Full wwPDB X-ray Structure Validation Report (i)

May 13, 2020 – 07:55 am BST

PDB ID	:	3P9U
Title	:	Crystal structure of TetX2 from Bacteroides thetaiotaomicron with substrate analogue
Authors	:	Walkiewicz, K.; Davlieva, M.; Sun, C.; Lau, K.; Shamoo, Y.
Deposited on	:	2010-10-18
Resolution	:	2.81 Å(reported)

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

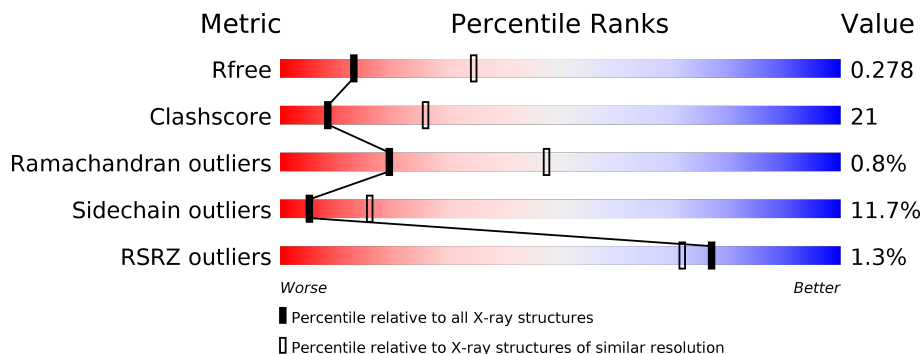|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.81 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	Percentile Ranks	Value
Rfree		0.278
Clashscore		21
Ramachandran outliers		0.8%
Sidechain outliers		11.7%
RSRZ outliers		1.3%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3617 (2.84-2.80)
Clashscore	141614	4060 (2.84-2.80)
Ramachandran outliers	138981	3978 (2.84-2.80)
Sidechain outliers	138945	3980 (2.84-2.80)
RSRZ outliers	127900	3552 (2.84-2.80)

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 on 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	378	2% ▮ 61% 29% 7% •
1	B	378	2% ▮ 60% 30% 7% •
1	C	378	% ▮ 60% 30% 8% •
1	D	378	% ▮ 60% 30% 7% •

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FAD	A	401	X	-	-	-
2	FAD	B	401	X	-	-	-
2	FAD	C	401	X	-	-	-
2	FAD	D	401	X	-	-	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 11909 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.
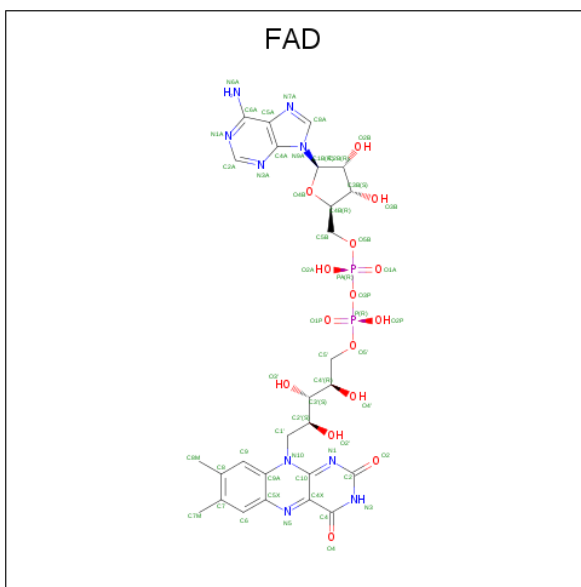
- Molecule 1 is a protein called TetX2 protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	368	Total	C	N	O	S	Se	0	0	0
			2909	1845	498	554	2	10			
1	B	365	Total	C	N	O	S	Se	0	0	0
			2885	1831	493	549	2	10			
1	C	366	Total	C	N	O	S	Se	0	0	0
			2893	1835	495	551	2	10			
1	D	367	Total	C	N	O	S	Se	0	0	0
			2900	1840	496	552	2	10			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	94	LYS	GLU	ENGINEERED MUTATION	UNP Q93L51
A	266	LYS	GLU	ENGINEERED MUTATION	UNP Q93L51
B	94	LYS	GLU	ENGINEERED MUTATION	UNP Q93L51
B	266	LYS	GLU	ENGINEERED MUTATION	UNP Q93L51
C	94	LYS	GLU	ENGINEERED MUTATION	UNP Q93L51
C	266	LYS	GLU	ENGINEERED MUTATION	UNP Q93L51
D	94	LYS	GLU	ENGINEERED MUTATION	UNP Q93L51
D	266	LYS	GLU	ENGINEERED MUTATION	UNP Q93L51

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).
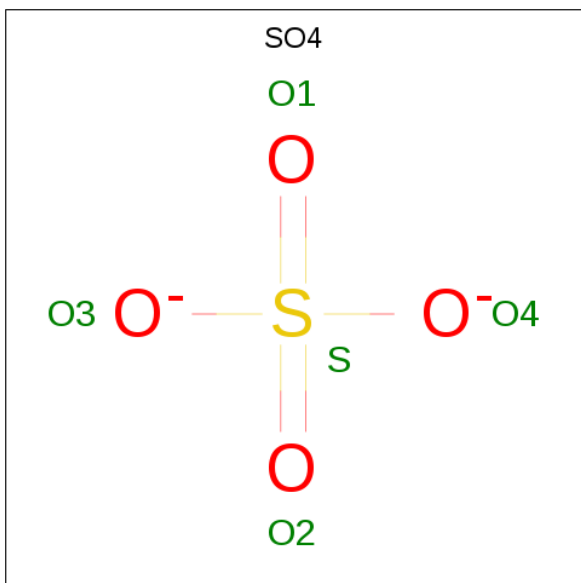
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 5	O 4	S 1	0	0
3	B	1	Total 5	O 4	S 1	0	0
3	C	1	Total 5	O 4	S 1	0	0
3	D	1	Total 5	O 4	S 1	0	0

- Molecule 4 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	23	Total 23	O 23	0	0
4	B	18	Total 18	O 18	0	0
4	C	22	Total 22	O 22	0	0
4	D	27	Total 27	O 27	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.
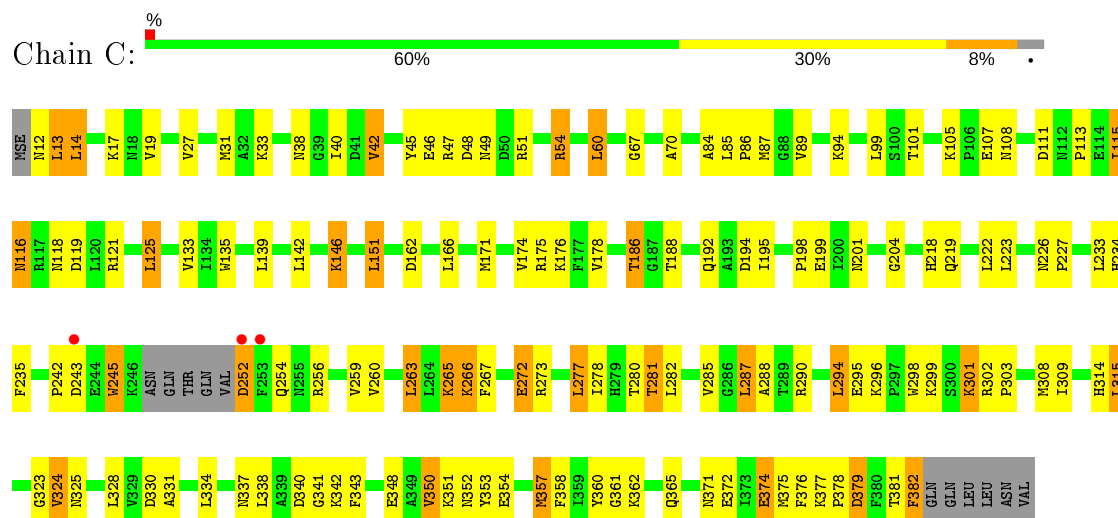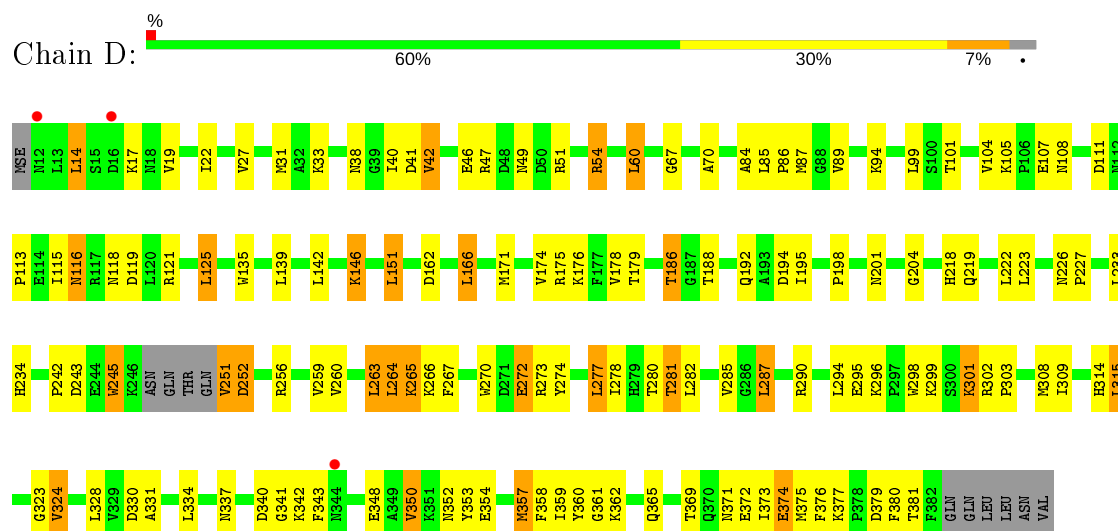
- Molecule 1: TetX2 protein
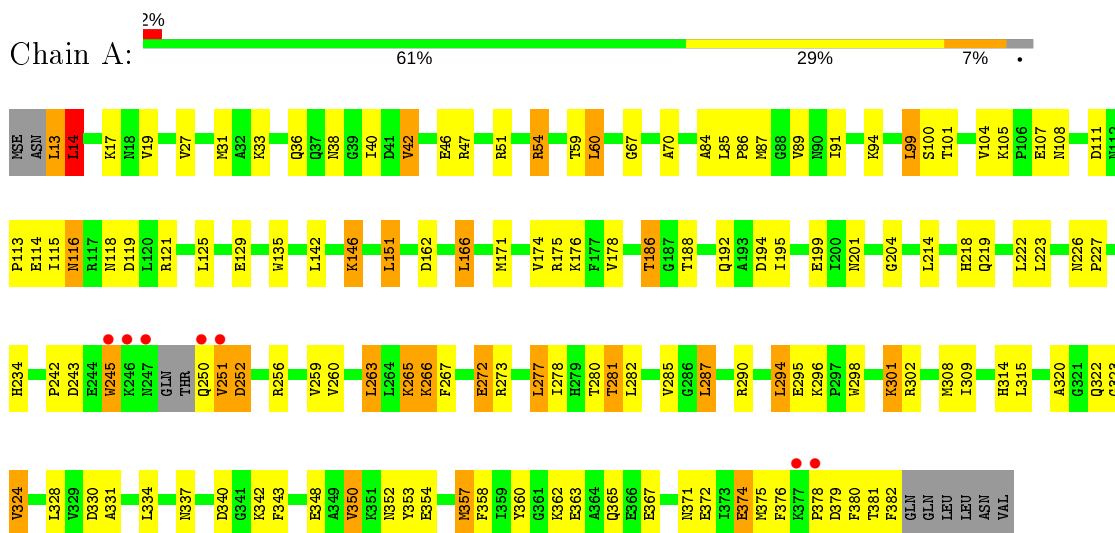
- Molecule 1: TetX2 protein

- Molecule 1: TetX2 protein

Chain C:

