HG3	2.09	0.52
1:B:8:ILE:O	1:B:35:ASP:HA	2.09	0.52
1:B:281:ASP:O	1:B:285:GLN:HG3	2.10	0.52
1:A:96:ARG:HA	1:A:96:ARG:NE	2.24	0.52
1:A:225:ALA:HB2	1:A:232:LEU:HD12	1.92	0.52
1:B:10:ALA:O	1:B:12:ARG:NH1	2.43	0.52
1:C:248:LEU:HD11	1:C:308:ALA:CB	2.40	0.52
1:C:373:ASP:HB3	1:C:390:ILE:HD11	1.91	0.52
1:C:524:MET:CE	1:C:528:ARG:HB2	2.40	0.52
1:C:379:LEU:HD12	1:C:417:MET:HE2	1.92	0.52
1:B:26:VAL:HG12	1:B:68:LEU:HD21	1.91	0.52
1:D:16:LEU:HD12	1:D:16:LEU:N	2.24	0.51
1:D:75:GLU:HG2	1:D:87:MET:HE1	1.91	0.51
1:B:424:LEU:HB3	1:B:430:LEU:HG	1.92	0.51
1:A:29:MET:SD	1:A:435:VAL:HG21	2.51	0.51
1:B:11:ASN:ND2	1:B:17:GLU:OE2	2.42	0.51
1:C:78:LEU:HD21	1:D:473:VAL:HG22	1.93	0.51
1:C:477:ALA:O	1:D:91:HIS:HE1	1.94	0.50
1:B:379:LEU:HD12	1:B:417:MET:HE2	1.93	0.50
1:A:473:VAL:HG22	1:B:78:LEU:HD21	1.94	0.50
1:A:485:HIS:HB2	1:A:497:HIS:CE1	2.46	0.50
1:C:33:ASN:O	1:C:39:ALA:HB2	2.12	0.50
1:C:468:VAL:HG12	1:C:472:LEU:HD22	1.94	0.50
1:B:441:LEU:HD23	1:B:441:LEU:C	2.33	0.50
1:D:8:ILE:O	1:D:35:ASP:HA	2.12	0.50
1:C:174:MET:SD	2:C:553:ACT:H3	2.52	0.49
1:A:516:ARG:HG3	1:B:89:ARG:O	2.13	0.49
1:C:129:THR:HG22	1:C:134:ILE:HG23	1.95	0.49
1:B:184:MET:HE1	1:B:392:MET:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:417:MET:O	1:B:421:ILE:HG13	2.12	0.49
1:A:134:ILE:HG13	1:A:134:ILE:O	2.13	0.49
1:A:547:ILE:N	1:A:547:ILE:HD12	2.28	0.49
1:B:360:ALA:HB3	1:B:435:VAL:CG2	2.42	0.49
1:D:167:LEU:HB2	1:D:254:ILE:HD13	1.94	0.49
1:D:382:THR:O	1:D:382:THR:CG2	2.60	0.49
1:B:141:ILE:HG12	1:B:141:ILE:O	2.13	0.48
1:A:157:PHE:CE1	1:A:315:ILE:HD12	2.48	0.48
1:A:363:SER:HB3	1:A:432:ALA:HB3	1.95	0.48
1:B:16:LEU:HD11	1:B:21:TRP:CE2	2.49	0.48
1:D:373:ASP:HB3	1:D:390:ILE:HD11	1.93	0.48
1:A:245:HIS:CD2	1:A:301:LYS:HE2	2.49	0.48
1:A:421:ILE:HG21	1:A:434:VAL:CG2	2.43	0.48
1:C:451:ARG:HB3	1:C:452:GLU:OE1	2.13	0.48
1:C:485:HIS:HB2	1:C:497:HIS:CE1	2.48	0.48
1:B:309:PHE:HB3	1:B:314:SER:OG	2.12	0.48
1:A:8:ILE:HD13	1:A:61:PHE:CZ	2.48	0.48
1:A:301:LYS:HA	1:A:304:GLU:OE1	2.14	0.48
1:B:141:ILE:HD12	3:B:6555:NAD:C4N	2.43	0.48
1:D:375:LEU:HD22	1:D:417:MET:CE	2.44	0.48
1:B:379:LEU:HD12	1:B:417:MET:CE	2.43	0.48
1:C:72:LYS:C	1:C:74:ASP:H	2.16	0.48
1:C:248:LEU:HD11	1:C:308:ALA:HB3	1.95	0.48
1:D:479:ALA:HB2	1:D:517:VAL:HG21	1.96	0.48
1:B:203:ILE:HD13	1:B:208:CYS:HB3	1.96	0.47
1:D:152:LEU:HD23	1:D:152:LEU:O	2.14	0.47
1:A:479:ALA:HB2	1:A:517:VAL:HG21	1.95	0.47
1:A:76:THR:CG2	1:A:98:LEU:HD22	2.42	0.47
1:A:178:GLN:N	1:A:179:PRO:HD2	2.30	0.47
1:B:152:LEU:HD23	1:B:152:LEU:O	2.14	0.47
1:D:363:SER:HB3	1:D:432:ALA:HB3	1.96	0.47
1:A:91:HIS:HE1	1:B:477:ALA:O	1.97	0.47
1:B:332:LEU:HD23	1:B:332:LEU:HA	1.79	0.47
1:D:327:ALA:HB1	1:D:332:LEU:HD12	1.95	0.47
1:A:20:GLY:O	1:A:23:GLN:HG2	2.14	0.47
1:B:485:HIS:HB2	1:B:497:HIS:CE1	2.49	0.47
1:C:134:ILE:HG13	1:C:134:ILE:O	2.14	0.47
1:C:382:THR:O	1:C:382:THR:CG2	2.62	0.47
1:B:254:ILE:HD12	1:B:309:PHE:CZ	2.50	0.47
1:B:320:GLY:HA3	1:B:451:ARG:HD2	1.95	0.47
1:B:379:LEU:HD22	1:B:416:LYS:HE2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:521:ASP:HB3	1:C:522:PRO:CD	2.44	0.47
1:A:375:LEU:HD22	1:A:379:LEU:HG	1.96	0.47
1:A:423:GLU:HG2	1:A:426:ARG:NH2	2.30	0.47
1:C:521:ASP:HB3	1:C:522:PRO:HD3	1.97	0.47
1:A:195:ASP:HA	1:A:277:LEU:HD11	1.97	0.47
1:D:112:GLU:CD	1:D:112:GLU:H	2.18	0.47
1:C:73:ASN:H	1:C:73:ASN:HD22	1.61	0.47
1:D:17:GLU:OE1	1:D:69:LYS:HE2	2.15	0.47
1:B:440:HIS:NE2	1:B:499:GLY:HA3	2.30	0.46
1:D:64:ILE:HG22	1:D:68:LEU:HD22	1.98	0.46
1:A:360:ALA:HB3	1:A:435:VAL:CG2	2.45	0.46
1:B:376:LEU:CD2	1:B:417:MET:HE3	2.45	0.46
1:C:121:GLY:HA2	4:C:7579:HOH:O	2.14	0.46
1:D:373:ASP:O	1:D:390:ILE:CD1	2.64	0.46
1:A:382:THR:O	1:A:382:THR:CG2	2.63	0.46
1:A:521:ASP:HB3	1:A:522:PRO:CD	2.45	0.46
1:B:169:ALA:HB3	1:B:259:ASP:OD2	2.16	0.46
1:C:468:VAL:HG12	1:C:472:LEU:CD2	2.45	0.46
1:A:320:GLY:HA3	1:A:451:ARG:HD2	1.97	0.46
1:A:215:ILE:HG12	1:A:236:LEU:HD21	1.97	0.46
1:B:250:ARG:CG	1:B:252:VAL:HG23	2.46	0.46
1:D:180:LEU:HD22	1:D:184:MET:HG3	1.97	0.46
1:A:179:PRO:HG2	1:A:207:TYR:O	2.16	0.46
1:B:57:ASP:HB2	4:B:6557:HOH:O	2.14	0.46
1:B:268:ILE:HD13	1:B:284:ARG:HD3	1.98	0.46
1:C:320:GLY:HA3	1:C:451:ARG:HD2	1.98	0.46
1:A:9:ARG:HH11	1:A:9:ARG:HG2	1.80	0.46
1:B:185:ASN:O	1:B:186:GLU:HB2	2.16	0.46
1:A:473:VAL:HG22	1:B:78:LEU:CD2	2.46	0.45
1:B:82:GLY:HA2	4:B:6586:HOH:O	2.15	0.45
1:B:378:GLU:O	1:B:381:PRO:HD3	2.16	0.45
1:C:80:GLN:HG2	1:D:465:ASP:CB	2.46	0.45
1:C:290:LEU:HD22	1:C:294:LEU:CD1	2.46	0.45
1:A:386:LEU:HD13	1:A:386:LEU:O	2.17	0.45
1:C:312:LYS:HG3	4:C:7714:HOH:O	2.15	0.45
1:D:127:GLN:HB3	1:D:128:MET:H	1.64	0.45
1:D:300:LYS:O	1:D:304:GLU:HG3	2.17	0.45
1:A:334:ASN:HB2	1:A:337:ASP:OD1	2.17	0.45
1:B:18:CYS:HB2	1:B:24:GLU:HG2	1.98	0.45
1:A:309:PHE:HB3	1:A:314:SER:OG	2.17	0.45
1:C:76:THR:HA	1:C:96:ARG:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:290:LEU:HD22	1:C:294:LEU:HD11	1.99	0.45
1:D:157:PHE:CE1	1:D:315:ILE:HD12	2.52	0.45
1:A:167:LEU:HD22	1:A:254:ILE:HD13	1.99	0.45
1:A:283:LEU:HD22	1:A:291:TYR:HB2	1.98	0.45
1:B:444:GLY:O	1:B:524:MET:SD	2.74	0.45
1:C:371:ARG:HD2	1:C:371:ARG:C	2.38	0.45
1:C:386:LEU:HD21	1:C:407:CYS:SG	2.56	0.45
1:B:376:LEU:HD23	1:B:417:MET:HE3	1.99	0.44
1:B:127:GLN:HB3	1:B:128:MET:H	1.59	0.44
1:B:387:HIS:O	1:B:390:ILE:HG22	2.16	0.44
1:D:29:MET:SD	1:D:435:VAL:HG21	2.58	0.44
