Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:45 PM GMT

PDB ID	:	4A99
Title	:	STRUCTURE OF THE TETRACYCLINE DEGRADING MONOOXYGENASE TETX IN COMPLEX WITH MINOCYCLINE
Authors	:	Volkers, G.; Palm, G.J.; Weiss, M.S.; Hinrichs, W.
Deposited on	:	2011-11-25
Resolution	:	2.18 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

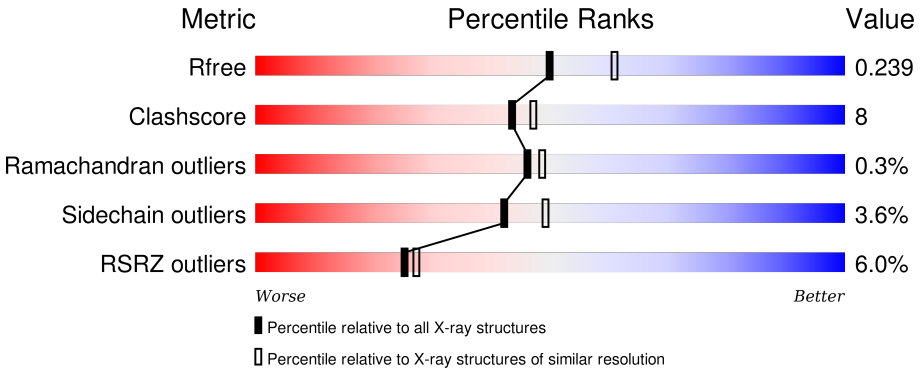
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.18 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}	91344	5130 (2.20-2.16)
Clashscore	102246	5965 (2.20-2.16)
Ramachandran outliers	100387	5863 (2.20-2.16)
Sidechain outliers	100360	5864 (2.20-2.16)
RSRZ outliers	91569	5142 (2.20-2.16)

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. 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	398	3% 79% 12% • 8%
1	B	398	5% 76% 14% • 8%
1	C	398	8% 78% 12% • 8%
1	D	398	6% 78% 12% • 8%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12662 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	0	0	0
			2886	1826	489	559	12			
1	B	368	Total	C	N	O	S	0	0	0
			2883	1826	489	556	12			
1	C	367	Total	C	N	O	S	0	0	0
			2868	1817	485	554	12			
1	D	367	Total	C	N	O	S	0	0	0
			2859	1812	485	550	12			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	MET	-	EXPRESSION TAG	UNP Q93L51
A	-8	GLY	-	EXPRESSION TAG	UNP Q93L51
A	-7	SER	-	EXPRESSION TAG	UNP Q93L51
A	-6	SER	-	EXPRESSION TAG	UNP Q93L51
A	-5	HIS	-	EXPRESSION TAG	UNP Q93L51
A	-4	HIS	-	EXPRESSION TAG	UNP Q93L51
A	-3	HIS	-	EXPRESSION TAG	UNP Q93L51
A	-2	HIS	-	EXPRESSION TAG	UNP Q93L51
A	-1	HIS	-	EXPRESSION TAG	UNP Q93L51
A	0	HIS	-	EXPRESSION TAG	UNP Q93L51
A	1	SER	-	EXPRESSION TAG	UNP Q93L51
A	2	SER	-	EXPRESSION TAG	UNP Q93L51
A	3	GLY	-	EXPRESSION TAG	UNP Q93L51
A	4	LEU	-	EXPRESSION TAG	UNP Q93L51
A	5	VAL	-	EXPRESSION TAG	UNP Q93L51
A	6	PRO	-	EXPRESSION TAG	UNP Q93L51
A	7	ARG	-	EXPRESSION TAG	UNP Q93L51
A	8	GLY	-	EXPRESSION TAG	UNP Q93L51
A	9	SER	-	EXPRESSION TAG	UNP Q93L51
A	10	HIS	-	EXPRESSION TAG	UNP Q93L51
B	-9	MET	-	EXPRESSION TAG	UNP Q93L51

Continued on next page...

Continued from previous page...

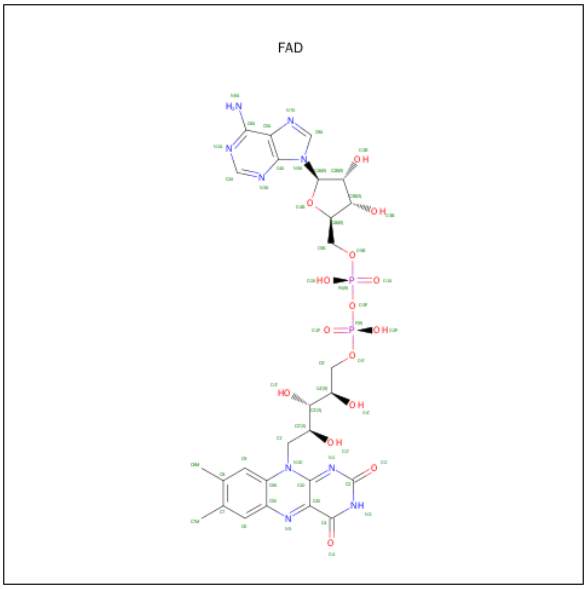
Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	GLY	-	EXPRESSION TAG	UNP Q93L51
B	-7	SER	-	EXPRESSION TAG	UNP Q93L51
B	-6	SER	-	EXPRESSION TAG	UNP Q93L51
B	-5	HIS	-	EXPRESSION TAG	UNP Q93L51
B	-4	HIS	-	EXPRESSION TAG	UNP Q93L51
B	-3	HIS	-	EXPRESSION TAG	UNP Q93L51
B	-2	HIS	-	EXPRESSION TAG	UNP Q93L51
B	-1	HIS	-	EXPRESSION TAG	UNP Q93L51
B	0	HIS	-	EXPRESSION TAG	UNP Q93L51
B	1	SER	-	EXPRESSION TAG	UNP Q93L51
B	2	SER	-	EXPRESSION TAG	UNP Q93L51
B	3	GLY	-	EXPRESSION TAG	UNP Q93L51
B	4	LEU	-	EXPRESSION TAG	UNP Q93L51
B	5	VAL	-	EXPRESSION TAG	UNP Q93L51
B	6	PRO	-	EXPRESSION TAG	UNP Q93L51
B	7	ARG	-	EXPRESSION TAG	UNP Q93L51
B	8	GLY	-	EXPRESSION TAG	UNP Q93L51
B	9	SER	-	EXPRESSION TAG	UNP Q93L51
B	10	HIS	-	EXPRESSION TAG	UNP Q93L51
C	-9	MET	-	EXPRESSION TAG	UNP Q93L51
C	-8	GLY	-	EXPRESSION TAG	UNP Q93L51
C	-7	SER	-	EXPRESSION TAG	UNP Q93L51
C	-6	SER	-	EXPRESSION TAG	UNP Q93L51
C	-5	HIS	-	EXPRESSION TAG	UNP Q93L51
C	-4	HIS	-	EXPRESSION TAG	UNP Q93L51
C	-3	HIS	-	EXPRESSION TAG	UNP Q93L51
C	-2	HIS	-	EXPRESSION TAG	UNP Q93L51
C	-1	HIS	-	EXPRESSION TAG	UNP Q93L51
C	0	HIS	-	EXPRESSION TAG	UNP Q93L51
C	1	SER	-	EXPRESSION TAG	UNP Q93L51
C	2	SER	-	EXPRESSION TAG	UNP Q93L51
C	3	GLY	-	EXPRESSION TAG	UNP Q93L51
C	4	LEU	-	EXPRESSION TAG	UNP Q93L51
C	5	VAL	-	EXPRESSION TAG	UNP Q93L51
C	6	PRO	-	EXPRESSION TAG	UNP Q93L51
C	7	ARG	-	EXPRESSION TAG	UNP Q93L51
C	8	GLY	-	EXPRESSION TAG	UNP Q93L51
C	9	SER	-	EXPRESSION TAG	UNP Q93L51
C	10	HIS	-	EXPRESSION TAG	UNP Q93L51
D	-9	MET	-	EXPRESSION TAG	UNP Q93L51
D	-8	GLY	-	EXPRESSION TAG	UNP Q93L51
D	-7	SER	-	EXPRESSION TAG	UNP Q93L51