• Molecule 1: TetX2 protein

Chain D:
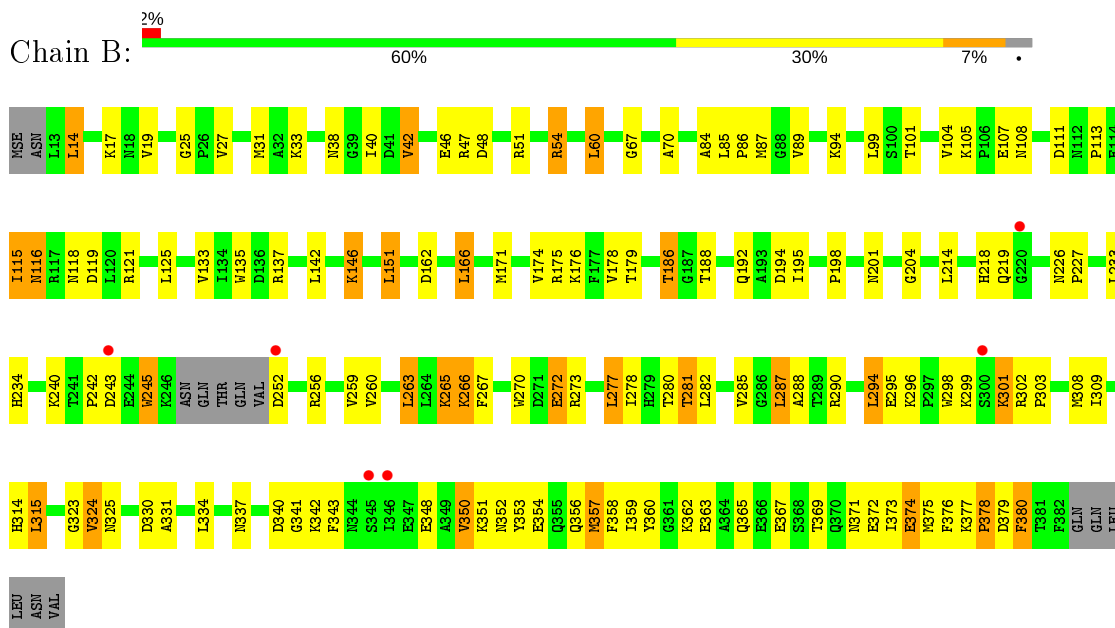
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	87.70Å　67.33Å　153.79Å 90.00°　100.31°　90.00°	Depositor
Resolution (Å)	48.45　–　2.81 48.45　–　2.81	Depositor EDS
% Data completeness (in resolution range)	88.3 (48.45-2.81) 88.5 (48.45-2.81)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	25.80 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.6.4_486	Depositor
R, R_{free}	0.238　,　0.282 0.235　,　0.278	Depositor DCC
R_{free} test set	2000 reflections (5.20%)	wwPDB-VP
Wilson B-factor (Å²)	28.7	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent k_{sol}(e/Å³), B_{sol}(Å²)	0.34 , 42.4	EDS
L-test for twinning[2]	$<|L|> = 0.52$, $<L^2> = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	11909	wwPDB-VP
Average B, all atoms (Å²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 52.69 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.6901e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[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: SO4, FAD

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	0.48	0/2957	0.62	2/3978 (0.1%)
1	B	0.46	0/2933	0.61	1/3945 (0.0%)
1	C	0.47	0/2941	0.62	0/3956
1	D	0.48	0/2948	0.61	0/3966
All	All	0.47	0/11779	0.62	3/15845 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	214	LEU	CA-CB-CG	5.32	127.53	115.30
1	A	214	LEU	CA-CB-CG	5.15	127.15	115.30
1	A	14	LEU	CB-CG-CD2	5.12	119.69	111.00

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	2909	0	2880	130	0
1	B	2885	0	2857	120	0
1	C	2893	0	2863	123	0
1	D	2900	0	2872	118	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	53	0	29	1	0
2	B	53	0	29	2	0
2	C	53	0	29	1	0
2	D	53	0	29	2	0
3	A	5	0	0	0	0
3	B	5	0	0	1	0
3	C	5	0	0	1	0
3	D	5	0	0	0	0
4	A	23	0	0	0	0
4	B	18	0	0	2	0
4	C	22	0	0	2	0
4	D	27	0	0	1	0
All	All	11909	0	11588	487	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 21.