1:D:332:LEU:HD23	1:D:332:LEU:HA	1.84	0.44
1:A:64:ILE:HG22	1:A:68:LEU:HD22	1.99	0.44
1:B:126:GLY:O	1:B:127:GLN:C	2.56	0.44
1:C:29:MET:CE	1:C:435:VAL:HG21	2.48	0.44
1:C:29:MET:SD	1:C:435:VAL:HG21	2.57	0.44
1:C:141:ILE:HG12	1:C:141:ILE:O	2.18	0.44
1:B:544:GLN:HE21	1:B:544:GLN:HB2	1.58	0.44
1:A:444:GLY:HA3	1:A:525:GLY:HA2	2.00	0.44
1:B:359:TRP:HA	1:B:435:VAL:O	2.17	0.44
1:B:521:ASP:HB3	1:B:522:PRO:HD3	2.00	0.44
1:C:355:GLY:HA3	1:C:442:ASP:OD1	2.17	0.44
1:C:75:GLU:HB3	1:C:87:MET:HE3	2.00	0.44
1:C:232:LEU:HD13	1:C:234:ILE:HG13	2.00	0.44
1:D:446:VAL:HG11	1:D:452:GLU:HG2	2.00	0.44
1:A:91:HIS:CD2	1:B:93:GLN:OE1	2.70	0.44
1:A:433:PRO:HB3	1:A:505:ASP:HA	2.00	0.44
1:B:292:VAL:CG1	1:B:296:LYS:HE3	2.48	0.44
1:C:16:LEU:HD11	1:C:21:TRP:CE2	2.53	0.44
1:D:180:LEU:O	1:D:184:MET:HG3	2.18	0.44
1:A:406:ILE:HG23	1:A:406:ILE:O	2.18	0.43
1:A:446:VAL:HG23	1:A:497:HIS:HB3	1.99	0.43
1:D:379:LEU:HD11	1:D:420:ALA:HB2	2.00	0.43
1:A:49:GLY:HA3	1:A:127:GLN:NE2	2.33	0.43
1:C:91:HIS:HE1	1:D:477:ALA:O	2.02	0.43
1:C:376:LEU:HD23	1:C:417:MET:CE	2.21	0.43
1:D:56:ARG:NH2	4:D:8670:HOH:O	2.48	0.43
1:D:379:LEU:HD22	1:D:416:LYS:HE2	1.99	0.43
1:D:524:MET:CE	1:D:528:ARG:HB2	2.47	0.43
1:A:152:LEU:O	1:A:152:LEU:HD23	2.18	0.43
1:A:281:ASP:O	1:A:285:GLN:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:390:ILE:HG23	1:D:391:ASP:N	2.33	0.43
1:A:197:LYS:HE3	1:A:197:LYS:HB2	1.86	0.43
1:A:472:LEU:HB3	1:B:98:LEU:HG	2.01	0.43
1:B:171:LEU:O	1:B:202:ARG:HD3	2.18	0.43
1:B:174:MET:HA	1:B:174:MET:CE	2.49	0.43
1:D:283:LEU:HD13	1:D:291:TYR:CD1	2.54	0.43
1:A:465:ASP:CB	1:B:80:GLN:HG2	2.48	0.43
1:C:363:SER:HB3	1:C:432:ALA:HB3	2.00	0.43
1:A:373:ASP:HB3	1:A:390:ILE:HD11	1.99	0.43
1:C:178:GLN:N	1:C:179:PRO:HD2	2.34	0.43
1:D:288:PRO:O	1:D:292:VAL:HG23	2.18	0.43
1:A:49:GLY:HA3	1:A:127:GLN:HE21	1.83	0.43
1:B:242:GLU:HB2	1:B:273:GLU:OE2	2.19	0.43
1:C:544:GLN:HE21	1:C:544:GLN:HB2	1.63	0.43
1:D:360:ALA:HB3	1:D:435:VAL:HG22	2.01	0.43
1:D:411:TYR:CE2	1:D:544:GLN:HG2	2.54	0.43
1:A:268:ILE:HD13	1:A:284:ARG:HD3	2.01	0.42
1:A:415:LYS:HE3	1:A:515:ALA:HB1	2.00	0.42
1:B:178:GLN:N	1:B:179:PRO:HD2	2.33	0.42
1:C:424:LEU:HB3	1:C:430:LEU:HG	2.00	0.42
1:A:115:HIS:O	1:A:119:LYS:CG	2.67	0.42
1:C:79:VAL:HB	1:C:99:LEU:HG	2.01	0.42
1:C:152:LEU:HD23	1:C:152:LEU:C	2.38	0.42
1:C:157:PHE:CE1	1:C:315:ILE:HD12	2.54	0.42
1:A:232:LEU:HD23	1:A:233:SER:N	2.34	0.42
1:B:342:VAL:HG21	1:B:452:GLU:HA	2.01	0.42
1:A:143:GLN:HB2	1:A:389:TRP:CZ2	2.55	0.42
1:C:293:ARG:NH2	4:C:7662:HOH:O	2.53	0.42
1:B:227:LEU:C	1:B:229:GLY:H	2.22	0.42
1:D:307:LEU:O	1:D:311:GLN:HG3	2.19	0.42
1:B:386:LEU:HD13	1:B:386:LEU:O	2.19	0.42
1:C:78:LEU:CD2	1:D:473:VAL:HG22	2.49	0.42
1:C:449:PRO:HD3	1:D:105:VAL:HG21	2.00	0.42
1:D:293:ARG:NH1	4:D:8648:HOH:O	2.51	0.42
1:A:80:GLN:HG2	1:B:465:ASP:HB2	2.02	0.42
1:B:162:LYS:HA	1:B:186:GLU:O	2.19	0.42
1:C:99:LEU:N	1:C:99:LEU:HD12	2.34	0.42
1:C:512:GLU:OE2	1:C:516:ARG:NH2	2.53	0.42
1:A:376:LEU:HA	1:A:417:MET:HE1	2.01	0.42
1:C:129:THR:CG2	1:C:134:ILE:HG23	2.50	0.42
1:C:126:GLY:O	1:C:127:GLN:C	2.57	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:466:TRP:HE3	1:D:524:MET:CE	2.30	0.41
1:C:72:LYS:C	1:C:74:ASP:N	2.72	0.41
1:C:96:ARG:HA	1:C:96:ARG:NE	2.35	0.41
1:D:26:VAL:HG22	1:D:481:TRP:CE3	2.55	0.41
1:D:75:GLU:HB3	1:D:87:MET:HE1	2.02	0.41
1:A:449:PRO:HD3	1:B:105:VAL:HG21	2.02	0.41
1:C:29:MET:HE1	1:C:435:VAL:HG21	2.03	0.41
1:C:108:TRP:CH2	1:D:449:PRO:HB2	2.55	0.41
1:D:110:ASP:CG	1:D:112:GLU:HG2	2.41	0.41
1:A:185:ASN:O	1:A:186:GLU:HB2	2.20	0.41
1:C:359:TRP:HA	1:C:435:VAL:O	2.20	0.41
1:C:390:ILE:HG23	1:C:391:ASP:N	2.36	0.41
1:A:449:PRO:HB2	1:B:108:TRP:CH2	2.56	0.41
1:C:180:LEU:HD22	1:C:184:MET:HG3	2.01	0.41
1:A:16:LEU:N	1:A:16:LEU:CD1	2.84	0.41
1:C:259:ASP:HB2	4:C:7614:HOH:O	2.20	0.41
1:D:119:LYS:HG2	1:D:119:LYS:H	1.58	0.41
1:D:379:LEU:HD23	1:D:379:LEU:HA	1.92	0.41
1:A:521:ASP:HB3	1:A:522:PRO:HD3	2.03	0.41
1:C:541:ALA:HA	1:C:546:ILE:HB	2.02	0.41
1:D:75:GLU:HB3	1:D:87:MET:CE	2.51	0.41
1:D:518:LEU:HD23	1:D:518:LEU:HA	1.88	0.41
1:B:163:GLY:O	1:B:226:LYS:HE3	2.21	0.41
3:C:7555:NAD:C4N	4:C:7663:HOH:O	2.69	0.41
1:D:16:LEU:HD12	1:D:16:LEU:H	1.86	0.41
1:D:232:LEU:HD13	1:D:234:ILE:HD11	2.03	0.41
1:D:466:TRP:CE3	1:D:524:MET:CE	3.04	0.41
1:A:129:THR:HG22	1:A:134:ILE:HG23	2.03	0.41
1:C:194:VAL:HG22	1:C:194:VAL:O	2.21	0.41
1:D:157:PHE:HE1	1:D:315:ILE:HD12	1.86	0.41
1:C:411:TYR:CE2	1:C:544:GLN:HB3	2.56	0.40
1:D:342:VAL:HA	1:D:346:ILE:HB	2.03	0.40
1:D:500:MET:HE1	1:D:517:VAL:HG13	2.03	0.40
1:B:60:ALA:O	1:B:64:ILE:HG13	2.21	0.40
1:D:178:GLN:N	1:D:179:PRO:HD2	2.36	0.40
1:D:500:MET:HE2	1:D:517:VAL:HG22	2.04	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	542/552 (98%)	520 (96%)	22 (4%)	0	100	100
1	B	544/552 (99%)	520 (96%)	24 (4%)	0	100	100
1	C	542/552 (98%)	518 (96%)	24 (4%)	0	100	100
1	D	542/552 (98%)	518 (96%)	22 (4%)	2 (0%)	34	37
All	All	2170/2208 (98%)	2076 (96%)	92 (4%)	2 (0%)	51	60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	451	ARG
1	D	106	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	432/440 (98%)	399 (92%)	33 (8%)	13	14
1	B	434/440 (99%)	406 (94%)	28 (6%)	17	19
1	C	432/440 (98%)	401 (93%)	31 (7%)	14	15
1	D	432/440 (98%)	400 (93%)	32 (7%)	13	14
All	All	1730/1760 (98%)	1606 (93%)	124 (7%)	14	15