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	-6	SER	-	EXPRESSION TAG	UNP Q93L51
D	-5	HIS	-	EXPRESSION TAG	UNP Q93L51
D	-4	HIS	-	EXPRESSION TAG	UNP Q93L51
D	-3	HIS	-	EXPRESSION TAG	UNP Q93L51
D	-2	HIS	-	EXPRESSION TAG	UNP Q93L51
D	-1	HIS	-	EXPRESSION TAG	UNP Q93L51
D	0	HIS	-	EXPRESSION TAG	UNP Q93L51
D	1	SER	-	EXPRESSION TAG	UNP Q93L51
D	2	SER	-	EXPRESSION TAG	UNP Q93L51
D	3	GLY	-	EXPRESSION TAG	UNP Q93L51
D	4	LEU	-	EXPRESSION TAG	UNP Q93L51
D	5	VAL	-	EXPRESSION TAG	UNP Q93L51
D	6	PRO	-	EXPRESSION TAG	UNP Q93L51
D	7	ARG	-	EXPRESSION TAG	UNP Q93L51
D	8	GLY	-	EXPRESSION TAG	UNP Q93L51
D	9	SER	-	EXPRESSION TAG	UNP Q93L51
D	10	HIS	-	EXPRESSION TAG	UNP Q93L51

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



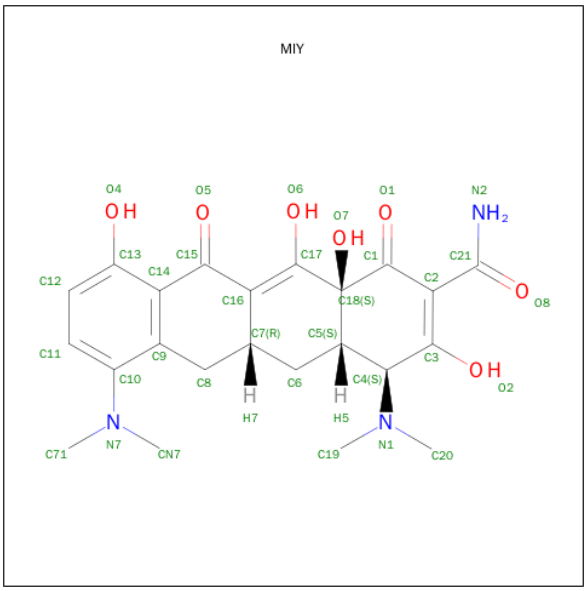
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

Continued on next page...

Continued from previous page...

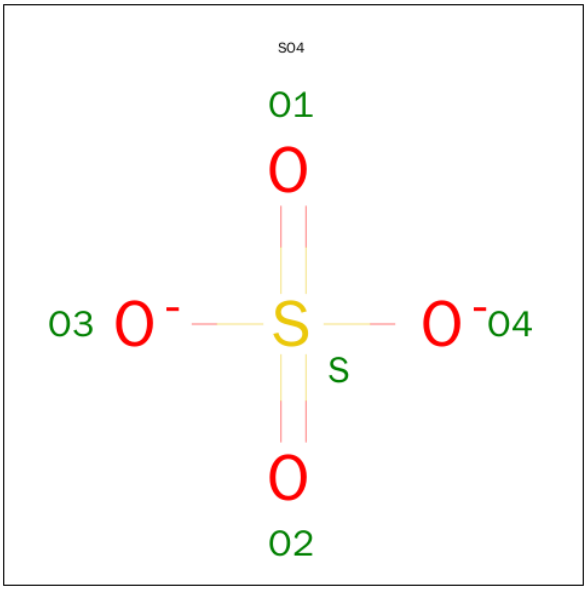
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C N O P 53 27 9 15 2	0	0
2	D	1	Total C N O P 53 27 9 15 2	0	0

- Molecule 3 is (4S,4AS,5AR,12AS)-4,7-BIS(DIMETHYLAMINO)-3,10,12,12A-TETRAHYDROXY-1,11-DIOXO-1,4,4A,5,5A,6,11,12A-OCTAHYDROTETRACENE-2-CARBOXAMIDE (three-letter code: MIY) (formula: $C_{23}H_{27}N_3O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 33 23 3 7	0	0
3	A	1	Total C N O 33 23 3 7	0	0
3	B	1	Total C N O 33 23 3 7	0	0
3	C	1	Total C N O 33 23 3 7	0	0
3	C	1	Total C N O 33 23 3 7	0	0
3	D	1	Total C N O 33 23 3 7	0	0
3	D	1	Total C N O 33 23 3 7	0	0
3	D	1	Total C N O 33 23 3 7	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	203	Total O 203 203	0	0

Continued on next page...