All (487) 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:D:31:MSE:HE2	1:D:331:ALA:HA	1.31	1.13
1:B:31:MSE:HE2	1:B:331:ALA:HA	1.26	1.10
1:A:31:MSE:HE2	1:A:331:ALA:HA	1.26	1.09
1:A:100:SER:HB2	1:D:359:ILE:HD11	1.35	1.08
1:C:31:MSE:HE2	1:C:331:ALA:HA	1.29	1.07
1:B:31:MSE:HE1	1:B:334:LEU:HB3	1.38	1.05
1:A:100:SER:HB2	1:D:359:ILE:CD1	1.86	1.05
1:D:31:MSE:HE1	1:D:334:LEU:HB3	1.34	1.04
1:C:31:MSE:HE1	1:C:334:LEU:HB3	1.37	1.03
1:A:31:MSE:HE1	1:A:334:LEU:HB3	1.37	1.02
1:C:175:ARG:HG2	1:C:308:MSE:SE	2.11	1.00
1:D:175:ARG:HG2	1:D:308:MSE:SE	2.14	0.97
1:A:175:ARG:HG2	1:A:308:MSE:SE	2.17	0.94
1:C:14:LEU:HD12	1:C:14:LEU:H	1.31	0.94
1:C:116:ASN:HD22	1:C:119:ASP:H	1.16	0.93
1:A:337:ASN:HD21	1:A:352:ASN:HD22	1.14	0.93
1:B:175:ARG:HG2	1:B:308:MSE:SE	2.20	0.92
1:B:337:ASN:HD21	1:B:352:ASN:HD22	1.07	0.92
1:D:14:LEU:H	1:D:14:LEU:HD12	1.34	0.92
1:A:116:ASN:HD22	1:A:119:ASP:H	1.19	0.91
1:B:116:ASN:HD22	1:B:119:ASP:H	1.12	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:LEU:HD12	1:B:14:LEU:H	1.35	0.90
1:C:337:ASN:HD21	1:C:352:ASN:HD22	1.09	0.90
1:D:337:ASN:HD21	1:D:352:ASN:HD22	1.16	0.88
1:D:116:ASN:HD22	1:D:119:ASP:H	1.21	0.87
1:A:14:LEU:H	1:A:14:LEU:HD23	1.38	0.87
1:D:54:ARG:H	1:D:54:ARG:HE	1.23	0.85
1:A:54:ARG:H	1:A:54:ARG:HE	1.19	0.84
1:B:54:ARG:H	1:B:54:ARG:HE	1.26	0.84
1:C:54:ARG:H	1:C:54:ARG:HE	1.26	0.83
1:A:91:ILE:HD12	1:A:382:PHE:CD2	2.15	0.81
1:B:116:ASN:ND2	1:B:119:ASP:H	1.78	0.81
1:C:226:ASN:HB2	3:C:1:SO4:O4	1.80	0.81
1:C:263:LEU:HB3	1:C:278:ILE:HD13	1.61	0.81
1:A:91:ILE:HD12	1:A:382:PHE:HD2	1.44	0.81
1:C:116:ASN:ND2	1:C:119:ASP:H	1.78	0.80
1:A:263:LEU:HB3	1:A:278:ILE:HD13	1.63	0.80
1:B:263:LEU:HB3	1:B:278:ILE:HD13	1.64	0.80
1:D:263:LEU:HB3	1:D:278:ILE:HD13	1.66	0.78
1:A:116:ASN:ND2	1:A:119:ASP:H	1.81	0.77
1:C:31:MSE:HE3	1:C:309:ILE:HG21	1.67	0.76
1:D:31:MSE:HE3	1:D:309:ILE:HG21	1.67	0.76
1:C:14:LEU:H	1:C:14:LEU:CD1	1.97	0.76
1:A:375:MSE:HE2	1:A:380:PHE:CE2	2.20	0.76
1:D:116:ASN:ND2	1:D:119:ASP:H	1.84	0.76
1:D:14:LEU:H	1:D:14:LEU:CD1	1.98	0.76
1:B:31:MSE:HE3	1:B:309:ILE:HG21	1.67	0.75
1:B:350:VAL:O	1:B:354:GLU:HG3	1.85	0.75
1:D:301:LYS:HD3	1:D:301:LYS:H	1.52	0.75
1:A:31:MSE:HE3	1:A:309:ILE:HG21	1.67	0.74
1:B:14:LEU:CD1	1:B:14:LEU:H	2.00	0.74
1:C:295:GLU:HG3	1:C:296:LYS:H	1.53	0.74
1:C:301:LYS:H	1:C:301:LYS:HD3	1.52	0.73
1:A:14:LEU:CD2	1:A:14:LEU:H	2.01	0.73
1:B:186:THR:HG21	1:B:372:GLU:OE1	1.89	0.73
1:B:295:GLU:HG3	1:B:296:LYS:H	1.53	0.72
1:B:84:ALA:HB1	1:B:113:PRO:HB2	1.72	0.72
1:B:277:LEU:O	1:B:281:THR:HG22	1.90	0.71
1:A:295:GLU:HG3	1:A:296:LYS:H	1.55	0.71
1:A:277:LEU:O	1:A:281:THR:HG22	1.91	0.71
1:B:301:LYS:HD3	1:B:301:LYS:H	1.54	0.71
1:C:350:VAL:O	1:C:354:GLU:HG3	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:MSE:HE1	1:A:334:LEU:CB	2.19	0.70
1:A:171:MSE:HE1	1:A:290:ARG:NE	2.06	0.69
1:D:295:GLU:HG3	1:D:296:LYS:H	1.57	0.69
1:C:31:MSE:HE1	1:C:334:LEU:CB	2.19	0.68
1:D:314:HIS:HE1	1:D:330:ASP:OD2	1.76	0.68
1:A:186:THR:HG21	1:A:372:GLU:OE1	1.93	0.68
1:C:186:THR:HG21	1:C:372:GLU:OE1	1.94	0.68
1:C:171:MSE:HE1	1:C:290:ARG:NE	2.08	0.68
1:A:84:ALA:HB1	1:A:113:PRO:HB2	1.74	0.68
1:C:277:LEU:O	1:C:281:THR:HG22	1.94	0.68
1:C:14:LEU:HD12	1:C:14:LEU:N	2.07	0.68
1:A:100:SER:HB2	1:D:359:ILE:HD12	1.72	0.68
1:B:337:ASN:ND2	1:B:352:ASN:HD22	1.88	0.67
1:D:171:MSE:HE1	1:D:290:ARG:NE	2.09	0.67
1:A:54:ARG:H	1:A:54:ARG:NE	1.92	0.67
1:A:19:VAL:HB	1:A:42:VAL:HG12	1.77	0.67
1:B:337:ASN:HD21	1:B:352:ASN:ND2	1.89	0.67
1:D:31:MSE:HE1	1:D:334:LEU:CB	2.17	0.67
1:B:219:GLN:HA	1:B:378:PRO:O	1.94	0.66
1:C:337:ASN:ND2	1:C:352:ASN:HD22	1.90	0.66
1:A:314:HIS:HE1	1:A:330:ASP:OD2	1.78	0.66
1:D:277:LEU:O	1:D:281:THR:HG22	1.95	0.66
1:D:19:VAL:HB	1:D:42:VAL:HG12	1.77	0.66
1:C:337:ASN:HD21	1:C:352:ASN:ND2	1.90	0.66
1:A:301:LYS:HD3	1:A:301:LYS:H	1.60	0.65
1:D:186:THR:HG21	1:D:372:GLU:OE1	1.96	0.65
1:A:121:ARG:O	1:A:125:LEU:HB2	1.96	0.64
1:A:99:LEU:HB3	1:D:359:ILE:HG23	1.79	0.64
1:C:116:ASN:HD21	1:C:118:ASN:HB2	1.61	0.64
1:A:178:VAL:HG13	1:A:302:ARG:NH1	2.13	0.64
1:C:194:ASP:OD1	1:C:234:HIS:HD2	1.81	0.64
1:D:256:ARG:O	1:D:260:VAL:HG23	1.98	0.64
1:C:219:GLN:HA	1:C:378:PRO:O	1.98	0.63
1:D:375:MSE:HA	1:D:380:PHE:CG	2.33	0.63
1:B:31:MSE:HE1	1:B:334:LEU:CB	2.22	0.63
1:A:350:VAL:O	1:A:354:GLU:HG3	1.97	0.63
1:C:54:ARG:NE	1:C:54:ARG:H	1.95	0.63
1:B:116:ASN:HD21	1:B:118:ASN:HB2	1.63	0.63
1:B:171:MSE:HE1	1:B:290:ARG:NE	2.12	0.63
1:A:108:ASN:HB3	1:A:111:ASP:OD2	1.97	0.62
1:A:372:GLU:O	1:A:376:PHE:HD2	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:171:MSE:HE1	1:C:290:ARG:CZ	2.29	0.62
1:D:17:LYS:HB3	1:D:162:ASP:CG	2.20	0.62
1:D:54:ARG:H	1:D:54:ARG:NE	1.93	0.62
1:A:380:PHE:CE2	1:A:382:PHE:HD1	2.18	0.62
1:C:12:ASN:HB3	1:C:13:LEU:HD13	1.80	0.62
1:D:116:ASN:HD21	1:D:118:ASN:HB2	1.63	0.62
1:D:194:ASP:OD1	1:D:234:HIS:HD2	1.82	0.62
1:D:14:LEU:N	1:D:14:LEU:HD12	2.11	0.62
1:B:178:VAL:HG13	1:B:302:ARG:NH1	2.14	0.62
1:B:31:MSE:HG3	1:B:309:ILE:HD13	1.82	0.62
1:A:194:ASP:OD1	1:A:234:HIS:HD2	1.83	0.62
1:B:314:HIS:HE1	1:B:330:ASP:OD2	1.82	0.61
1:B:105:LYS:HE3	1:B:107:GLU:OE2	2.00	0.61
1:D:108:ASN:HB3	1:D:111:ASP:OD2	2.01	0.61
1:C:121:ARG:O	1:C:125:LEU:HB2	2.00	0.61
1:A:116:ASN:HD21	1:A:118:ASN:HB2	1.64	0.61
1:A:27:VAL:HG12	1:A:309:ILE:HD12	1.83	0.61
1:D:178:VAL:HG13	1:D:302:ARG:NH1	2.15	0.61
1:C:17:LYS:HB3	1:C:162:ASP:CG	2.21	0.61
1:B:121:ARG:O	1:B:125:LEU:HB2	2.00	0.61
1:D:171:MSE:HE1	1:D:290:ARG:CZ	2.30	0.61
1:D:84:ALA:HB1	1:D:113:PRO:HB2	1.82	0.60
1:B:54:ARG:H	1:B:54:ARG:NE	1.96	0.60
1:C:19:VAL:HB	1:C:42:VAL:HG12	1.83	0.60
1:D:350:VAL:O	1:D:354:GLU:HG3	2.02	0.60
1:C:84:ALA:HB1	1:C:113:PRO:HB2	1.83	0.60
1:C:87:MSE:HE1	1:C:227:PRO:HD2	1.84	0.59
1:A:17:LYS:HB3	1:A:162:ASP:CG	2.22	0.59
1:C:314:HIS:HE1	1:C:330:ASP:OD2	1.84	0.59
1:B:301:LYS:HD3	1:B:301:LYS:N	2.18	0.59
1:D:372:GLU:O	1:D:376:PHE:HD2	1.85	0.59
1:D:54:ARG:N	1:D:54:ARG:HE	1.98	0.59
1:A:171:MSE:HE1	1:A:290:ARG:CZ	2.32	0.59
1:C:178:VAL:HG13	1:C:302:ARG:NH1	2.18	0.59
1:B:17:LYS:HB3	1:B:162:ASP:CG	2.23	0.59
1:B:194:ASP:OD1	1:B:234:HIS:HD2	1.85	0.59
1:A:31:MSE:HG3	1:A:309:ILE:HD13	1.84	0.59
1:B:108:ASN:HB3	1:B:111:ASP:OD2	2.03	0.59
1:C:142:LEU:CD2	1:C:151:LEU:HD22	2.33	0.58
1:D:142:LEU:CD2	1:D:151:LEU:HD22	2.33	0.58
1:A:105:LYS:HE3	1:A:107:GLU:OE2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:301:LYS:N	1:C:301:LYS:HD3	2.17	0.58
1:B:19:VAL:HB	1:B:42:VAL:HG12	1.85	0.58
1:C:31:MSE:HG3	1:C:309:ILE:HD13	1.85	0.58
1:C:371:ASN:OD1	1:C:375:MSE:HE3	2.03	0.58
1:D:121:ARG:O	1:D:125:LEU:HB2	2.03	0.58
1:D:357:MSE:HE3	1:D:358:PHE:CD2	2.38	0.58
1:B:87:MSE:HE1	1:B:227:PRO:HD2	1.85	0.58
1:D:259:VAL:HG12	1:D:263:LEU:HD22	1.86	0.58
1:D:301:LYS:HD3	1:D:301:LYS:N	2.18	0.57