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ARG
1	A	23	GLN
1	A	24	GLU
1	A	33	ASN
1	A	56	ARG
1	A	68	LEU
1	A	87	MET
1	A	98	LEU
1	A	119	LYS
1	A	122	LEU
1	A	180	LEU
1	A	202	ARG
1	A	214	SER
1	A	227	LEU
1	A	232	LEU
1	A	237	LEU
1	A	253	LYS
1	A	283	LEU
1	A	290	LEU
1	A	332	LEU
1	A	333	GLU
1	A	371	ARG
1	A	375	LEU
1	A	386	LEU
1	A	394	GLN
1	A	423	GLU
1	A	472	LEU
1	A	500	MET
1	A	509	LEU
1	A	516	ARG
1	A	524	MET
1	A	528	ARG
1	A	544	GLN
1	B	23	GLN
1	B	33	ASN
1	B	56	ARG
1	B	68	LEU
1	B	87	MET
1	B	98	LEU
1	B	122	LEU
1	B	123	MET
1	B	180	LEU
1	B	183	THR

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Mol	Chain	Res	Type
1	B	202	ARG
1	B	216	GLU
1	B	232	LEU
1	B	237	LEU
1	B	250	ARG
1	B	253	LYS
1	B	283	LEU
1	B	290	LEU
1	B	332	LEU
1	B	375	LEU
1	B	434	VAL
1	B	472	LEU
1	B	500	MET
1	B	509	LEU
1	B	516	ARG
1	B	524	MET
1	B	528	ARG
1	B	544	GLN
1	C	23	GLN
1	C	56	ARG
1	C	68	LEU
1	C	87	MET
1	C	93	GLN
1	C	98	LEU
1	C	119	LYS
1	C	122	LEU
1	C	180	LEU
1	C	183	THR
1	C	202	ARG
1	C	227	LEU
1	C	232	LEU
1	C	237	LEU
1	C	244	HIS
1	C	248	LEU
1	C	283	LEU
1	C	290	LEU
1	C	332	LEU
1	C	333	GLU
1	C	339	PRO
1	C	371	ARG
1	C	375	LEU
1	C	434	VAL