Continued from previous page...

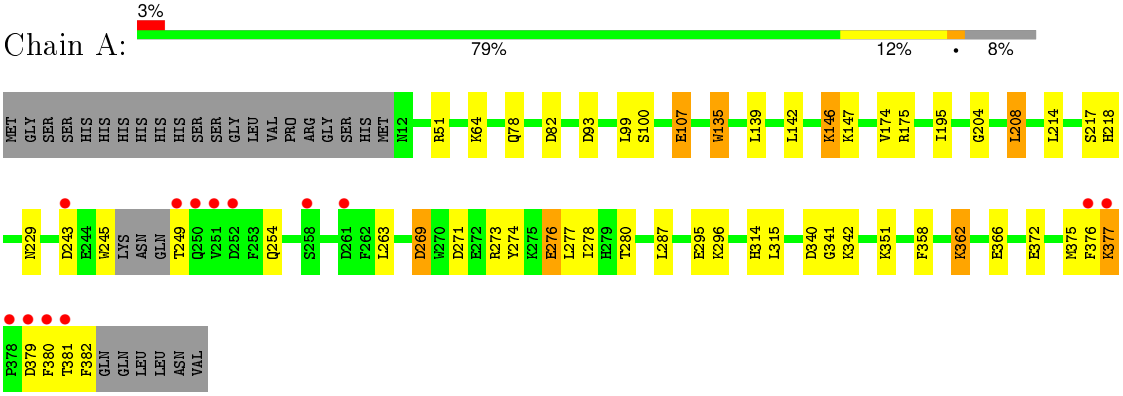
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	189	Total O 189 189	0	0
5	C	134	Total O 134 134	0	0
5	D	114	Total O 114 114	0	0

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 errors 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.

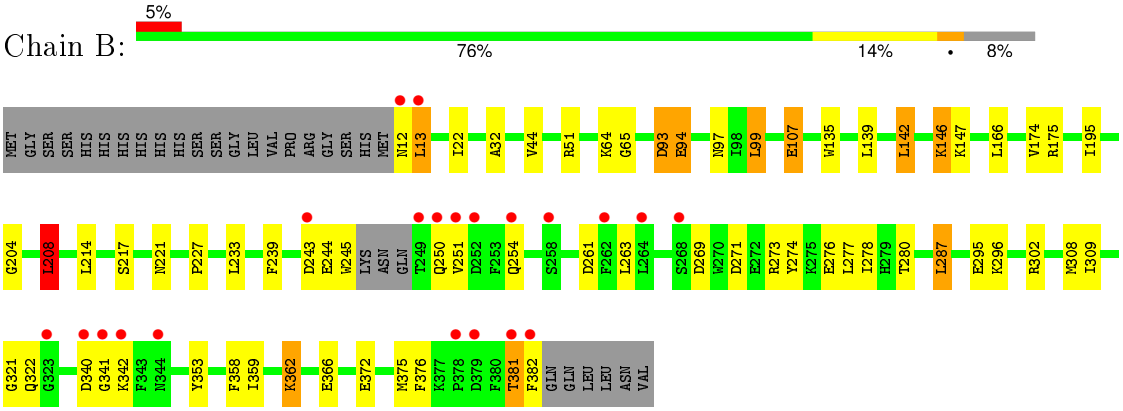
- Molecule 1: TETX2 PROTEIN

Chain A:



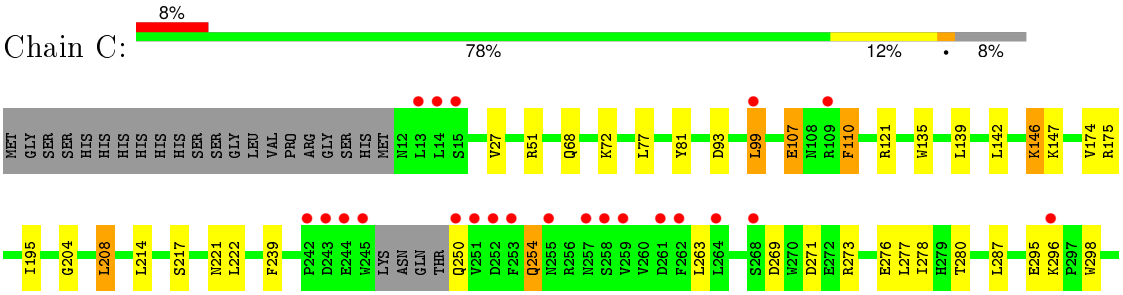
- Molecule 1: TETX2 PROTEIN

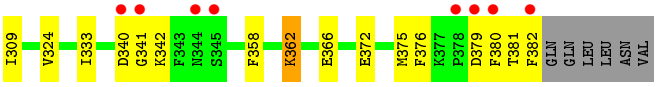
Chain B:



- Molecule 1: TETX2 PROTEIN

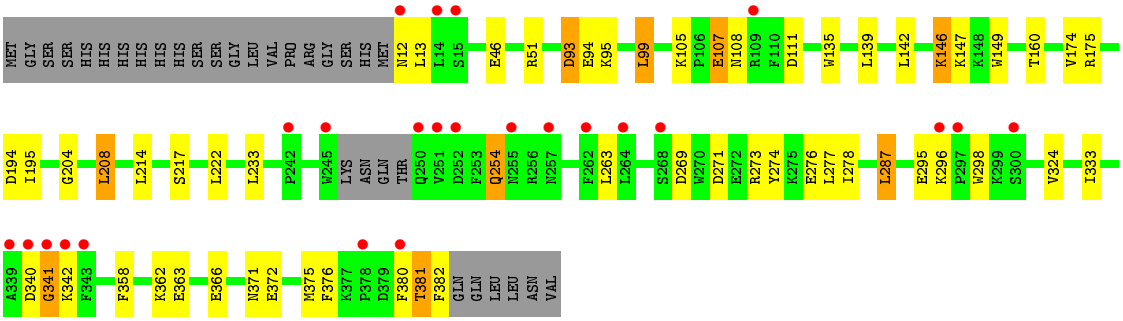
Chain C:





- Molecule 1: TETX2 PROTEIN

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	68.88Å 80.33Å 86.63Å 110.82° 90.27° 93.39°	Depositor
Resolution (Å)	80.94 – 2.18 47.66 – 2.18	Depositor EDS
% Data completeness (in resolution range)	95.5 (80.94-2.18) 85.2 (47.66-2.18)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.50 (at 2.18Å)	Xtriage
Refinement program	REFMAC 5.6.0116	Depositor
R, R_{free}	0.185 , 0.235 0.188 , 0.239	Depositor DCC
R_{free} test set	4301 reflections (5.24%)	DCC
Wilson B-factor (Å^2)	31.1	Xtriage
Anisotropy	0.278	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 48.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 86442 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	12662	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.68% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: MIY, 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	0.90	5/2944 (0.2%)	0.89	3/3988 (0.1%)
1	B	0.92	3/2941 (0.1%)	0.99	10/3983 (0.3%)
1	C	0.79	1/2926 (0.0%)	0.83	4/3965 (0.1%)
1	D	0.82	3/2917 (0.1%)	0.85	6/3954 (0.2%)
All	All	0.86	12/11728 (0.1%)	0.89	23/15890 (0.1%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	94	GLU	CD-OE2	-9.28	1.15	1.25
1	B	94	GLU	CD-OE1	-6.89	1.18	1.25
1	A	135	TRP	CD2-CE2	5.91	1.48	1.41
1	A	78	GLN	CD-NE2	-5.83	1.18	1.32
1	A	276	GLU	CD-OE1	5.72	1.31	1.25
1	D	371	ASN	CG-ND2	-5.59	1.18	1.32
1	A	245	TRP	CD2-CE2	5.40	1.47	1.41
1	B	276	GLU	CD-OE1	5.22	1.31	1.25
1	C	298	TRP	CD2-CE2	5.17	1.47	1.41
1	D	298	TRP	CD2-CE2	5.17	1.47	1.41
1	A	78	GLN	CD-OE1	-5.06	1.12	1.24
1	D	46	GLU	CD-OE2	5.03	1.31	1.25

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	175	ARG	NE-CZ-NH2	-13.46	113.57	120.30
1	A	175	ARG	NE-CZ-NH2	-11.04	114.78	120.30
1	B	94	GLU	OE1-CD-OE2	-10.97	110.13	123.30
1	B	93	ASP	CB-CG-OD2	9.83	127.15	118.30
1	B	175	ARG	NE-CZ-NH1	9.81	125.20	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	287	LEU	CA-CB-CG	9.75	137.72	115.30
1	A	175	ARG	NE-CZ-NH1	9.72	125.16	120.30
1	B	93	ASP	CB-CG-OD1	8.78	126.20	118.30
1	B	93	ASP	OD1-CG-OD2	-8.77	106.64	123.30
1	D	287	LEU	CA-CB-CG	8.54	134.94	115.30
1	D	175	ARG	NE-CZ-NH2	-7.53	116.53	120.30
1	C	175	ARG	NE-CZ-NH2	-6.87	116.87	120.30
1	B	208	LEU	CA-CB-CG	6.61	130.50	115.30
1	C	175	ARG	NE-CZ-NH1	6.35	123.47	120.30
1	B	99	LEU	CA-CB-CG	6.03	129.18	115.30
1	A	82	ASP	CB-CG-OD1	5.86	123.58	118.30
1	D	175	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	D	111	ASP	CB-CG-OD2	-5.85	113.04	118.30
1	D	93	ASP	CB-CG-OD1	5.70	123.43	118.30
1	C	121	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	C	99	LEU	CA-CB-CG	5.43	127.80	115.30
1	D	94	GLU	OE1-CD-OE2	-5.36	116.86	123.30
1	B	302	ARG	NE-CZ-NH2	-5.04	117.78	120.30

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	2886	0	2800	39	0
1	B	2883	0	2797	51	0
1	C	2868	0	2771	39	0
1	D	2859	0	2761	42	0
2	A	53	0	31	4	0
2	B	53	0	31	3	0
2	C	53	0	31	2	0
2	D	53	0	31	3	0
3	A	66	0	48	3	0
3	B	33	0	24	2	0
3	C	66	0	49	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	99	0	73	7	0
4	A	5	0	0	0	0
4	B	15	0	0	0	0
4	C	15	0	0	0	0
4	D	15	0	0	0	0
5	A	203	0	0	6	0
5	B	189	0	0	10	0
5	C	134	0	0	2	0
5	D	114	0	0	3	0
All	All	12662	0	11447	189	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 8.