1:C:94:LYS:HD3	1:C:218:HIS:NE2	2.20	0.57
1:D:94:LYS:HD3	1:D:218:HIS:NE2	2.19	0.57
1:A:380:PHE:CD2	1:A:382:PHE:CD1	2.93	0.57
1:A:242:PRO:HG2	1:A:245:TRP:CZ2	2.38	0.57
1:A:272:GLU:H	1:A:272:GLU:CD	2.07	0.57
1:B:171:MSE:HE1	1:B:290:ARG:CZ	2.35	0.57
1:C:201:ASN:HB3	1:C:280:THR:HG21	1.86	0.57
1:B:40:ILE:HD12	1:B:40:ILE:N	2.20	0.57
1:C:375:MSE:O	1:C:376:PHE:HB2	2.04	0.56
1:C:259:VAL:HG12	1:C:263:LEU:HD22	1.86	0.56
1:C:372:GLU:O	1:C:376:PHE:HD2	1.88	0.56
1:A:378:PRO:O	1:A:379:ASP:HB2	2.06	0.56
1:C:108:ASN:HB3	1:C:111:ASP:OD2	2.06	0.56
1:D:260:VAL:O	1:D:264:LEU:HB2	2.05	0.56
1:B:14:LEU:HD12	1:B:14:LEU:N	2.12	0.56
1:D:337:ASN:ND2	1:D:352:ASN:HD22	1.96	0.56
1:B:372:GLU:O	1:B:376:PHE:HD2	1.88	0.56
1:A:245:TRP:CD1	1:A:245:TRP:N	2.73	0.56
1:B:27:VAL:HG12	1:B:309:ILE:HD12	1.87	0.56
1:B:84:ALA:CB	1:B:113:PRO:HB2	2.36	0.56
1:D:371:ASN:OD1	1:D:375:MSE:HE3	2.06	0.56
1:B:201:ASN:HB3	1:B:280:THR:HG21	1.87	0.56
1:C:186:THR:HG22	1:C:188:THR:H	1.71	0.56
1:B:142:LEU:CD2	1:B:151:LEU:HD22	2.35	0.56
1:B:166:LEU:HD21	1:B:174:VAL:O	2.06	0.56
1:B:54:ARG:N	1:B:54:ARG:HE	2.00	0.56
1:C:105:LYS:HE3	1:C:107:GLU:OE2	2.05	0.56
1:C:323:GLY:O	1:C:324:VAL:HG12	2.06	0.56
1:D:105:LYS:HE3	1:D:107:GLU:OE2	2.05	0.56
1:D:272:GLU:H	1:D:272:GLU:CD	2.09	0.56
1:A:40:ILE:N	1:A:40:ILE:HD12	2.21	0.55
1:A:337:ASN:HD21	1:A:352:ASN:ND2	1.94	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:375:MSE:O	1:D:376:PHE:HB2	2.05	0.55
1:D:116:ASN:HD22	1:D:119:ASP:N	2.00	0.55
1:C:218:HIS:O	1:C:219:GLN:HG2	2.07	0.55
1:C:166:LEU:HD21	1:C:174:VAL:O	2.07	0.55
1:D:287:LEU:HD23	1:D:287:LEU:C	2.27	0.54
1:B:38:ASN:HB2	1:B:40:ILE:HD13	1.88	0.54
1:A:375:MSE:O	1:A:376:PHE:HB2	2.07	0.54
1:C:357:MSE:HE3	1:C:358:PHE:CD2	2.43	0.54
1:C:298:TRP:CH2	1:C:357:MSE:HE2	2.43	0.54
1:D:186:THR:HG22	1:D:188:THR:H	1.73	0.54
1:D:340:ASP:O	1:D:342:LYS:HG3	2.08	0.54
1:B:94:LYS:HD3	1:B:218:HIS:NE2	2.23	0.54
1:D:49:ASN:HB2	4:D:410:HOH:O	2.07	0.54
1:D:87:MSE:HE1	1:D:227:PRO:HD2	1.89	0.54
1:B:259:VAL:HG12	1:B:263:LEU:HD22	1.90	0.54
1:C:54:ARG:HE	1:C:54:ARG:N	1.99	0.54
1:A:259:VAL:HG12	1:A:263:LEU:HD22	1.90	0.53
1:B:357:MSE:HE3	1:B:358:PHE:CD2	2.42	0.53
1:D:166:LEU:HD21	1:D:174:VAL:O	2.09	0.53
1:D:218:HIS:O	1:D:219:GLN:HG2	2.08	0.53
1:A:94:LYS:HD3	1:A:218:HIS:NE2	2.22	0.53
1:B:377:LYS:C	1:B:379:ASP:H	2.12	0.53
1:B:375:MSE:O	1:B:376:PHE:HB2	2.07	0.53
1:D:94:LYS:HD3	1:D:218:HIS:CE1	2.42	0.53
1:A:337:ASN:ND2	1:A:352:ASN:HD22	1.94	0.53
1:A:142:LEU:CD2	1:A:151:LEU:HD22	2.39	0.53
1:A:54:ARG:HE	1:A:54:ARG:N	1.98	0.53
1:A:301:LYS:N	1:A:301:LYS:HD3	2.23	0.53
1:B:146:LYS:H	1:B:146:LYS:CE	2.21	0.53
1:B:226:ASN:HB2	3:B:1:SO4:O3	2.08	0.53
1:B:25:GLY:HA2	4:B:418:HOH:O	2.07	0.53
1:B:371:ASN:OD1	1:B:375:MSE:HE3	2.09	0.53
1:B:115:ILE:HG13	1:B:116:ASN:N	2.23	0.53
1:C:27:VAL:HG12	1:C:309:ILE:HD12	1.91	0.53
1:B:242:PRO:HG2	1:B:245:TRP:CZ2	2.44	0.53
1:A:201:ASN:HB3	1:A:280:THR:HG21	1.90	0.52
1:A:287:LEU:HD23	1:A:287:LEU:C	2.30	0.52
1:B:265:LYS:HA	1:B:265:LYS:HE3	1.91	0.52
1:C:49:ASN:HB2	4:C:422:HOH:O	2.09	0.52
1:A:166:LEU:HD21	1:A:174:VAL:O	2.09	0.52
1:D:85:LEU:HD12	1:D:86:PRO:HD2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:LYS:HD3	1:A:218:HIS:CE1	2.44	0.52
1:C:116:ASN:HD22	1:C:119:ASP:N	1.96	0.52
1:A:85:LEU:HD12	1:A:86:PRO:HD2	1.92	0.52
1:D:242:PRO:HG2	1:D:245:TRP:CZ2	2.44	0.52
1:D:14:LEU:HD11	1:D:341:GLY:HA2	1.92	0.52
1:A:186:THR:HG22	1:A:188:THR:H	1.74	0.52
1:A:323:GLY:O	1:A:324:VAL:HG12	2.09	0.52
1:B:266:LYS:HG3	1:B:267:PHE:HD2	1.74	0.52
1:A:84:ALA:CB	1:A:113:PRO:HB2	2.39	0.52
1:A:87:MSE:HE1	1:A:227:PRO:HD2	1.91	0.52
1:B:146:LYS:H	1:B:146:LYS:HZ3	1.56	0.52
1:C:245:TRP:CD1	1:C:245:TRP:N	2.76	0.52
1:A:146:LYS:CE	1:A:146:LYS:H	2.23	0.52
1:C:256:ARG:HD2	1:C:282:LEU:O	2.10	0.52
1:C:94:LYS:HD3	1:C:218:HIS:CE1	2.45	0.52
1:D:245:TRP:CD1	1:D:245:TRP:N	2.76	0.51
1:C:256:ARG:O	1:C:260:VAL:HG23	2.10	0.51
1:D:27:VAL:HG12	1:D:309:ILE:HD12	1.91	0.51
1:A:265:LYS:HE3	1:A:265:LYS:HA	1.92	0.51
1:A:357:MSE:HE3	1:A:358:PHE:CD2	2.45	0.51
1:C:265:LYS:HA	1:C:265:LYS:HE3	1.91	0.51
1:C:357:MSE:HA	1:C:360:TYR:CE2	2.45	0.51
1:B:298:TRP:CH2	1:B:357:MSE:HE2	2.46	0.51
1:C:45:TYR:O	2:C:401:FAD:H2A	2.10	0.51
1:D:337:ASN:HD21	1:D:352:ASN:ND2	1.94	0.51
1:A:115:ILE:HG13	1:A:116:ASN:N	2.25	0.51
1:A:204:GLY:HA3	1:A:273:ARG:HG2	1.93	0.51
1:B:218:HIS:O	1:B:219:GLN:HG2	2.11	0.51
1:D:324:VAL:HG12	2:D:401:FAD:O2	2.10	0.51
1:A:218:HIS:O	1:A:219:GLN:HG2	2.10	0.51
1:D:31:MSE:HG3	1:D:309:ILE:HD13	1.92	0.51
1:D:40:ILE:N	1:D:40:ILE:HD12	2.25	0.51
1:B:314:HIS:O	1:B:315:LEU:C	2.48	0.51
1:C:146:LYS:CE	1:C:146:LYS:H	2.24	0.51
1:B:151:LEU:N	1:B:151:LEU:HD23	2.26	0.50
1:C:266:LYS:HG3	1:C:267:PHE:HD2	1.77	0.50
1:C:314:HIS:O	1:C:315:LEU:C	2.49	0.50
1:A:33:LYS:O	1:A:33:LYS:HD2	2.11	0.50
1:B:377:LYS:C	1:B:379:ASP:N	2.64	0.50
1:D:146:LYS:H	1:D:146:LYS:CE	2.24	0.50
1:A:100:SER:CB	1:D:359:ILE:HD11	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:242:PRO:HG2	1:C:245:TRP:CZ2	2.46	0.50
1:B:323:GLY:O	1:B:324:VAL:HG12	2.11	0.50
1:C:340:ASP:O	1:C:342:LYS:HG3	2.12	0.50
1:D:265:LYS:HA	1:D:265:LYS:HE3	1.92	0.50
1:B:287:LEU:HD23	1:B:287:LEU:C	2.32	0.50
1:B:67:GLY:O	1:B:70:ALA:HB3	2.11	0.50
1:A:375:MSE:HG3	1:A:376:PHE:CD2	2.47	0.50
1:B:340:ASP:O	1:B:342:LYS:HG3	2.12	0.50
1:D:201:ASN:HB3	1:D:280:THR:HG21	1.93	0.50
1:A:340:ASP:O	1:A:342:LYS:HG3	2.12	0.49
1:A:357:MSE:HA	1:A:360:TYR:CE2	2.47	0.49
1:B:85:LEU:HD12	1:B:86:PRO:HD2	1.94	0.49
1:D:323:GLY:O	1:D:324:VAL:HG12	2.12	0.49
1:A:116:ASN:HD22	1:A:119:ASP:N	2.00	0.49
1:B:357:MSE:HA	1:B:360:TYR:CE2	2.47	0.49
1:D:204:GLY:HA3	1:D:273:ARG:HG2	1.94	0.49
1:B:186:THR:HG22	1:B:188:THR:H	1.77	0.49
1:B:245:TRP:N	1:B:245:TRP:CD1	2.76	0.49
1:C:38:ASN:HB2	1:C:40:ILE:HD13	1.94	0.48
1:D:198:PRO:HB3	1:D:233:LEU:HB2	1.95	0.48
1:B:204:GLY:HA3	1:B:273:ARG:HG2	1.94	0.48
1:C:379:ASP:OD2	1:C:379:ASP:C	2.51	0.48
1:A:91:ILE:CD1	1:A:382:PHE:HD2	2.20	0.48
1:B:94:LYS:HD3	1:B:218:HIS:CE1	2.48	0.48
1:C:287:LEU:HD23	1:C:287:LEU:C	2.33	0.48
1:A:251:VAL:HG13	1:A:252:ASP:N	2.29	0.48
1:A:31:MSE:HE2	1:A:331:ALA:CA	2.20	0.48
1:C:375:MSE:O	1:C:376:PHE:CB	2.62	0.48
1:A:256:ARG:HD2	1:A:282:LEU:O	2.13	0.48
1:B:377:LYS:O	1:B:379:ASP:N	2.46	0.48
1:D:251:VAL:HG13	1:D:252:ASP:N	2.29	0.48
1:C:40:ILE:HD12	1:C:40:ILE:N	2.29	0.48
1:D:194:ASP:OD1	1:D:234:HIS:CD2	2.66	0.48
1:B:369:THR:O	1:B:373:ILE:HG13	2.13	0.48
1:C:175:ARG:HD3	1:C:308:MSE:HE1	1.96	0.48
1:D:298:TRP:CH2	1:D:357:MSE:HE2	2.48	0.48
1:D:38:ASN:HB2	1:D:40:ILE:HD13	1.96	0.47
1:D:314:HIS:O	1:D:315:LEU:C	2.52	0.47
1:C:14:LEU:HD11	1:C:341:GLY:HA2	1.96	0.47
1:C:198:PRO:HB3	1:C:233:LEU:HB2	1.96	0.47
1:C:146:LYS:HZ3	1:C:146:LYS:H	1.61	0.47