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Mol	Chain	Res	Type
1	C	472	LEU
1	C	473	VAL
1	C	500	MET
1	C	509	LEU
1	C	524	MET
1	C	528	ARG
1	C	544	GLN
1	D	9	ARG
1	D	23	GLN
1	D	56	ARG
1	D	68	LEU
1	D	87	MET
1	D	98	LEU
1	D	119	LYS
1	D	122	LEU
1	D	180	LEU
1	D	183	THR
1	D	202	ARG
1	D	227	LEU
1	D	232	LEU
1	D	237	LEU
1	D	253	LYS
1	D	282	ARG
1	D	283	LEU
1	D	290	LEU
1	D	312	LYS
1	D	314	SER
1	D	332	LEU
1	D	333	GLU
1	D	371	ARG
1	D	375	LEU
1	D	417	MET
1	D	472	LEU
1	D	500	MET
1	D	509	LEU
1	D	516	ARG
1	D	524	MET
1	D	528	ARG
1	D	544	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	HIS
1	A	544	GLN
1	B	91	HIS
1	B	244	HIS
1	B	544	GLN
1	C	23	GLN
1	C	73	ASN
1	C	249	ASN
1	C	544	GLN
1	D	91	HIS
1	D	244	HIS
1	D	544	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

8 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	B	6555	-	42,48,48	1.74	4 (9%)	50,73,73	1.59	4 (8%)
2	ACT	C	553	-	3,3,3	2.05	2 (66%)	3,3,3	0.83	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	ACT	D	553	-	3,3,3	2.01	1 (33%)	3,3,3	0.84	0
3	NAD	A	5555	-	42,48,48	1.74	5 (11%)	50,73,73	1.60	4 (8%)
3	NAD	D	8555	-	42,48,48	1.77	6 (14%)	50,73,73	1.60	4 (8%)
3	NAD	C	7555	-	42,48,48	1.72	6 (14%)	50,73,73	1.59	4 (8%)
2	ACT	B	553	-	3,3,3	2.03	2 (66%)	3,3,3	0.74	0
2	ACT	A	553	-	3,3,3	1.93	2 (66%)	3,3,3	0.85	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAD	B	6555	-	-	4/26/62/62	0/5/5/5
3	NAD	A	5555	-	-	4/26/62/62	0/5/5/5
3	NAD	D	8555	-	-	4/26/62/62	0/5/5/5
3	NAD	C	7555	-	-	4/26/62/62	0/5/5/5

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	6555	NAD	O7N-C7N	7.33	1.37	1.24
3	D	8555	NAD	O7N-C7N	7.32	1.37	1.24
3	C	7555	NAD	O7N-C7N	6.96	1.37	1.24
3	A	5555	NAD	O7N-C7N	6.91	1.37	1.24
3	A	5555	NAD	C2A-N3A	4.75	1.39	1.32
3	B	6555	NAD	C2A-N3A	4.62	1.39	1.32
3	D	8555	NAD	C2A-N3A	4.25	1.38	1.32
3	C	7555	NAD	C2A-N3A	4.12	1.38	1.32
3	A	5555	NAD	C2A-N1A	3.81	1.40	1.33
3	C	7555	NAD	C2A-N1A	3.74	1.40	1.33
3	D	8555	NAD	C2A-N1A	3.56	1.40	1.33
3	B	6555	NAD	C2A-N1A	3.56	1.40	1.33
3	D	8555	NAD	C2N-N1N	3.40	1.38	1.35
3	B	6555	NAD	C2N-N1N	3.12	1.38	1.35
3	A	5555	NAD	C2N-N1N	3.11	1.38	1.35
2	D	553	ACT	O-C	2.86	1.34	1.22
3	C	7555	NAD	PN-O3	2.82	1.62	1.59
2	C	553	ACT	O-C	2.80	1.34	1.22
2	B	553	ACT	O-C	2.78	1.34	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	553	ACT	O-C	2.65	1.33	1.22
3	C	7555	NAD	C2N-N1N	2.64	1.37	1.35
3	D	8555	NAD	C4N-C3N	2.28	1.42	1.39
3	C	7555	NAD	C4N-C3N	2.22	1.42	1.39
2	B	553	ACT	OXT-C	-2.16	1.20	1.30
3	A	5555	NAD	C4N-C3N	2.13	1.42	1.39
2	C	553	ACT	OXT-C	-2.13	1.21	1.30
3	D	8555	NAD	C6N-N1N	2.05	1.40	1.35
2	A	553	ACT	OXT-C	-2.00	1.21	1.30