All (189) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:ASP:HB2	5:A:2163:HOH:O	1.28	1.29
1:A:218:HIS:HD2	5:A:2063:HOH:O	1.43	0.99
1:B:381:THR:HA	5:B:2185:HOH:O	1.64	0.96
1:D:12:ASN:HD21	1:D:341:GLY:CA	1.83	0.92
1:D:12:ASN:HD21	1:D:341:GLY:HA2	1.35	0.91
1:C:333:ILE:HD11	3:C:392:MIY:HN73	1.52	0.91
3:D:392:MIY:O2	3:D:392:MIY:H192	1.70	0.89
1:D:146:LYS:HE2	1:D:147:LYS:H	1.45	0.81
1:A:269:ASP:CB	5:A:2163:HOH:O	2.02	0.80
1:D:139:LEU:HD21	1:D:142:LEU:HD13	1.64	0.79
1:C:139:LEU:HD21	1:C:142:LEU:HD13	1.65	0.78
1:C:146:LYS:HE2	1:C:147:LYS:H	1.50	0.77
1:A:379:ASP:HB3	1:B:65:GLY:O	1.87	0.75
1:B:146:LYS:HE2	1:B:147:LYS:H	1.53	0.74
1:B:174:VAL:HG22	1:B:174:VAL:O	1.87	0.73
1:A:146:LYS:HE2	1:A:147:LYS:H	1.53	0.73
1:A:362:LYS:O	1:A:366:GLU:HG2	1.90	0.71
1:C:250:GLN:N	5:C:2103:HOH:O	2.24	0.70
1:C:174:VAL:HG22	1:C:174:VAL:O	1.92	0.69
1:B:322:GLN:OE1	5:B:2176:HOH:O	2.09	0.69
1:C:362:LYS:O	1:C:366:GLU:HG2	1.92	0.69
1:B:244:GLU:CD	1:B:244:GLU:H	1.96	0.69
1:C:333:ILE:HD11	3:C:392:MIY:CN7	2.23	0.68
1:D:93:ASP:HB3	1:D:99:LEU:HD11	1.75	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:340:ASP:C	1:D:342:LYS:H	1.97	0.68
1:B:321:GLY:O	5:B:2174:HOH:O	2.10	0.68
1:A:99:LEU:HB3	1:B:359:ILE:HG23	1.75	0.67
1:A:99:LEU:HD22	1:B:359:ILE:O	1.94	0.67
1:D:362:LYS:O	1:D:366:GLU:HG2	1.94	0.67
1:D:51:ARG:HG2	5:D:2017:HOH:O	1.94	0.67
1:B:340:ASP:C	1:B:342:LYS:H	1.98	0.66
1:A:372:GLU:O	1:A:376:PHE:HD2	1.79	0.66
1:B:139:LEU:HD21	1:B:142:LEU:HD13	1.79	0.65
1:A:340:ASP:C	1:A:342:LYS:H	1.99	0.65
1:C:208:LEU:HD12	1:C:214:LEU:HD11	1.79	0.65
1:D:174:VAL:O	1:D:174:VAL:HG22	1.96	0.65
3:D:392:MIY:C19	3:D:392:MIY:O2	2.43	0.65
1:D:271:ASP:OD1	1:D:273:ARG:HD3	1.97	0.65
1:C:340:ASP:C	1:C:342:LYS:H	2.00	0.64
1:C:295:GLU:HG3	1:C:296:LYS:HG2	1.79	0.64
1:A:174:VAL:HG22	1:A:174:VAL:O	1.97	0.64
1:C:93:ASP:HB3	1:C:99:LEU:HD21	1.81	0.63
3:D:393:MIY:H712	3:D:393:MIY:C8	2.30	0.62
1:A:263:LEU:HB3	1:A:278:ILE:HD13	1.82	0.62
1:B:263:LEU:HB3	1:B:278:ILE:HD13	1.81	0.62
1:C:217:SER:HB2	1:C:382:PHE:CE2	2.35	0.62
1:D:208:LEU:HD12	1:D:214:LEU:HD11	1.83	0.61
1:B:271:ASP:OD1	1:B:273:ARG:HD3	2.01	0.61
1:D:381:THR:HG23	5:D:2110:HOH:O	2.01	0.61
1:D:358:PHE:O	1:D:362:LYS:HB2	2.01	0.60
2:D:389:FAD:N1	2:D:389:FAD:H2'	2.15	0.60
1:A:358:PHE:O	1:A:362:LYS:HB2	2.00	0.60
1:D:12:ASN:ND2	1:D:341:GLY:CA	2.62	0.60
1:A:139:LEU:HD21	1:A:142:LEU:HD13	1.84	0.59
1:C:271:ASP:OD1	1:C:273:ARG:HD3	2.02	0.59
1:B:358:PHE:O	1:B:362:LYS:HB2	2.01	0.59
1:A:195:ILE:HD12	1:A:277:LEU:HD12	1.85	0.58
1:B:142:LEU:HD22	1:B:174:VAL:CG2	2.34	0.58
1:A:271:ASP:OD1	1:A:273:ARG:HD3	2.03	0.58
2:B:389:FAD:N1	2:B:389:FAD:H2'	2.19	0.58
1:C:195:ILE:HD12	1:C:277:LEU:HD12	1.86	0.57
1:D:217:SER:HB2	1:D:382:PHE:CE2	2.39	0.57
1:B:217:SER:HB2	1:B:382:PHE:CE2	2.39	0.57
1:B:372:GLU:O	1:B:376:PHE:HD2	1.88	0.56
2:C:389:FAD:H2'	2:C:389:FAD:N1	2.19	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:358:PHE:O	1:C:362:LYS:HB2	2.05	0.56
1:D:295:GLU:HG3	1:D:296:LYS:HG2	1.87	0.56
1:B:208:LEU:HD12	1:B:214:LEU:HD11	1.87	0.55
1:B:243:ASP:CB	5:B:2147:HOH:O	2.55	0.55
1:C:333:ILE:CD1	3:C:392:MIY:HN73	2.32	0.55
1:A:274:TYR:O	1:A:277:LEU:HB3	2.07	0.55
1:A:93:ASP:HB3	1:A:99:LEU:HD11	1.89	0.54
1:B:243:ASP:HA	5:B:2147:HOH:O	2.05	0.54
1:B:295:GLU:HG3	1:B:296:LYS:HG2	1.89	0.54
3:C:392:MIY:O5	3:C:392:MIY:O6	2.24	0.54
1:A:204:GLY:HA3	1:A:273:ARG:HG2	1.91	0.53
1:A:295:GLU:HG3	1:A:296:LYS:HG2	1.90	0.53
1:D:105:LYS:HD2	1:D:108:ASN:ND2	2.24	0.53
1:A:142:LEU:HD22	1:A:174:VAL:CG2	2.39	0.52
1:A:379:ASP:O	1:A:379:ASP:CG	2.47	0.52
1:C:204:GLY:HA3	1:C:273:ARG:HG2	1.92	0.52
1:A:64:LYS:NZ	5:A:2039:HOH:O	2.41	0.52
1:B:274:TYR:O	1:B:277:LEU:HB3	2.09	0.52
1:C:324:VAL:HG12	2:C:389:FAD:O2	2.10	0.51
1:A:217:SER:HB2	1:A:382:PHE:CE1	2.45	0.51
3:A:392:MIY:HN72	3:C:392:MIY:N2	2.26	0.50
3:D:393:MIY:H712	3:D:393:MIY:H81	1.94	0.50
1:A:229:ASN:ND2	5:A:2028:HOH:O	2.39	0.50
1:B:362:LYS:O	1:B:366:GLU:HG2	2.11	0.49
1:A:100:SER:HB2	1:B:359:ILE:HG12	1.94	0.49
1:D:274:TYR:O	1:D:277:LEU:HB3	2.11	0.49
1:A:377:LYS:NZ	1:A:377:LYS:HB2	2.28	0.49
1:D:340:ASP:C	1:D:342:LYS:N	2.66	0.49
2:A:389:FAD:N1	2:A:389:FAD:H2'	2.28	0.49
1:D:204:GLY:HA3	1:D:273:ARG:HG2	1.95	0.49
1:B:245:TRP:O	5:B:2148:HOH:O	2.20	0.48
1:B:340:ASP:C	1:B:342:LYS:N	2.66	0.48
1:D:12:ASN:CG	1:D:13:LEU:H	2.17	0.48