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Full wwPDB X-ray Structure Validation Report

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:85:LEU:HD12	1:C:86:PRO:HD2	1.97	0.47
1:A:314:HIS:O	1:A:315:LEU:C	2.50	0.47
1:B:294:LEU:HB2	1:B:365:GLN:OE1	2.14	0.47
1:D:195:ILE:CD1	1:D:277:LEU:HD23	2.45	0.47
1:B:357:MSE:HA	1:B:360:TYR:CZ	2.49	0.47
1:C:116:ASN:ND2	1:C:119:ASP:N	2.55	0.47
1:D:375:MSE:O	1:D:376:PHE:CB	2.62	0.47
1:B:240:LYS:NZ	4:B:416:HOH:O	2.48	0.47
1:B:272:GLU:CD	1:B:272:GLU:H	2.17	0.47
1:C:324:VAL:O	1:C:328:LEU:N	2.45	0.47
1:A:125:LEU:HD21	1:A:135:TRP:HZ2	1.80	0.47
1:C:125:LEU:HD12	1:C:125:LEU:HA	1.81	0.47
1:C:204:GLY:HA3	1:C:273:ARG:HG2	1.96	0.46
1:C:195:ILE:CD1	1:C:277:LEU:HD23	2.45	0.46
1:C:272:GLU:H	1:C:272:GLU:CD	2.19	0.46
1:C:195:ILE:HD12	1:C:277:LEU:HD23	1.96	0.46
1:D:67:GLY:O	1:D:70:ALA:HB3	2.16	0.46
1:D:256:ARG:HD2	1:D:282:LEU:O	2.15	0.46
1:A:357:MSE:HA	1:A:360:TYR:CZ	2.50	0.46
1:B:116:ASN:HD22	1:B:119:ASP:N	1.95	0.46
1:B:266:LYS:HE2	1:B:266:LYS:HB3	1.86	0.46
1:B:14:LEU:HD11	1:B:341:GLY:HA2	1.98	0.46
1:C:357:MSE:HA	1:C:360:TYR:CZ	2.50	0.46
1:D:266:LYS:HG3	1:D:267:PHE:HD2	1.80	0.46
1:D:151:LEU:HD23	1:D:151:LEU:N	2.31	0.46
1:D:294:LEU:HG	1:D:365:GLN:OE1	2.16	0.46
1:D:377:LYS:C	1:D:379:ASP:H	2.19	0.46
1:A:266:LYS:HG3	1:A:267:PHE:HD2	1.80	0.46
1:A:380:PHE:CD2	1:A:382:PHE:HD1	2.34	0.46
1:A:256:ARG:O	1:A:260:VAL:HG23	2.15	0.46
1:C:294:LEU:HB2	1:C:365:GLN:OE1	2.16	0.46
1:C:67:GLY:O	1:C:70:ALA:HB3	2.16	0.46
1:D:46:GLU:HG2	1:D:135:TRP:CZ3	2.51	0.46
1:A:125:LEU:HD12	1:A:125:LEU:HA	1.85	0.45
1:A:194:ASP:OD1	1:A:234:HIS:CD2	2.68	0.45
1:B:31:MSE:HG3	1:B:309:ILE:CD1	2.46	0.45
1:A:31:MSE:HG3	1:A:309:ILE:CD1	2.46	0.45
1:A:358:PHE:HD1	1:A:362:LYS:HE3	1.81	0.45
1:A:13:LEU:HD11	1:A:38:ASN:O	2.15	0.45
1:B:195:ILE:CD1	1:B:277:LEU:HD23	2.46	0.45
1:A:199:GLU:OE1	1:A:199:GLU:N	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:375:MSE:HB3	1:D:380:PHE:CE2	2.50	0.45
1:C:302:ARG:NH2	4:C:418:HOH:O	2.50	0.45
1:C:358:PHE:HD1	1:C:362:LYS:HE3	1.81	0.45
1:B:135:TRP:O	1:B:137:ARG:HG2	2.16	0.45
1:B:380:PHE:CD2	1:B:380:PHE:C	2.89	0.45
1:B:60:LEU:HD12	1:B:60:LEU:HA	1.77	0.45
1:C:361:GLY:O	1:C:365:GLN:HG3	2.16	0.45
1:D:107:GLU:CD	1:D:107:GLU:H	2.20	0.45
1:D:33:LYS:O	1:D:33:LYS:HD2	2.16	0.45
1:A:375:MSE:O	1:A:376:PHE:CB	2.64	0.45
1:C:31:MSE:HG3	1:C:309:ILE:CD1	2.47	0.45
1:C:382:PHE:CD2	1:C:382:PHE:N	2.84	0.45
1:A:67:GLY:O	1:A:70:ALA:HB3	2.17	0.45
1:C:194:ASP:OD1	1:C:234:HIS:CD2	2.66	0.45
1:A:38:ASN:HB2	1:A:40:ILE:HD13	1.99	0.45
1:C:381:THR:CG2	1:C:382:PHE:N	2.79	0.45
1:D:343:PHE:HD1	1:D:348:GLU:HB3	1.82	0.44
1:A:294:LEU:HB2	1:A:365:GLN:OE1	2.17	0.44
1:A:371:ASN:OD1	1:A:375:MSE:HE3	2.15	0.44
1:B:350:VAL:HG23	1:B:354:GLU:OE2	2.17	0.44
1:A:99:LEU:HG	1:D:359:ILE:O	2.18	0.44
1:A:375:MSE:HG3	1:A:376:PHE:CE2	2.52	0.44
1:B:133:VAL:HG11	1:B:135:TRP:CE2	2.52	0.44
1:D:31:MSE:HE2	1:D:331:ALA:CA	2.23	0.44
1:A:195:ILE:CD1	1:A:277:LEU:HD23	2.47	0.44
1:B:358:PHE:HD1	1:B:362:LYS:HE3	1.83	0.44
1:D:357:MSE:HA	1:D:360:TYR:CE2	2.53	0.44
1:A:175:ARG:HD3	1:A:308:MSE:HE1	2.00	0.44
1:B:195:ILE:HD12	1:B:277:LEU:HD23	1.99	0.44
1:B:343:PHE:HD1	1:B:348:GLU:HB3	1.82	0.44
1:C:266:LYS:HE2	1:C:266:LYS:HB3	1.89	0.44
1:C:350:VAL:HG23	1:C:354:GLU:OE2	2.18	0.44
1:C:222:LEU:HD12	1:C:223:LEU:N	2.33	0.44
1:A:324:VAL:HG12	2:A:401:FAD:O2	2.18	0.43
1:B:256:ARG:HD2	1:B:282:LEU:O	2.17	0.43
1:B:363:GLU:O	1:B:367:GLU:HG3	2.19	0.43
1:C:84:ALA:CB	1:C:113:PRO:HB2	2.47	0.43
1:D:116:ASN:ND2	1:D:119:ASP:N	2.60	0.43
1:A:60:LEU:HA	1:A:60:LEU:HD12	1.68	0.43
1:C:377:LYS:HA	1:C:378:PRO:HD3	1.84	0.43
1:D:125:LEU:HD12	1:D:125:LEU:HA	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:226:ASN:C	1:D:226:ASN:OD1	2.57	0.43
1:B:375:MSE:O	1:B:376:PHE:CB	2.64	0.43
1:B:302:ARG:HA	1:B:303:PRO:HD2	1.70	0.43
1:B:116:ASN:ND2	1:B:119:ASP:N	2.57	0.43
1:B:146:LYS:NZ	1:B:146:LYS:H	2.16	0.43
1:C:13:LEU:HD11	1:C:38:ASN:O	2.18	0.43
1:A:146:LYS:H	1:A:146:LYS:HZ3	1.65	0.43
1:A:375:MSE:HE2	1:A:380:PHE:HE2	1.79	0.43
1:C:133:VAL:HG11	1:C:135:TRP:CE2	2.54	0.43
1:B:324:VAL:HG13	1:B:325:ASN:N	2.34	0.43
1:B:46:GLU:HG3	1:B:48:ASP:H	1.84	0.43
1:C:302:ARG:HA	1:C:303:PRO:HD2	1.70	0.43
1:D:270:TRP:HE3	1:D:274:TYR:CD2	2.37	0.43
1:D:195:ILE:HD12	1:D:277:LEU:HD23	2.01	0.43
1:D:324:VAL:O	1:D:328:LEU:N	2.48	0.43
1:B:256:ARG:O	1:B:260:VAL:HG13	2.19	0.43
1:B:178:VAL:O	1:B:299:LYS:HG2	2.19	0.43
1:B:186:THR:CG2	1:B:372:GLU:OE1	2.64	0.43
1:C:46:GLU:HG2	1:C:135:TRP:CZ3	2.54	0.43
1:D:84:ALA:CB	1:D:113:PRO:HB2	2.47	0.43
1:D:369:THR:O	1:D:373:ILE:HG13	2.19	0.43
1:C:287:LEU:HD23	1:C:288:ALA:C	2.40	0.42
1:A:151:LEU:N	1:A:151:LEU:HD23	2.33	0.42
1:A:324:VAL:O	1:A:328:LEU:N	2.47	0.42
1:B:324:VAL:HG12	2:B:401:FAD:O2	2.19	0.42
1:A:320:ALA:HB3	1:A:322:GLN:OE1	2.19	0.42
1:A:343:PHE:HD1	1:A:348:GLU:HB3	1.83	0.42
1:C:125:LEU:HD21	1:C:135:TRP:HZ2	1.85	0.42
1:D:222:LEU:HD12	1:D:223:LEU:N	2.35	0.42
1:A:116:ASN:ND2	1:A:119:ASP:N	2.59	0.42
1:C:151:LEU:HD23	1:C:151:LEU:N	2.35	0.42
1:D:358:PHE:HD1	1:D:362:LYS:HE3	1.84	0.42
1:A:146:LYS:HE2	1:A:146:LYS:H	1.85	0.42
1:C:178:VAL:O	1:C:299:LYS:HG2	2.20	0.42
1:C:46:GLU:HG3	1:C:48:ASP:H	1.85	0.42
1:D:115:ILE:HG13	1:D:116:ASN:N	2.35	0.42
1:D:375:MSE:HG3	1:D:376:PHE:CD2	2.55	0.42
1:A:380:PHE:CE2	1:A:382:PHE:CD1	3.04	0.42
1:C:226:ASN:OD1	1:C:226:ASN:C	2.58	0.42
1:B:348:GLU:O	1:B:351:LYS:HB3	2.20	0.42
1:C:199:GLU:N	1:C:199:GLU:OE1	2.42	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:PHE:HD2	1:A:382:PHE:CE1	2.38	0.42
1:B:294:LEU:HD22	1:B:365:GLN:OE1	2.20	0.42
1:C:235:PHE:CE2	1:C:277:LEU:HD22	2.55	0.42
1:A:107:GLU:H	1:A:107:GLU:CD	2.23	0.41
1:A:36:GLN:OE1	1:A:129:GLU:HG3	2.20	0.41
1:C:33:LYS:O	1:C:33:LYS:HD2	2.19	0.41
1:D:266:LYS:HB3	1:D:266:LYS:HE2	1.90	0.41
2:B:401:FAD:H1'1	2:B:401:FAD:H9	1.69	0.41
1:C:115:ILE:HG13	1:C:116:ASN:N	2.36	0.41
1:C:334:LEU:HD21	1:C:338:LEU:HD11	2.02	0.41
1:C:60:LEU:HD12	1:C:60:LEU:HA	1.79	0.41
1:B:125:LEU:HD21	1:B:135:TRP:HZ2	1.86	0.41
1:B:356:GLN:O	1:B:359:ILE:HB	2.21	0.41
1:D:361:GLY:O	1:D:365:GLN:HG3	2.20	0.41
1:A:363:GLU:O	1:A:367:GLU:HG3	2.19	0.41
1:B:33:LYS:O	1:B:33:LYS:HD2	2.21	0.41
1:A:266:LYS:HB3	1:A:266:LYS:HE2	1.91	0.41
1:C:60:LEU:O	1:C:115:ILE:HG22	2.21	0.41
1:A:272:GLU:CD	1:A:272:GLU:N	2.73	0.41
1:A:380:PHE:CD2	1:A:382:PHE:CE1	3.08	0.41
1:A:13:LEU:HG	1:A:40:ILE:HD11	2.03	0.41
1:B:142:LEU:HD23	1:B:151:LEU:HD22	2.02	0.41
1:C:348:GLU:HG2	1:C:351:LYS:NZ	2.36	0.41
1:D:302:ARG:HA	1:D:303:PRO:HD2	1.70	0.41
1:D:22:ILE:HG13	1:D:139:LEU:HD22	2.02	0.41
1:D:40:ILE:CG2	1:D:41:ASP:N	2.84	0.41
1:A:314:HIS:CE1	1:A:330:ASP:OD2	2.67	0.41
1:B:46:GLU:HG2	1:B:135:TRP:CZ3	2.56	0.41
1:B:287:LEU:HD23	1:B:288:ALA:C	2.41	0.41
1:C:252:ASP:OD1	1:C:254:GLN:HB2	2.20	0.41
2:D:401:FAD:H1'1	2:D:401:FAD:H9	1.85	0.41
1:A:40:ILE:N	1:A:40:ILE:CD1	2.83	0.41
1:A:59:THR:OG1	1:A:114:GLU:HB3	2.20	0.41
1:B:175:ARG:HD3	1:B:308:MSE:HE1	2.03	0.41
1:C:324:VAL:HG13	1:C:325:ASN:N	2.35	0.41
1:A:245:TRP:CD1	1:A:250:GLN:N	2.89	0.41
1:A:298:TRP:CH2	1:A:357:MSE:HE2	2.55	0.41
1:A:60:LEU:HG	1:A:324:VAL:HG11	2.03	0.41
1:B:375:MSE:HG3	1:B:376:PHE:CD2	2.56	0.41
1:C:294:LEU:HD22	1:C:365:GLN:OE1	2.21	0.41
1:D:60:LEU:HD12	1:D:60:LEU:HA	1.77	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:LEU:HD12	1:A:223:LEU:N	2.36	0.40
1:B:115:ILE:HG13	1:B:116:ASN:H	1.86	0.40
1:C:343:PHE:HD1	1:C:348:GLU:HB3	1.84	0.40
1:D:146:LYS:HE2	1:D:146:LYS:H	1.86	0.40
1:D:298:TRP:O	1:D:299:LYS:C	2.58	0.40
1:A:226:ASN:C	1:A:226:ASN:OD1	2.60	0.40
1:A:46:GLU:HG2	1:A:135:TRP:CZ3	2.57	0.40
1:B:218:HIS:HB3	1:B:270:TRP:CZ2	2.55	0.40
1:A:195:ILE:HD12	1:A:277:LEU:HD23	2.04	0.40
1:B:198:PRO:HB3	1:B:233:LEU:HB2	2.01	0.40
1:D:139:LEU:CD1	1:D:151:LEU:HB3	2.51	0.40
1:B:226:ASN:C	1:B:226:ASN:OD1	2.59	0.40
1:C:139:LEU:CD1	1:C:151:LEU:HB3	2.52	0.40
1:D:31:MSE:HG3	1:D:309:ILE:CD1	2.51	0.40
1:D:125:LEU:HD21	1:D:135:TRP:HZ2	1.86	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	364/378 (96%)	323 (89%)	39 (11%)	2 (0%)	29	59
1	B	361/378 (96%)	324 (90%)	33 (9%)	4 (1%)	14	39
1	C	362/378 (96%)	325 (90%)	34 (9%)	3 (1%)	19	47
1	D	363/378 (96%)	326 (90%)	34 (9%)	3 (1%)	19	47
All	All	1450/1512 (96%)	1298 (90%)	140 (10%)	12 (1%)	19	47

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	51	ARG
1	A	51	ARG
1	B	51	ARG
1	D	51	ARG
1	A	374	GLU
1	B	374	GLU
1	C	315	LEU
1	C	374	GLU
1	D	315	LEU
1	B	315	LEU
1	D	374	GLU
1	B	378	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	318/317 (100%)	281 (88%)	37 (12%)	5	16
1	B	315/317 (99%)	278 (88%)	37 (12%)	5	16
1	C	316/317 (100%)	279 (88%)	37 (12%)	5	16
1	D	317/317 (100%)	280 (88%)	37 (12%)	5	16
All	All	1266/1268 (100%)	1118 (88%)	148 (12%)	5	16

All (148) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LEU
1	A	14	LEU
1	A	42	VAL
1	A	47	ARG
1	A	54	ARG
1	A	60	LEU
1	A	89	VAL
1	A	99	LEU
1	A	101	THR
1	A	104	VAL

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Mol	Chain	Res	Type
1	A	116	ASN
1	A	146	LYS
1	A	151	LEU
1	A	166	LEU
1	A	176	LYS
1	A	186	THR
1	A	192	GLN
1	A	243	ASP
1	A	245	TRP
1	A	251	VAL
1	A	252	ASP
1	A	263	LEU
1	A	265	LYS
1	A	266	LYS
1	A	272	GLU
1	A	277	LEU
1	A	281	THR
1	A	285	VAL
1	A	287	LEU
1	A	294	LEU
1	A	301	LYS
1	A	324	VAL
1	A	350	VAL
1	A	353	TYR
1	A	357	MSE
1	A	374	GLU
1	A	381	THR
1	B	14	LEU
1	B	42	VAL
1	B	47	ARG
1	B	54	ARG
1	B	60	LEU
1	B	89	VAL
1	B	99	LEU
1	B	101	THR
1	B	104	VAL
1	B	115	ILE
1	B	116	ASN
1	B	146	LYS
1	B	151	LEU
1	B	166	LEU
1	B	176	LYS

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Mol	Chain	Res	Type
1	B	179	THR
1	B	186	THR
1	B	192	GLN
1	B	243	ASP
1	B	245	TRP
1	B	252	ASP
1	B	263	LEU
1	B	265	LYS
1	B	266	LYS
1	B	272	GLU
1	B	277	LEU
1	B	281	THR
1	B	285	VAL
1	B	287	LEU
1	B	294	LEU
1	B	301	LYS
1	B	324	VAL
1	B	350	VAL
1	B	353	TYR
1	B	357	MSE
1	B	374	GLU
1	B	380	PHE
1	C	13	LEU
1	C	14	LEU
1	C	42	VAL
1	C	47	ARG
1	C	54	ARG
1	C	60	LEU
1	C	89	VAL
1	C	99	LEU
1	C	101	THR
1	C	115	ILE
1	C	116	ASN
1	C	125	LEU
1	C	146	LYS
1	C	151	LEU
1	C	176	LYS
1	C	186	THR
1	C	192	GLN
1	C	243	ASP
1	C	245	TRP
1	C	252	ASP