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	8555	NAD	C4B-O4B-C1B	-6.27	104.18	109.92
3	B	6555	NAD	C4B-O4B-C1B	-6.26	104.19	109.92
3	C	7555	NAD	N3A-C2A-N1A	-6.02	120.50	128.67
3	D	8555	NAD	N3A-C2A-N1A	-6.02	120.50	128.67
3	B	6555	NAD	N3A-C2A-N1A	-5.94	120.61	128.67
3	A	5555	NAD	C4B-O4B-C1B	-5.94	104.49	109.92
3	C	7555	NAD	C4B-O4B-C1B	-5.92	104.51	109.92
3	A	5555	NAD	N3A-C2A-N1A	-5.91	120.65	128.67
3	C	7555	NAD	C3N-C7N-N7N	4.76	123.60	117.74
3	A	5555	NAD	C3N-C7N-N7N	4.75	123.59	117.74
3	B	6555	NAD	C3N-C7N-N7N	4.48	123.25	117.74
3	D	8555	NAD	C3N-C7N-N7N	4.39	123.15	117.74
3	D	8555	NAD	O7N-C7N-N7N	-2.82	118.54	122.62
3	B	6555	NAD	O7N-C7N-N7N	-2.68	118.74	122.62
3	C	7555	NAD	O7N-C7N-N7N	-2.67	118.76	122.62
3	A	5555	NAD	O7N-C7N-N7N	-2.50	119.01	122.62

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	5555	NAD	O4D-C1D-N1N-C2N
3	A	5555	NAD	O4D-C1D-N1N-C6N
3	A	5555	NAD	C2D-C1D-N1N-C2N
3	A	5555	NAD	C2D-C1D-N1N-C6N
3	B	6555	NAD	O4D-C1D-N1N-C2N
3	B	6555	NAD	O4D-C1D-N1N-C6N
3	B	6555	NAD	C2D-C1D-N1N-C2N
3	B	6555	NAD	C2D-C1D-N1N-C6N

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Mol	Chain	Res	Type	Atoms
3	C	7555	NAD	O4D-C1D-N1N-C2N
3	C	7555	NAD	O4D-C1D-N1N-C6N
3	C	7555	NAD	C2D-C1D-N1N-C2N
3	C	7555	NAD	C2D-C1D-N1N-C6N
3	D	8555	NAD	O4D-C1D-N1N-C2N
3	D	8555	NAD	O4D-C1D-N1N-C6N
3	D	8555	NAD	C2D-C1D-N1N-C2N
3	D	8555	NAD	C2D-C1D-N1N-C6N

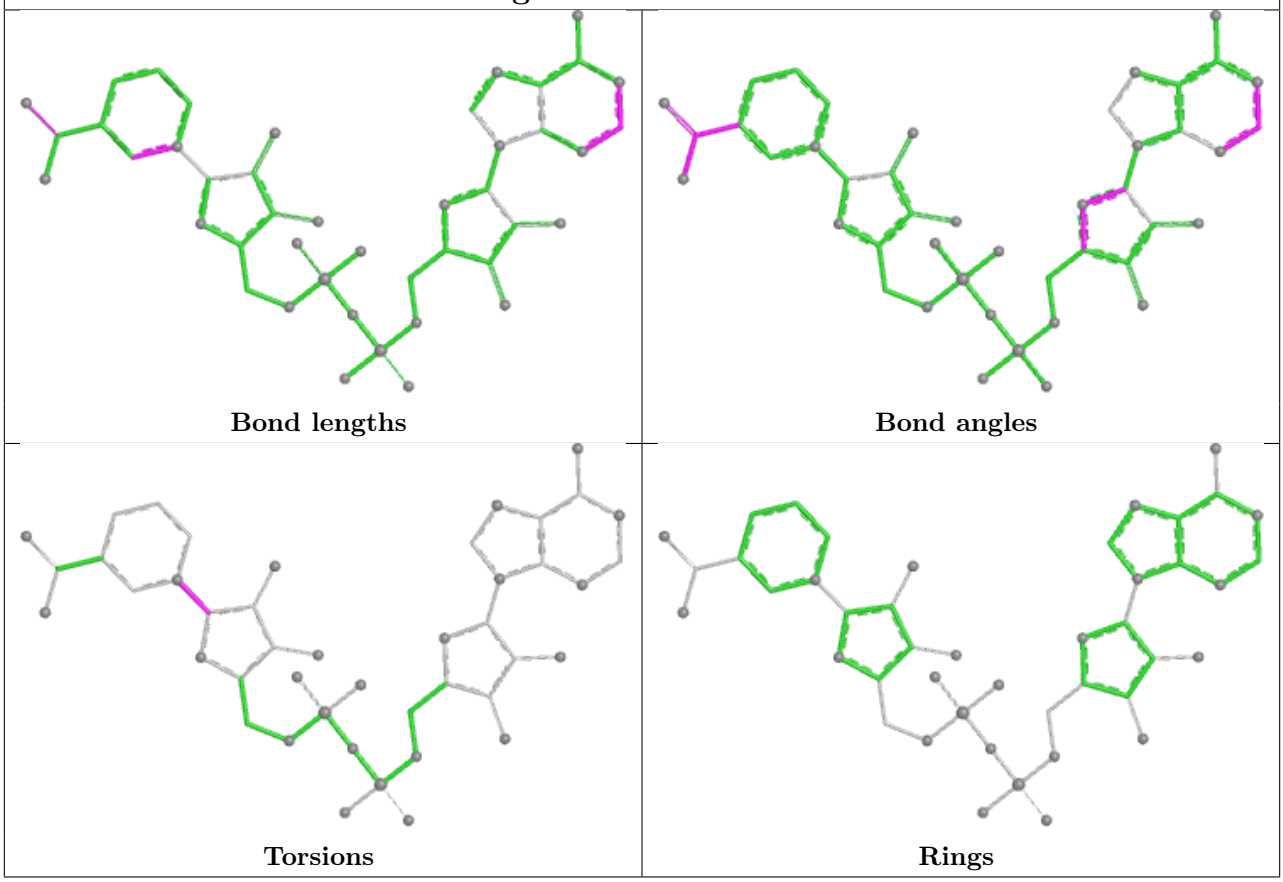
There are no ring outliers.