1:C:174:VAL:CG2	1:C:174:VAL:O	2.60	0.48
1:A:208:LEU:HD12	1:A:214:LEU:HD11	1.96	0.48
1:B:166:LEU:HB2	1:B:308:MET:HG2	1.96	0.48
1:C:72:LYS:CG	1:C:77:LEU:HD22	2.44	0.48
1:D:208:LEU:HD23	1:D:273:ARG:NH2	2.29	0.47
1:D:324:VAL:HG12	2:D:389:FAD:O2	2.14	0.47
1:C:195:ILE:HD13	1:C:280:THR:CG2	2.44	0.47
1:B:195:ILE:HD12	1:B:277:LEU:HD12	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:340:ASP:C	1:C:342:LYS:N	2.68	0.47
1:B:93:ASP:HB3	1:B:99:LEU:HD21	1.96	0.47
1:A:380:PHE:CZ	1:A:382:PHE:HA	2.49	0.47
1:D:263:LEU:HB3	1:D:278:ILE:HD13	1.97	0.47
1:B:51:ARG:HB3	1:B:135:TRP:CZ2	2.50	0.47
1:A:340:ASP:C	1:A:342:LYS:N	2.68	0.47
1:B:204:GLY:HA3	1:B:273:ARG:HG2	1.97	0.47
1:D:195:ILE:HD12	1:D:277:LEU:HD12	1.96	0.46
1:D:95:LYS:HE3	5:D:2037:HOH:O	2.15	0.46
1:C:342:LYS:HG3	5:C:2123:HOH:O	2.15	0.46
1:C:222:LEU:N	1:C:222:LEU:HD12	2.31	0.46
1:C:380:PHE:CZ	1:C:382:PHE:HA	2.51	0.46
1:B:243:ASP:CA	5:B:2147:HOH:O	2.63	0.46
1:C:208:LEU:HD12	1:C:214:LEU:CD1	2.46	0.46
3:D:393:MIY:O5	3:D:393:MIY:O6	2.33	0.45
1:C:51:ARG:HB3	1:C:135:TRP:CZ2	2.51	0.45
1:B:93:ASP:OD1	1:B:97:ASN:HB2	2.16	0.45
1:C:375:MET:HE3	1:C:375:MET:HB3	1.62	0.45
1:D:208:LEU:HD12	1:D:214:LEU:CD1	2.46	0.45
1:D:333:ILE:HD11	3:D:393:MIY:H713	1.98	0.45
1:C:107:GLU:H	1:C:107:GLU:HG3	1.34	0.45
1:D:51:ARG:HB3	1:D:135:TRP:CZ2	2.52	0.45
1:D:375:MET:HB3	1:D:375:MET:HE3	1.57	0.45
1:D:107:GLU:HG3	1:D:107:GLU:H	1.31	0.45
1:B:375:MET:HE2	1:B:375:MET:HB3	1.62	0.44
1:D:372:GLU:O	1:D:376:PHE:HD2	2.00	0.44
3:C:391:MIY:H203	3:C:391:MIY:H5	1.77	0.44
1:B:174:VAL:CG2	1:B:174:VAL:O	2.57	0.44
1:B:261:ASP:OD1	5:B:2151:HOH:O	2.21	0.44
2:B:389:FAD:H1'1	2:B:389:FAD:H9	1.75	0.44
1:B:227:PRO:HA	1:B:233:LEU:HD12	2.00	0.44
1:A:195:ILE:HD13	1:A:280:THR:CG2	2.48	0.44
1:D:222:LEU:HD22	1:D:375:MET:HE3	2.00	0.43
1:C:27:VAL:HG12	1:C:309:ILE:HD12	2.00	0.43
1:C:263:LEU:HB3	1:C:278:ILE:HD13	2.00	0.43
3:B:391:MIY:O6	3:B:391:MIY:O5	2.35	0.43
3:A:391:MIY:O6	3:A:391:MIY:O5	2.35	0.43
1:A:314:HIS:O	1:A:315:LEU:C	2.56	0.43
1:B:107:GLU:H	1:B:107:GLU:HG3	1.31	0.43
1:B:22:ILE:HG13	1:B:139:LEU:HD22	2.00	0.43
1:C:208:LEU:HD23	1:C:273:ARG:NH2	2.34	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:LEU:HD12	1:B:214:LEU:CD1	2.49	0.43
1:C:221:ASN:HD22	1:C:239:PHE:HB3	1.84	0.43
1:B:146:LYS:H	1:B:146:LYS:HG3	1.38	0.43
2:D:389:FAD:H1'1	2:D:389:FAD:H9	1.79	0.43
1:C:72:LYS:HG3	1:C:77:LEU:HD22	2.00	0.43
2:A:389:FAD:H6	3:A:391:MIY:C19	2.48	0.43
1:D:142:LEU:HD12	1:D:142:LEU:HA	1.88	0.43
3:B:391:MIY:H5	3:B:391:MIY:H203	1.74	0.42
1:B:245:TRP:HA	1:B:250:GLN:HE21	1.85	0.42
1:B:195:ILE:HD13	1:B:280:THR:CG2	2.49	0.42
1:C:110:PHE:CD1	1:C:110:PHE:N	2.88	0.42
1:D:174:VAL:O	1:D:174:VAL:CG2	2.67	0.42
1:A:51:ARG:HB3	1:A:135:TRP:CZ2	2.54	0.42
1:C:254:GLN:HB3	1:C:254:GLN:HE21	1.72	0.42
1:B:221:ASN:HD22	1:B:239:PHE:HB3	1.84	0.42
1:A:218:HIS:HE1	1:A:269:ASP:OD2	2.02	0.42
1:A:195:ILE:CD1	1:A:277:LEU:HD12	2.48	0.42
1:D:254:GLN:HE21	1:D:254:GLN:HB3	1.73	0.42
1:C:372:GLU:O	1:C:376:PHE:HD2	2.02	0.42
1:A:142:LEU:HD22	1:A:174:VAL:HG22	2.02	0.42
1:A:107:GLU:H	1:A:107:GLU:HG3	1.20	0.42
1:D:363:GLU:OE1	3:D:393:MIY:O6	2.37	0.41
1:D:380:PHE:CZ	1:D:382:PHE:HA	2.55	0.41
1:D:149:TRP:O	1:D:160:THR:HA	2.20	0.41
1:B:13:LEU:H	1:B:13:LEU:HG	1.72	0.41
1:C:142:LEU:HA	1:C:142:LEU:HD12	1.88	0.41
1:B:64:LYS:NZ	5:B:2037:HOH:O	2.40	0.41
1:C:68:GLN:NE2	1:C:81:TYR:OH	2.53	0.41
2:A:389:FAD:H9	5:A:2185:HOH:O	2.21	0.41
1:B:244:GLU:O	1:B:250:GLN:HG2	2.20	0.41
1:D:295:GLU:HG3	1:D:296:LYS:H	1.85	0.41
1:A:362:LYS:O	1:A:366:GLU:CG	2.65	0.41
1:D:263:LEU:HA	1:D:263:LEU:HD23	1.87	0.41
1:B:244:GLU:CD	1:B:244:GLU:N	2.71	0.41
2:B:389:FAD:H9	5:B:2170:HOH:O	2.21	0.41
1:D:194:ASP:HA	1:D:233:LEU:O	2.21	0.40
1:B:94:GLU:N	1:B:94:GLU:OE1	2.52	0.40
3:C:392:MIY:H203	3:C:392:MIY:H5	1.68	0.40
1:A:375:MET:CE	1:A:376:PHE:CE2	3.05	0.40
2:A:389:FAD:H1'1	2:A:389:FAD:H9	1.81	0.40
1:B:32:ALA:HB2	1:B:44:VAL:CG2	2.51	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:309:ILE:HG21	1:B:309:ILE:HD13	1.91	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	364/398 (92%)	352 (97%)	11 (3%)	1 (0%)	46	48
1	B	364/398 (92%)	350 (96%)	12 (3%)	2 (0%)	34	33
1	C	363/398 (91%)	348 (96%)	14 (4%)	1 (0%)	46	48
1	D	363/398 (91%)	348 (96%)	14 (4%)	1 (0%)	46	48
All	All	1454/1592 (91%)	1398 (96%)	51 (4%)	5 (0%)	46	48