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Mol	Chain	Res	Type
1	C	263	LEU
1	C	265	LYS
1	C	266	LYS
1	C	272	GLU
1	C	277	LEU
1	C	281	THR
1	C	285	VAL
1	C	287	LEU
1	C	294	LEU
1	C	301	LYS
1	C	324	VAL
1	C	350	VAL
1	C	353	TYR
1	C	357	MSE
1	C	374	GLU
1	C	379	ASP
1	C	382	PHE
1	D	14	LEU
1	D	42	VAL
1	D	47	ARG
1	D	54	ARG
1	D	60	LEU
1	D	89	VAL
1	D	99	LEU
1	D	101	THR
1	D	104	VAL
1	D	116	ASN
1	D	125	LEU
1	D	146	LYS
1	D	151	LEU
1	D	166	LEU
1	D	176	LYS
1	D	179	THR
1	D	186	THR
1	D	192	GLN
1	D	243	ASP
1	D	245	TRP
1	D	251	VAL
1	D	252	ASP
1	D	263	LEU
1	D	264	LEU
1	D	265	LYS

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Mol	Chain	Res	Type
1	D	272	GLU
1	D	277	LEU
1	D	281	THR
1	D	285	VAL
1	D	287	LEU
1	D	301	LYS
1	D	324	VAL
1	D	350	VAL
1	D	353	TYR
1	D	357	MSE
1	D	374	GLU
1	D	381	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	116	ASN
1	A	234	HIS
1	A	314	HIS
1	A	352	ASN
1	A	356	GLN
1	B	116	ASN
1	B	234	HIS
1	B	314	HIS
1	B	352	ASN
1	B	356	GLN
1	C	116	ASN
1	C	234	HIS
1	C	314	HIS
1	C	352	ASN
1	C	356	GLN
1	D	116	ASN
1	D	218	HIS
1	D	234	HIS
1	D	314	HIS
1	D	352	ASN
1	D	356	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 carbohydrates 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	SO4	C	1	-	4,4,4	0.26	0	6,6,6	0.46	0
3	SO4	A	1	-	4,4,4	0.14	0	6,6,6	0.22	0
3	SO4	B	1	-	4,4,4	0.31	0	6,6,6	0.54	0
3	SO4	D	1	-	4,4,4	0.18	0	6,6,6	0.58	0
2	FAD	B	401	-	51,58,58	2.38	13 (25%)	60,89,89	2.07	14 (23%)
2	FAD	C	401	-	51,58,58	2.43	11 (21%)	60,89,89	2.06	13 (21%)
2	FAD	A	401	-	51,58,58	2.43	13 (25%)	60,89,89	2.21	15 (25%)
2	FAD	D	401	-	51,58,58	2.38	12 (23%)	60,89,89	2.31	17 (28%)

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
2	FAD	A	401	-	1/1/9/9	4/30/50/50	0/6/6/6
2	FAD	D	401	-	1/1/9/9	4/30/50/50	0/6/6/6
2	FAD	B	401	-	1/1/9/9	6/30/50/50	0/6/6/6
2	FAD	C	401	-	1/1/9/9	6/30/50/50	0/6/6/6

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	FAD	O2'-C2'	-8.75	1.24	1.43
2	B	401	FAD	O2'-C2'	-8.35	1.25	1.43
2	A	401	FAD	O2'-C2'	-8.03	1.26	1.43
2	D	401	FAD	O2'-C2'	-7.93	1.26	1.43
2	B	401	FAD	O4-C4	7.08	1.42	1.24
2	A	401	FAD	O4-C4	6.96	1.42	1.24
2	C	401	FAD	O4-C4	6.68	1.41	1.24
2	D	401	FAD	O4-C4	6.60	1.41	1.24
2	C	401	FAD	C2B-C1B	-5.23	1.45	1.53
2	C	401	FAD	C1'-N10	-4.99	1.43	1.48
2	A	401	FAD	C1'-N10	-4.66	1.43	1.48
2	A	401	FAD	C2B-C1B	-4.62	1.46	1.53
2	D	401	FAD	C1'-N10	-4.57	1.43	1.48
2	D	401	FAD	C2B-C1B	-4.47	1.47	1.53
2	D	401	FAD	C6A-N6A	4.45	1.50	1.34
2	C	401	FAD	C2B-C3B	-4.38	1.41	1.53
2	B	401	FAD	C2'-C3'	4.37	1.61	1.53
2	D	401	FAD	C2B-C3B	-4.37	1.41	1.53
2	A	401	FAD	C6A-N6A	4.31	1.49	1.34
2	D	401	FAD	C2'-C3'	4.31	1.61	1.53
2	A	401	FAD	C2B-C3B	-4.28	1.41	1.53
2	B	401	FAD	C2B-C3B	-4.27	1.41	1.53
2	B	401	FAD	C6A-N6A	4.24	1.49	1.34
2	A	401	FAD	C2'-C3'	4.05	1.61	1.53
2	C	401	FAD	C2'-C3'	3.98	1.61	1.53
2	C	401	FAD	C6A-N6A	3.97	1.48	1.34
2	B	401	FAD	C2B-C1B	-3.80	1.48	1.53
2	B	401	FAD	C1'-N10	-3.72	1.44	1.48
2	B	401	FAD	C7M-C7	3.11	1.57	1.51
2	D	401	FAD	C7M-C7	2.92	1.56	1.51
2	A	401	FAD	C4'-C3'	-2.85	1.48	1.53
2	C	401	FAD	C7M-C7	2.72	1.56	1.51
2	A	401	FAD	C7M-C7	2.65	1.56	1.51
2	A	401	FAD	O5'-C5'	-2.52	1.35	1.44
2	D	401	FAD	C2-N3	-2.48	1.33	1.38
2	B	401	FAD	C3B-C4B	-2.32	1.47	1.53
2	A	401	FAD	O4'-C4'	-2.30	1.38	1.43
2	B	401	FAD	P-O2P	-2.26	1.44	1.55
2	B	401	FAD	O4B-C1B	-2.21	1.38	1.41
2	B	401	FAD	C9A-N10	-2.17	1.35	1.38
2	A	401	FAD	C3B-C4B	-2.17	1.47	1.53
2	B	401	FAD	C2A-N3A	2.16	1.35	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	FAD	O5'-C5'	-2.14	1.36	1.44
2	C	401	FAD	O4B-C1B	-2.08	1.38	1.41
2	C	401	FAD	P-O2P	-2.08	1.45	1.55
2	A	401	FAD	P-O2P	-2.07	1.45	1.55
2	C	401	FAD	C2-N3	-2.06	1.34	1.38
2	D	401	FAD	P-O2P	-2.04	1.45	1.55
2	D	401	FAD	C4X-N5	2.01	1.36	1.33

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	401	FAD	C1B-N9A-C4A	-9.39	110.14	126.64
2	C	401	FAD	C1B-N9A-C4A	-8.76	111.25	126.64
2	A	401	FAD	C1B-N9A-C4A	-8.20	112.24	126.64
2	A	401	FAD	C4-N3-C2	6.71	120.81	115.14
2	B	401	FAD	C1B-N9A-C4A	-6.59	115.06	126.64
2	B	401	FAD	C4-N3-C2	5.90	120.12	115.14
2	D	401	FAD	C1'-N10-C9A	5.78	122.84	118.29
2	B	401	FAD	C1'-C2'-C3'	5.56	125.34	109.79
2	D	401	FAD	C4-N3-C2	5.26	119.59	115.14
2	A	401	FAD	O2'-C2'-C1'	5.11	121.90	109.59
2	A	401	FAD	C1'-N10-C9A	4.99	122.22	118.29
2	C	401	FAD	C4-N3-C2	4.96	119.33	115.14
2	A	401	FAD	C1'-C2'-C3'	4.82	123.25	109.79
2	D	401	FAD	O2'-C2'-C1'	4.64	120.76	109.59
2	C	401	FAD	O2'-C2'-C3'	4.56	120.20	109.10
2	D	401	FAD	C1'-C2'-C3'	4.49	122.35	109.79
2	C	401	FAD	C1'-C2'-C3'	4.32	121.86	109.79
2	C	401	FAD	N3A-C2A-N1A	-4.16	122.18	128.68
2	A	401	FAD	N3A-C2A-N1A	-4.14	122.20	128.68
2	B	401	FAD	N3A-C2A-N1A	-4.08	122.30	128.68
2	D	401	FAD	N3A-C2A-N1A	-3.94	122.52	128.68
2	B	401	FAD	O2'-C2'-C3'	3.53	117.69	109.10
2	C	401	FAD	O2'-C2'-C1'	3.47	117.95	109.59
2	B	401	FAD	O5'-C5'-C4'	3.39	118.41	109.36
2	B	401	FAD	P-O3P-PA	-3.28	121.58	132.83
2	D	401	FAD	O2'-C2'-C3'	3.20	116.89	109.10
2	D	401	FAD	C4X-N5-C5X	3.19	119.96	116.77
2	D	401	FAD	O5'-C5'-C4'	3.18	117.86	109.36
2	B	401	FAD	C4X-N5-C5X	3.16	119.93	116.77
2	B	401	FAD	O4B-C1B-C2B	-3.16	102.30	106.93
2	C	401	FAD	C1'-N10-C9A	3.16	120.78	118.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	FAD	P-O3P-PA	-3.10	122.20	132.83
2	B	401	FAD	O2'-C2'-C1'	3.06	116.97	109.59
2	C	401	FAD	C4'-C3'-C2'	3.06	119.73	113.36
2	C	401	FAD	O5'-C5'-C4'	3.05	117.50	109.36
2	A	401	FAD	C3B-C2B-C1B	3.01	105.50	100.98
2	D	401	FAD	C4-C4X-C10	-3.00	117.97	119.95
2	A	401	FAD	C4X-C4-N3	-2.99	119.35	123.43
2	D	401	FAD	C4-C4X-N5	2.92	121.93	118.60
2	A	401	FAD	C5X-C9A-N10	2.72	119.69	117.72
2	B	401	FAD	C4X-C4-N3	-2.72	119.71	123.43
2	D	401	FAD	C3B-C2B-C1B	2.71	105.06	100.98
2	C	401	FAD	C4X-N5-C5X	2.70	119.47	116.77
2	B	401	FAD	C5X-C9A-N10	2.63	119.62	117.72
2	D	401	FAD	C1'-N10-C10	-2.63	116.06	118.41
2	A	401	FAD	P-O3P-PA	-2.61	123.86	132.83
2	A	401	FAD	O5'-C5'-C4'	2.38	115.71	109.36
2	A	401	FAD	O2'-C2'-C3'	2.36	114.85	109.10
2	D	401	FAD	C4'-C3'-C2'	2.34	118.24	113.36
2	A	401	FAD	C4A-C5A-N7A	-2.27	107.04	109.40
2	D	401	FAD	C4A-C5A-N7A	-2.22	107.09	109.40
2	D	401	FAD	O4'-C4'-C5'	-2.19	104.99	109.92
2	A	401	FAD	O3'-C3'-C2'	2.15	114.00	108.81
2	A	401	FAD	C4X-N5-C5X	2.15	118.92	116.77
2	B	401	FAD	C1'-N10-C9A	2.12	119.97	118.29
2	B	401	FAD	C4A-C5A-N7A	-2.12	107.19	109.40
2	C	401	FAD	C4A-C5A-N7A	-2.09	107.22	109.40
2	C	401	FAD	O4'-C4'-C5'	-2.02	105.37	109.92
2	D	401	FAD	C4X-C4-N3	-2.02	120.67	123.43

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	401	FAD	C2'
2	C	401	FAD	C2'
2	A	401	FAD	C2'
2	D	401	FAD	C2'

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	401	FAD	C2'-C1'-N10-C9A
2	B	401	FAD	N10-C1'-C2'-O2'

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Mol	Chain	Res	Type	Atoms
2	B	401	FAD	O2'-C2'-C3'-O3'
2	B	401	FAD	O2'-C2'-C3'-C4'
2	C	401	FAD	N10-C1'-C2'-O2'
2	C	401	FAD	O2'-C2'-C3'-O3'
2	C	401	FAD	O2'-C2'-C3'-C4'
2	A	401	FAD	N10-C1'-C2'-O2'
2	A	401	FAD	O2'-C2'-C3'-O3'
2	A	401	FAD	O2'-C2'-C3'-C4'
2	D	401	FAD	N10-C1'-C2'-O2'
2	D	401	FAD	O2'-C2'-C3'-O3'
2	D	401	FAD	O2'-C2'-C3'-C4'
2	B	401	FAD	O4B-C4B-C5B-O5B
2	C	401	FAD	O4B-C4B-C5B-O5B
2	B	401	FAD	C3B-C4B-C5B-O5B
2	A	401	FAD	O4B-C4B-C5B-O5B
2	C	401	FAD	C3B-C4B-C5B-O5B
2	D	401	FAD	O4B-C4B-C5B-O5B
2	C	401	FAD	C2'-C3'-C4'-O4'