4 monomers are involved in 4 short contacts:

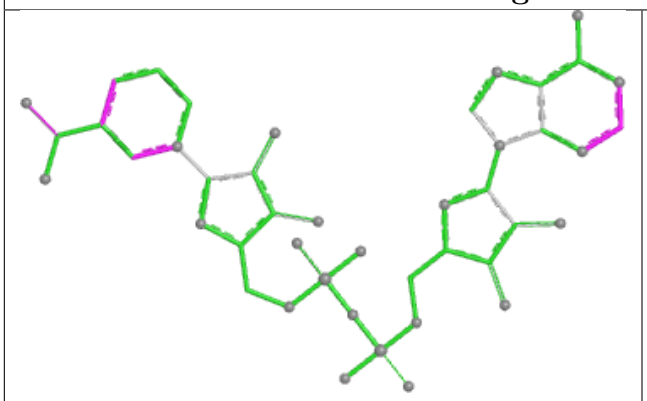
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	6555	NAD	1	0
2	C	553	ACT	1	0
3	C	7555	NAD	1	0
2	B	553	ACT	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

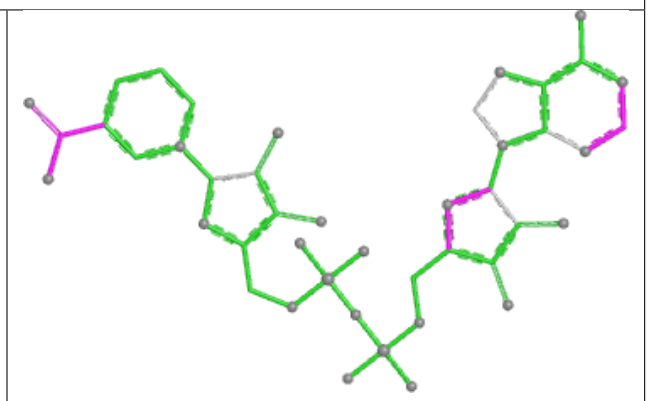
Ligand NAD B 6555



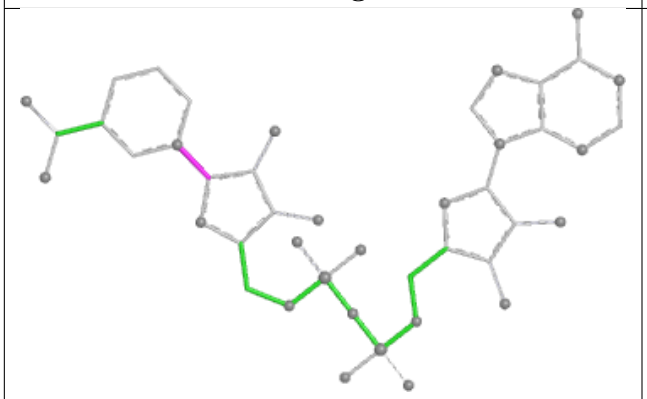
Ligand NAD A 5555



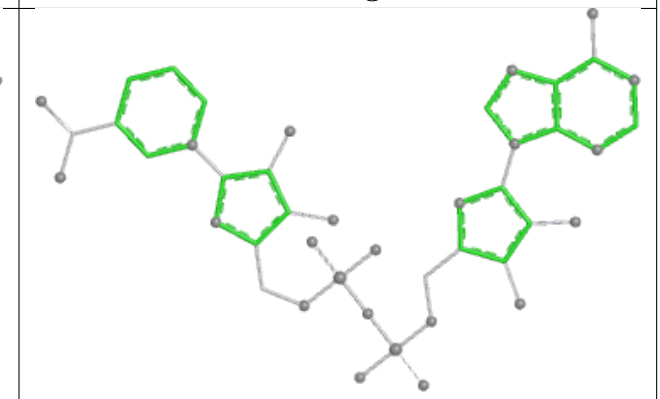
Bond lengths



Bond angles

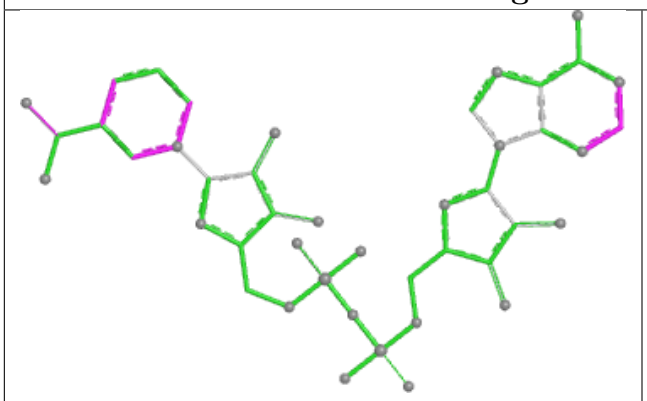


Torsions

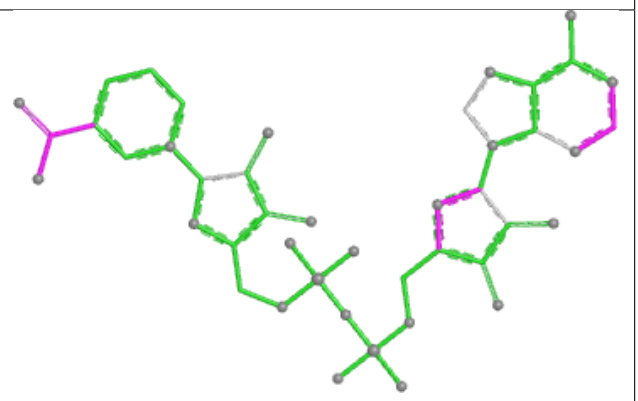


Rings

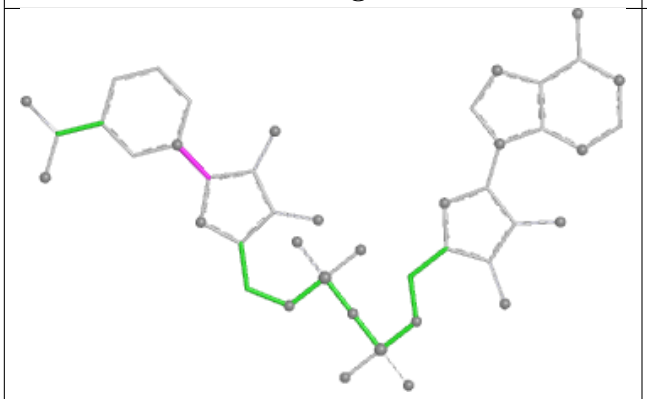
Ligand NAD D 8555



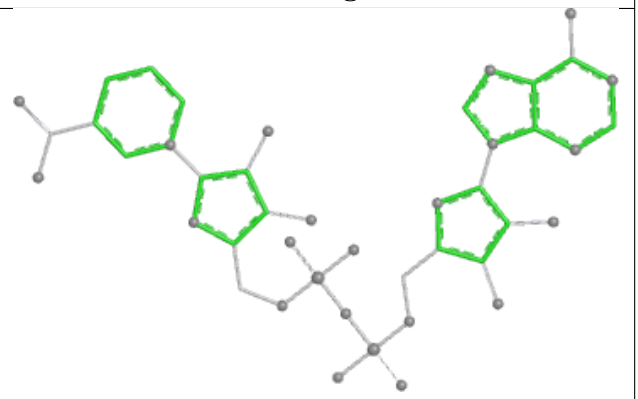
Bond lengths



Bond angles

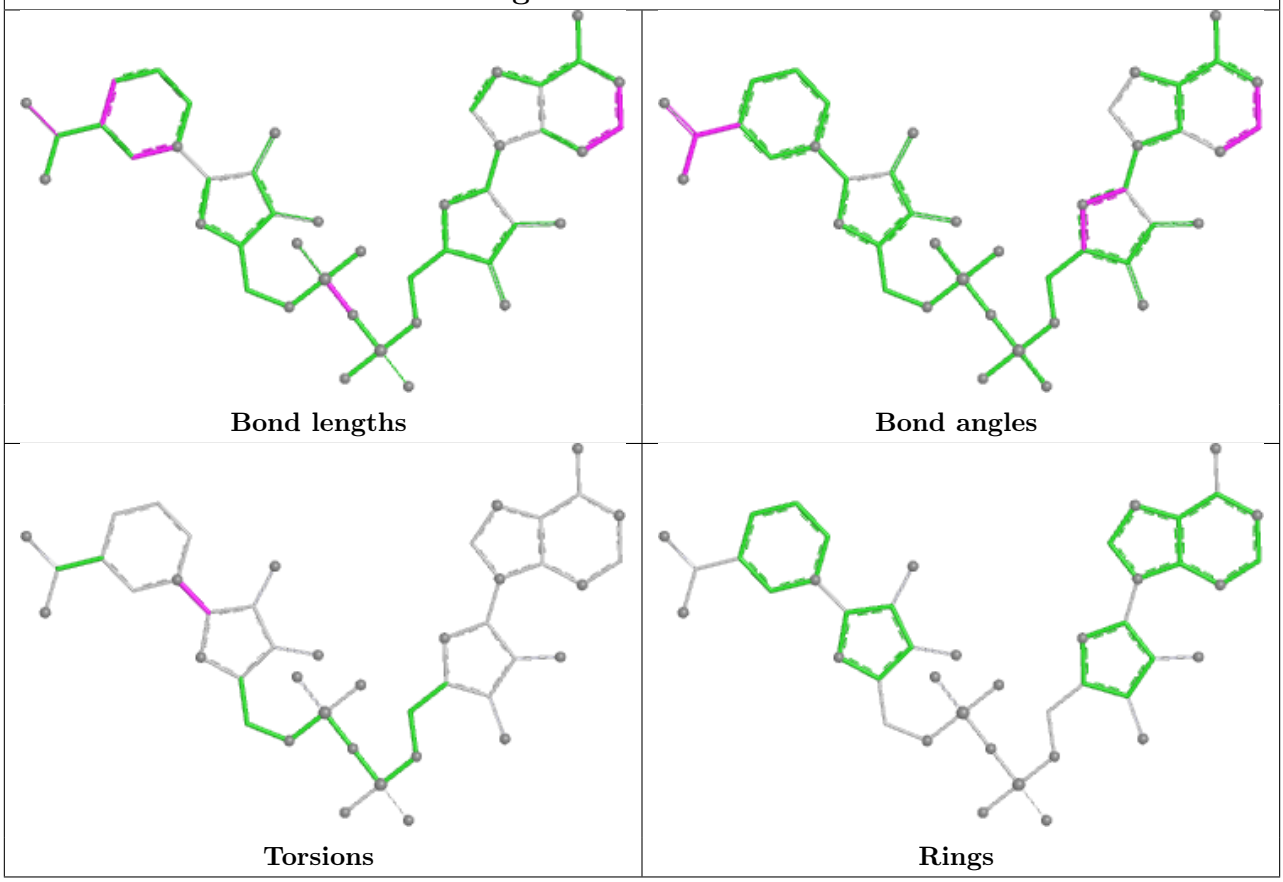


Torsions



Rings

Ligand NAD C 7555



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	544/552 (98%)	-0.36	5 (0%)	84	83	16, 25, 38, 53	0
1	B	546/552 (98%)	-0.32	5 (0%)	84	83	17, 27, 42, 55	0