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	13	LEU
1	A	341	GLY
1	B	341	GLY
1	D	341	GLY
1	C	341	GLY

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	312/345 (90%)	299 (96%)	13 (4%)	36	42
1	B	310/345 (90%)	298 (96%)	12 (4%)	39	45
1	C	307/345 (89%)	296 (96%)	11 (4%)	42	49
1	D	305/345 (88%)	296 (97%)	9 (3%)	48	57
All	All	1234/1380 (89%)	1189 (96%)	45 (4%)	42	49

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	107	GLU
1	A	146	LYS
1	A	208	LEU
1	A	243	ASP
1	A	249	THR
1	A	254	GLN
1	A	269	ASP
1	A	276	GLU
1	A	287	LEU
1	A	351	LYS
1	A	362	LYS
1	A	377	LYS
1	A	381	THR
1	B	12	ASN
1	B	107	GLU
1	B	142	LEU
1	B	146	LYS
1	B	208	LEU
1	B	251	VAL
1	B	254	GLN
1	B	269	ASP
1	B	287	LEU
1	B	353	TYR
1	B	362	LYS
1	B	381	THR
1	C	107	GLU
1	C	110	PHE
1	C	146	LYS
1	C	208	LEU
1	C	254	GLN
1	C	269	ASP
1	C	276	GLU
1	C	287	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	362	LYS
1	C	379	ASP
1	C	381	THR
1	D	99	LEU
1	D	107	GLU
1	D	146	LYS
1	D	208	LEU
1	D	254	GLN
1	D	269	ASP
1	D	276	GLU
1	D	287	LEU
1	D	381	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	GLN
1	A	78	GLN
1	A	130	ASN
1	A	190	ASN
1	A	218	HIS
1	A	221	ASN
1	A	254	GLN
1	A	370	GLN
1	A	371	ASN
1	B	108	ASN
1	B	130	ASN
1	B	190	ASN
1	B	221	ASN
1	B	250	GLN
1	B	254	GLN
1	B	370	GLN
1	B	371	ASN
1	C	12	ASN
1	C	68	GLN
1	C	130	ASN
1	C	190	ASN
1	C	218	HIS
1	C	221	ASN
1	C	254	GLN
1	C	279	HIS
1	C	371	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	12	ASN
1	D	108	ASN
1	D	130	ASN
1	D	190	ASN
1	D	221	ASN
1	D	254	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