There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1	SO4	1	0
3	B	1	SO4	1	0
2	B	401	FAD	2	0
2	C	401	FAD	1	0
2	A	401	FAD	1	0
2	D	401	FAD	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 FAD B 401

Bond lengths

Bond angles

Torsions

Rings

Ligand FAD C 401

Bond lengths

Bond angles

Torsions

Rings

Ligand FAD A 401

Bond lengths

Bond angles

Torsions

Rings

Ligand FAD D 401

Bond lengths

Bond angles

Torsions

Rings
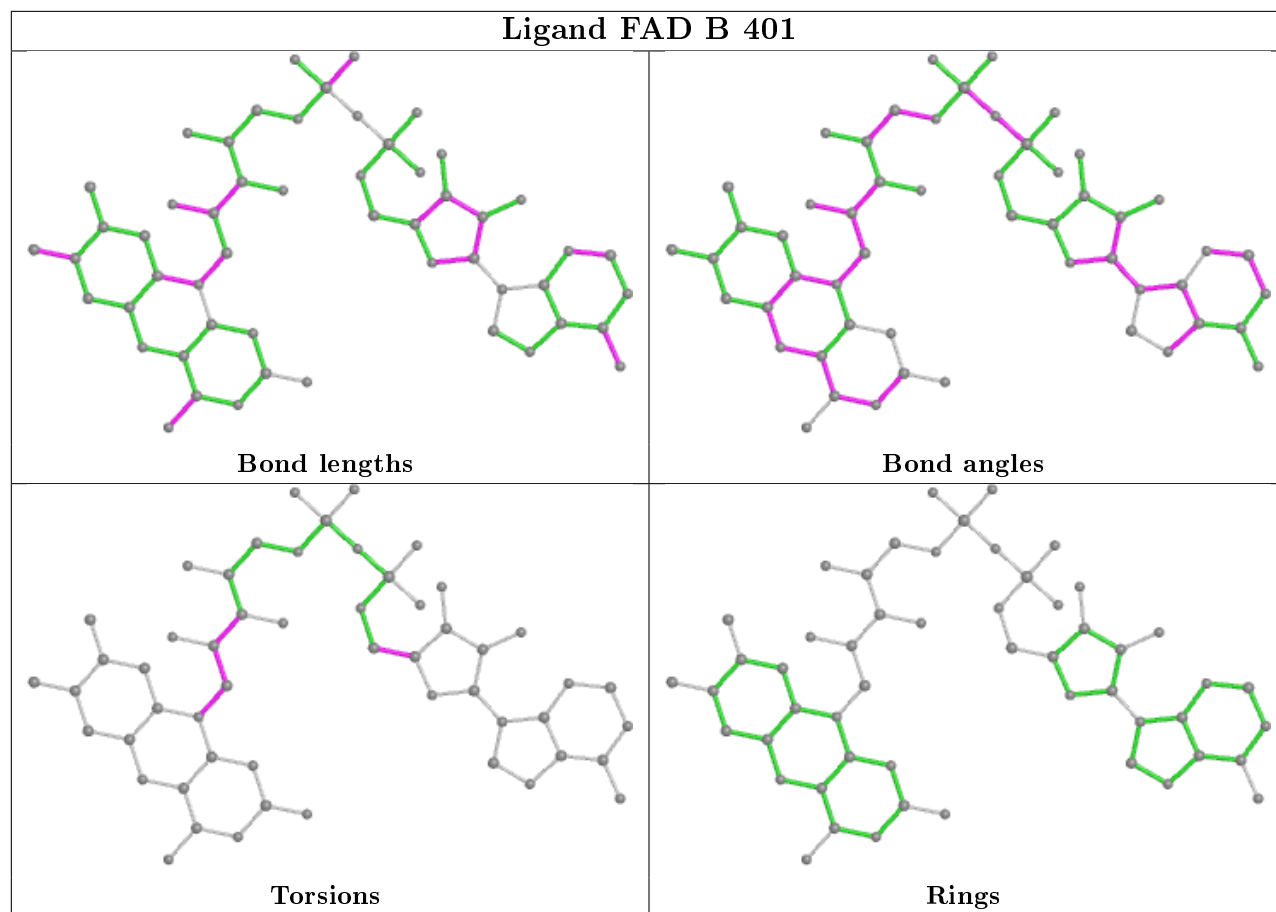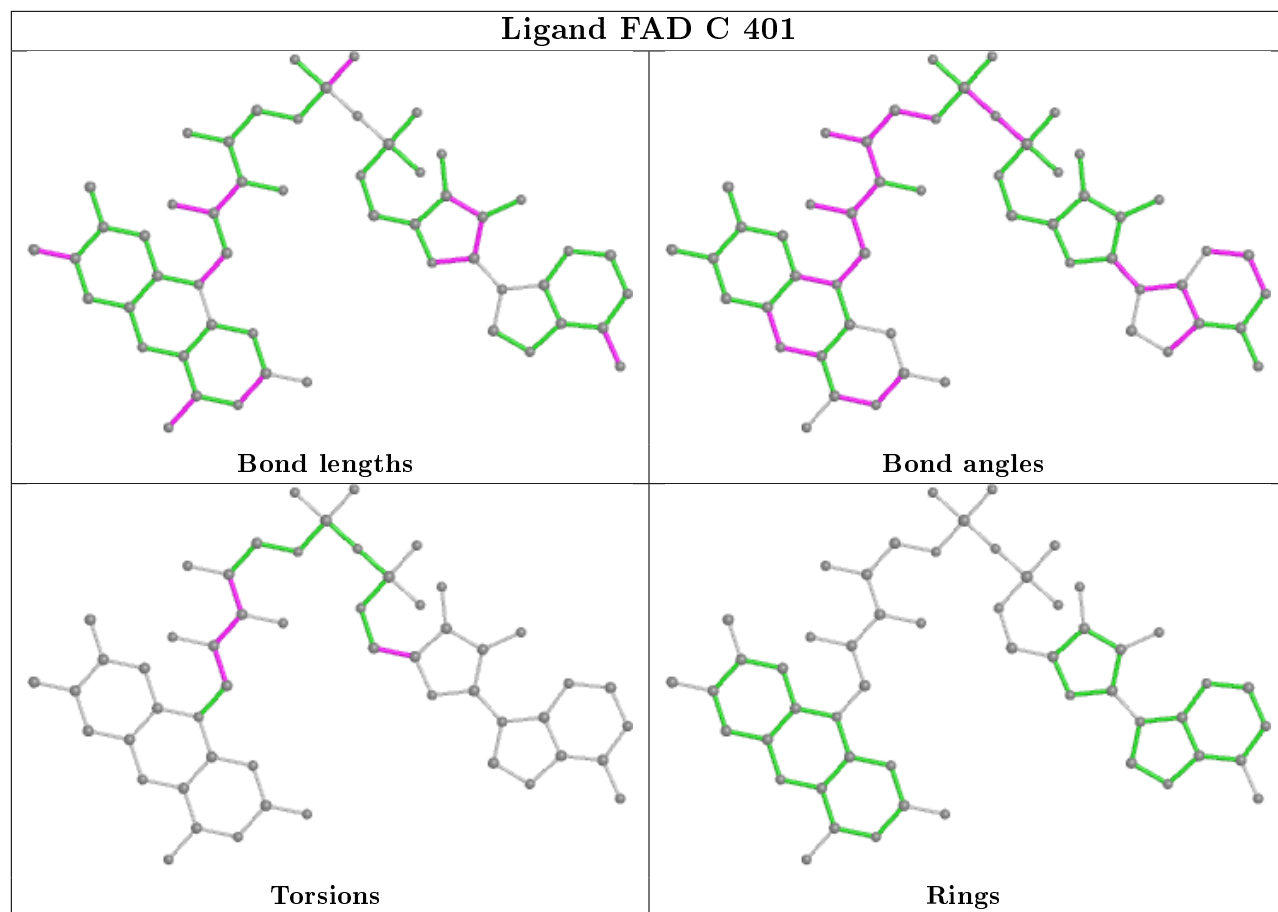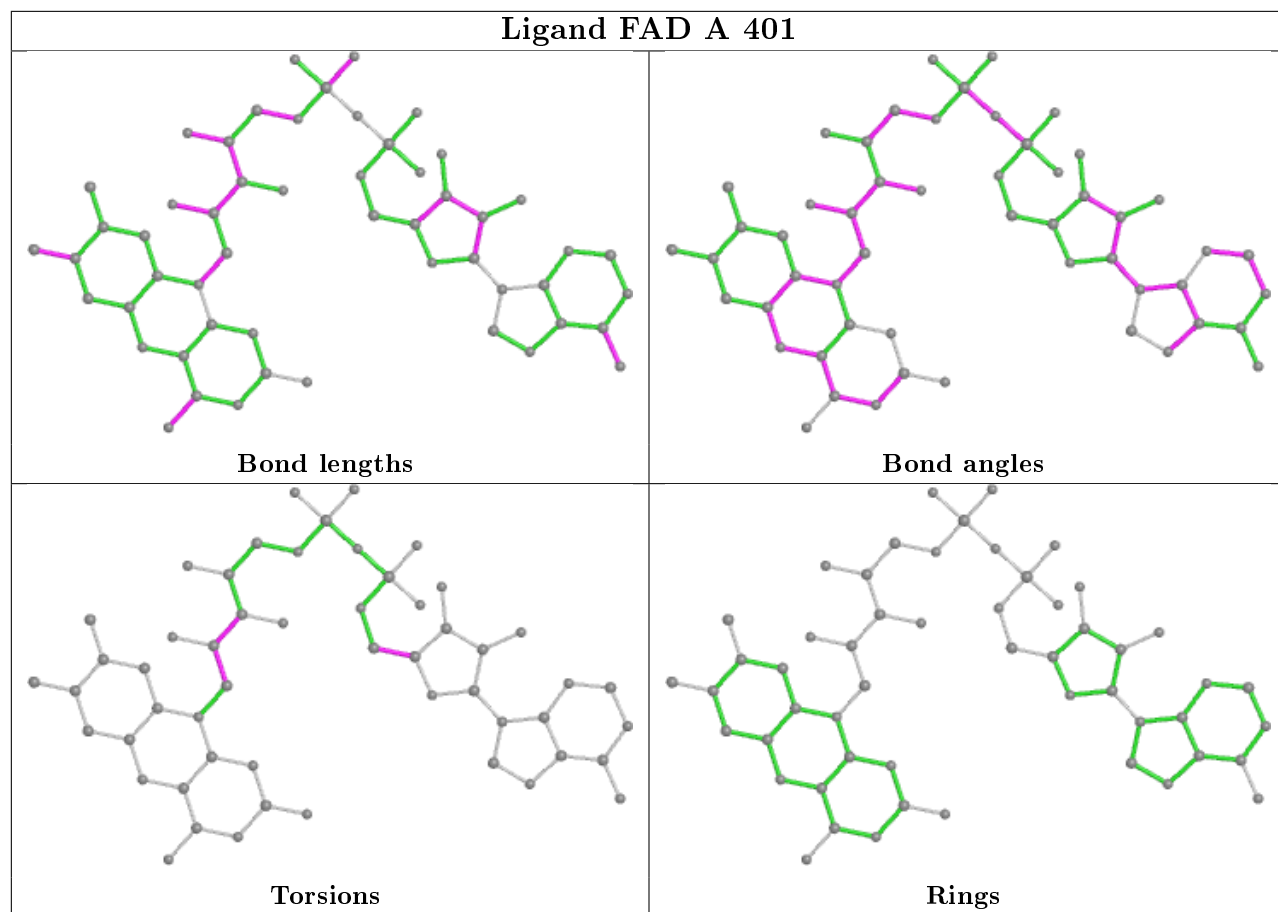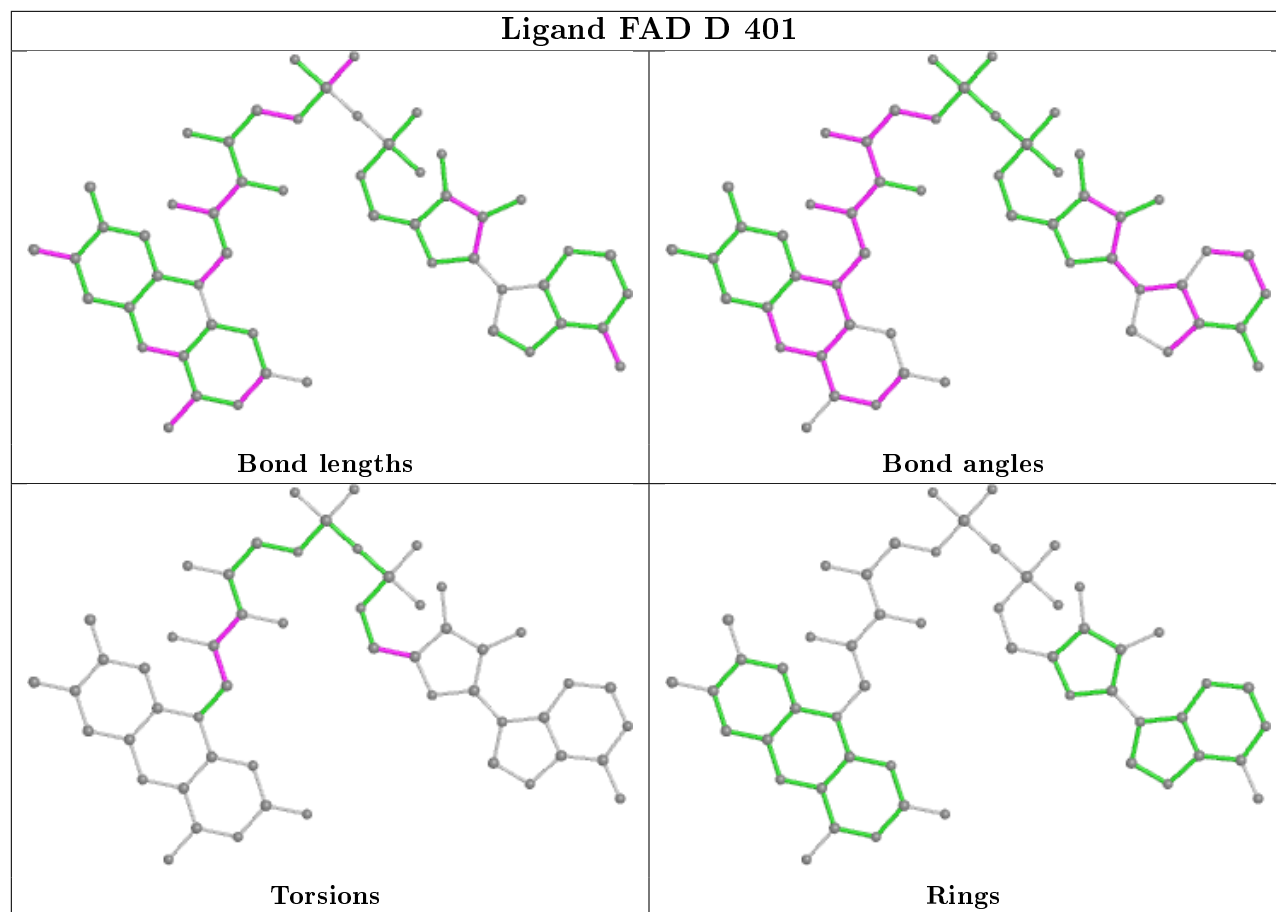
5.7 Other polymers (i)