1	C	544/552 (98%)	-0.39	0	100	100	17, 25, 38, 52	0
1	D	544/552 (98%)	-0.31	0	100	100	18, 29, 42, 62	0
All	All	2178/2208 (98%)	-0.34	10 (0%)	91	90	16, 26, 40, 62	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	227	LEU	3.8
1	A	227	LEU	2.6
1	A	282	ARG	2.6
1	B	524	MET	2.6
1	A	524	MET	2.5
1	A	498	ALA	2.5
1	B	484	PHE	2.4
1	A	468	VAL	2.1
1	B	250	ARG	2.1
1	B	473	VAL	2.1

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

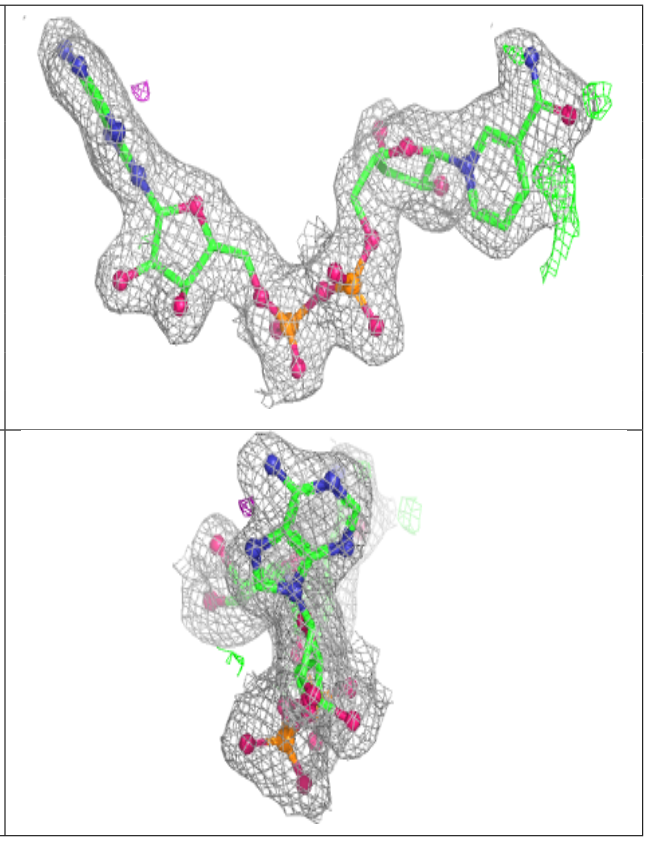
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ACT	B	553	4/4	0.88	0.23	27,28,28,29	0
2	ACT	D	553	4/4	0.92	0.16	25,26,26,27	0
3	NAD	B	6555	44/44	0.95	0.11	21,25,28,30	0
3	NAD	D	8555	44/44	0.95	0.12	24,28,30,34	0
3	NAD	C	7555	44/44	0.96	0.11	18,22,24,26	0
3	NAD	A	5555	44/44	0.97	0.09	18,22,27,29	0
2	ACT	A	553	4/4	0.98	0.11	22,22,23,25	0
2	ACT	C	553	4/4	0.99	0.11	18,20,20,23	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.

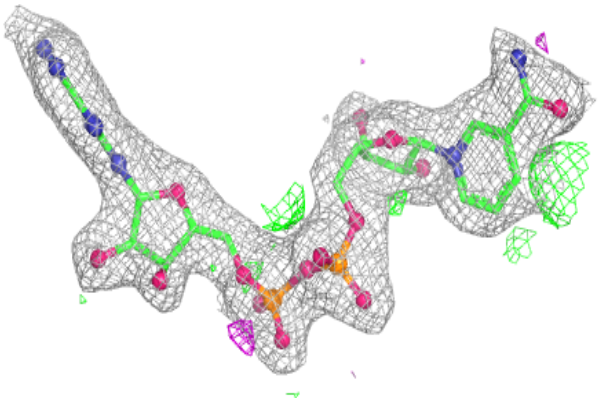
Electron density around NAD B 6555:

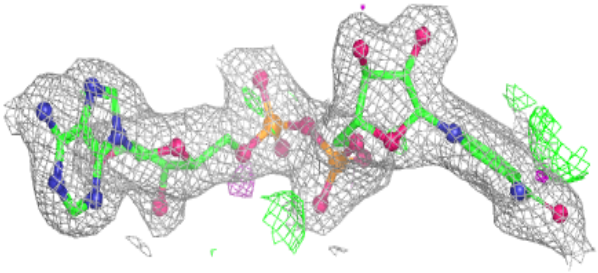
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

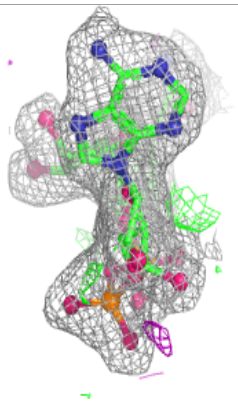


Electron density around NAD D 8555:

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

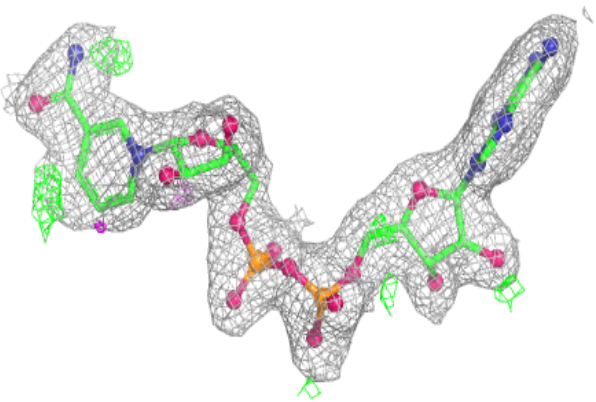


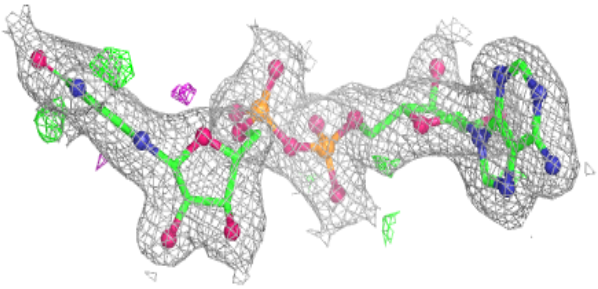


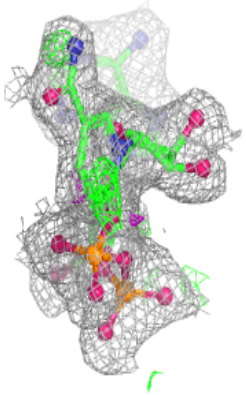


Electron density around NAD C 7555:

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

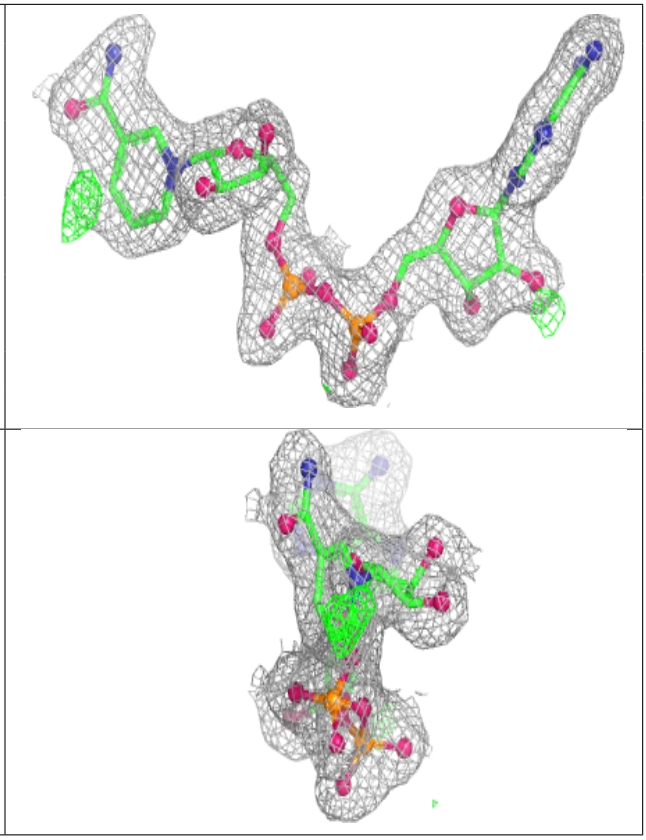






Electron density around NAD A 5555:

$2mF_o$-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.