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 (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(Å²)	Q<0.9
1	A	358/378 (94%)	-0.16	7 (1%)	65	56	7, 20, 58, 90	0
1	B	355/378 (93%)	-0.06	6 (1%)	70	63	8, 22, 51, 74	0
1	C	356/378 (94%)	-0.11	3 (0%)	86	82	7, 22, 51, 73	0
1	D	357/378 (94%)	-0.12	3 (0%)	86	82	7, 20, 50, 74	0
All	All	1426/1512 (94%)	-0.11	19 (1%)	77	72	7, 21, 51, 90	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	250	GLN	4.7
1	A	378	PRO	3.5
1	D	12	ASN	3.3
1	C	243	ASP	3.0
1	B	243	ASP	2.9
1	B	300	SER	2.7
1	A	377	LYS	2.7
1	B	220	GLY	2.5
1	A	247	ASN	2.5
1	C	252	ASP	2.4
1	B	346	ILE	2.3
1	A	246	LYS	2.3
1	D	344	ASN	2.3
1	B	345	SER	2.2
1	D	16	ASP	2.1
1	A	245	TRP	2.1
1	B	252	ASP	2.1
1	A	251	VAL	2.1
1	C	253	PHE	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 carbohydrates 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	FAD	B	401	53/53	0.97	0.14	6,14,21,28	0
2	FAD	C	401	53/53	0.97	0.14	5,15,26,37	0
2	FAD	A	401	53/53	0.97	0.14	5,12,24,28	0
2	FAD	D	401	53/53	0.97	0.15	3,13,25,28	0
3	SO4	C	1	5/5	0.98	0.10	8,10,22,30	0
3	SO4	A	1	5/5	0.98	0.11	7,14,25,26	0
3	SO4	B	1	5/5	0.98	0.13	12,19,29,31	0
3	SO4	D	1	5/5	0.98	0.13	7,11,13,13	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 FAD B 401:

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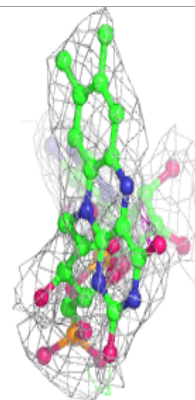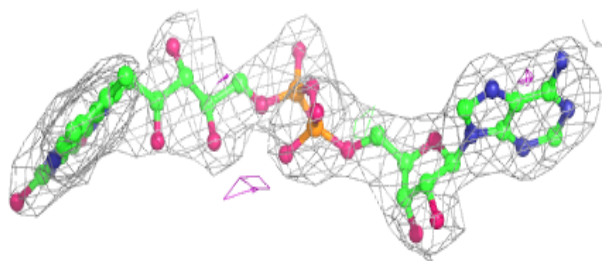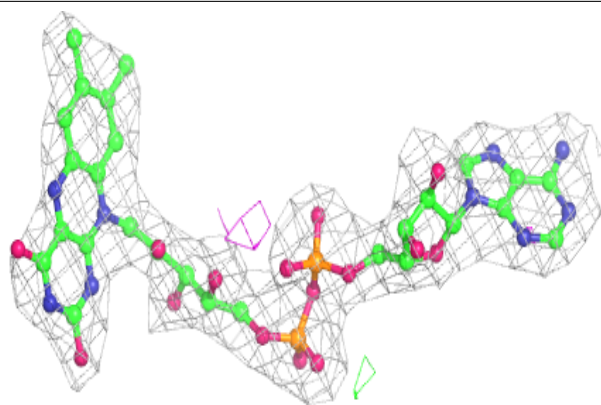
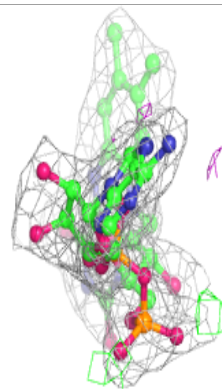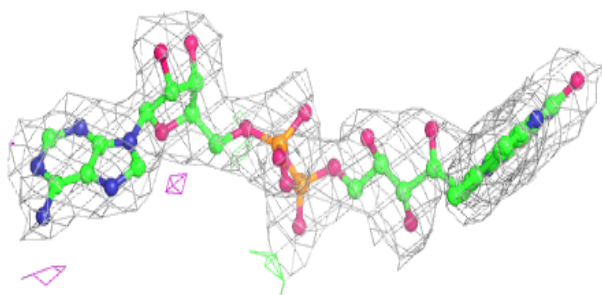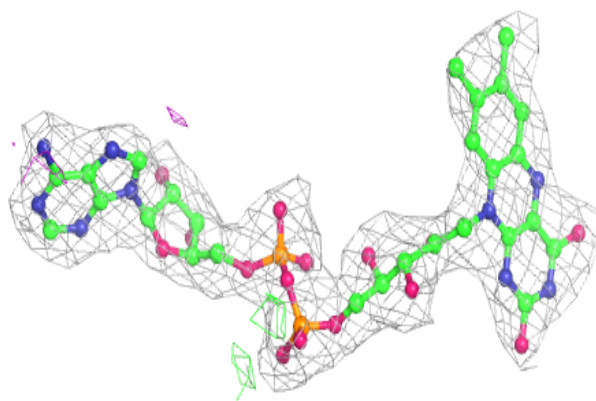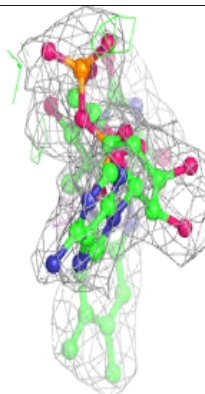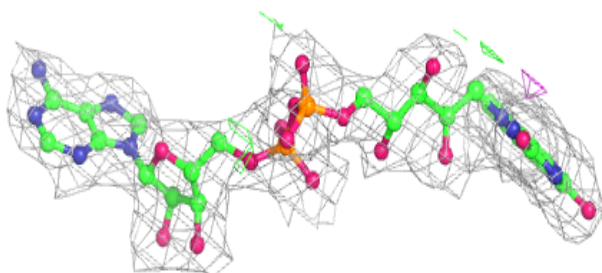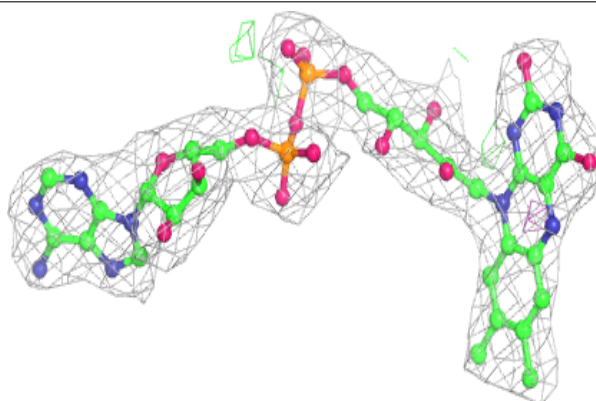

Electron density around FAD C 401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
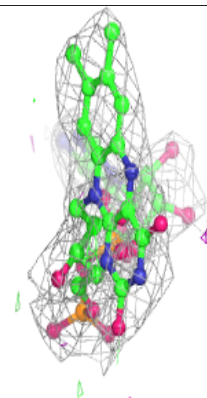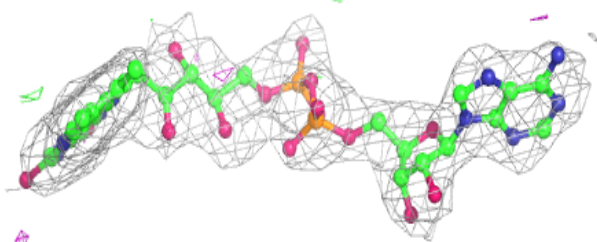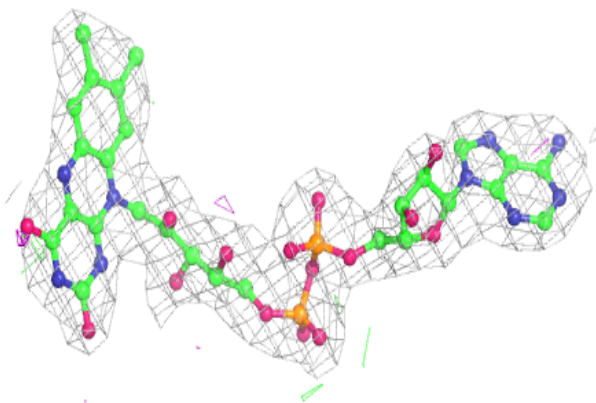
Electron density around FAD A 401:

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

Electron density around FAD D 401:

$2mF_o$-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.