22 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	SO4	A	1383	-	4,4,4	0.51	0	6,6,6	0.32	0
2	FAD	A	389	-	48,58,58	1.36	7 (14%)	54,89,89	2.54	11 (20%)
3	MIY	A	391	-	35,36,36	1.41	4 (11%)	40,58,58	1.65	9 (22%)
3	MIY	A	392	-	35,36,36	1.28	4 (11%)	40,58,58	2.21	12 (30%)
4	SO4	B	1383	-	4,4,4	0.58	0	6,6,6	0.36	0
4	SO4	B	1384	-	4,4,4	0.53	0	6,6,6	0.28	0
4	SO4	B	1385	-	4,4,4	0.58	0	6,6,6	0.15	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	FAD	B	389	-	48,58,58	1.59	9 (18%)	54,89,89	2.52	10 (18%)
3	MIY	B	391	-	35,36,36	1.27	5 (14%)	40,58,58	1.73	10 (25%)
4	SO4	C	1383	-	4,4,4	0.74	0	6,6,6	0.28	0
4	SO4	C	1384	-	4,4,4	0.50	0	6,6,6	0.39	0
4	SO4	C	1385	-	4,4,4	0.43	0	6,6,6	0.22	0
2	FAD	C	389	-	48,58,58	1.49	7 (14%)	54,89,89	2.68	16 (29%)
3	MIY	C	391	-	35,36,36	1.09	1 (2%)	40,58,58	1.87	10 (25%)
3	MIY	C	392	-	35,36,36	1.53	7 (20%)	40,58,58	2.54	12 (30%)
4	SO4	D	1383	-	4,4,4	0.83	0	6,6,6	0.23	0
4	SO4	D	1384	-	4,4,4	0.57	0	6,6,6	0.41	0
4	SO4	D	1385	-	4,4,4	0.60	0	6,6,6	0.26	0
2	FAD	D	389	-	48,58,58	1.51	8 (16%)	54,89,89	2.73	9 (16%)
3	MIY	D	391	-	35,36,36	1.06	2 (5%)	40,58,58	1.81	9 (22%)
3	MIY	D	392	-	35,36,36	1.35	6 (17%)	40,58,58	2.37	13 (32%)
3	MIY	D	393	-	35,36,36	1.07	3 (8%)	40,58,58	2.81	14 (35%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SO4	A	1383	-	-	0/0/0/0	0/0/0/0
2	FAD	A	389	-	-	0/30/50/50	0/6/6/6
3	MIY	A	391	-	-	0/12/70/70	0/4/4/4
3	MIY	A	392	-	-	0/12/70/70	0/4/4/4
4	SO4	B	1383	-	-	0/0/0/0	0/0/0/0
4	SO4	B	1384	-	-	0/0/0/0	0/0/0/0
4	SO4	B	1385	-	-	0/0/0/0	0/0/0/0
2	FAD	B	389	-	-	0/30/50/50	0/6/6/6
3	MIY	B	391	-	-	0/12/70/70	0/4/4/4
4	SO4	C	1383	-	-	0/0/0/0	0/0/0/0
4	SO4	C	1384	-	-	0/0/0/0	0/0/0/0
4	SO4	C	1385	-	-	0/0/0/0	0/0/0/0
2	FAD	C	389	-	-	0/30/50/50	0/6/6/6
3	MIY	C	391	-	-	0/12/70/70	0/4/4/4
3	MIY	C	392	-	-	0/12/70/70	0/4/4/4
4	SO4	D	1383	-	-	0/0/0/0	0/0/0/0
4	SO4	D	1384	-	-	0/0/0/0	0/0/0/0
4	SO4	D	1385	-	-	0/0/0/0	0/0/0/0
2	FAD	D	389	-	-	0/30/50/50	0/6/6/6

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MIY	D	391	-	-	0/12/70/70	0/4/4/4
3	MIY	D	392	-	-	0/12/70/70	0/4/4/4
3	MIY	D	393	-	-	0/12/70/70	0/4/4/4

All (63) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	392	MIY	C16-C17	-3.79	1.31	1.36
2	D	389	FAD	O5'-C5'	-3.52	1.30	1.44
2	B	389	FAD	O5'-C5'	-3.45	1.30	1.44
3	A	391	MIY	C6-C5	-3.33	1.48	1.53
2	C	389	FAD	O5'-C5'	-3.21	1.31	1.44
2	A	389	FAD	O5'-C5'	-2.59	1.34	1.44
2	D	389	FAD	C6-C5X	-2.55	1.37	1.41
2	A	389	FAD	O4B-C4B	-2.54	1.39	1.45
3	D	392	MIY	C14-C13	-2.40	1.37	1.41
3	B	391	MIY	C5-C4	-2.35	1.51	1.54
3	D	391	MIY	C6-C5	-2.32	1.49	1.53
2	B	389	FAD	C4-C4X	-2.30	1.36	1.41
3	A	391	MIY	C18-C1	-2.28	1.51	1.55
3	D	392	MIY	C18-C1	-2.23	1.51	1.55
3	B	391	MIY	C18-C1	-2.08	1.51	1.55
2	D	389	FAD	O2'-C2'	-2.07	1.38	1.43
2	B	389	FAD	C6-C5X	-2.04	1.38	1.41
2	C	389	FAD	O2'-C2'	-2.04	1.38	1.43
3	D	393	MIY	O1-C1	2.01	1.26	1.22
3	D	392	MIY	O1-C1	2.03	1.26	1.22
3	B	391	MIY	C14-C15	2.03	1.51	1.46
3	C	391	MIY	C2-C21	2.04	1.51	1.47
3	C	392	MIY	O7-C18	2.06	1.45	1.42
3	B	391	MIY	C11-C10	2.08	1.43	1.39
2	A	389	FAD	C5X-N5	2.11	1.38	1.35
3	C	392	MIY	C4-C3	2.15	1.56	1.51
2	B	389	FAD	C10-N1	2.21	1.39	1.35
3	C	392	MIY	C18-C17	2.23	1.54	1.52
3	D	393	MIY	C14-C9	2.26	1.44	1.40
3	A	392	MIY	O5-C15	2.26	1.28	1.23
3	A	392	MIY	C14-C15	2.31	1.52	1.46
3	A	391	MIY	C14-C15	2.36	1.52	1.46
3	D	392	MIY	C4-C3	2.36	1.56	1.51
3	A	392	MIY	C7-C16	2.38	1.54	1.51
3	D	392	MIY	C14-C15	2.39	1.52	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	392	MIY	C5-C4	2.43	1.57	1.54
2	D	389	FAD	C2A-N1A	2.49	1.38	1.33
3	B	391	MIY	C18-C5	2.57	1.55	1.53
2	B	389	FAD	O4'-C4'	2.58	1.49	1.43
2	A	389	FAD	C2A-N3A	2.58	1.36	1.32
3	C	392	MIY	O5-C15	2.60	1.28	1.23
2	B	389	FAD	C2A-N1A	2.63	1.38	1.33
3	D	392	MIY	O7-C18	2.64	1.46	1.42
2	A	389	FAD	C1'-N10	2.79	1.51	1.48
3	D	393	MIY	O5-C15	2.87	1.29	1.23
3	D	391	MIY	C18-C5	2.91	1.55	1.53
2	D	389	FAD	C2A-N3A	3.04	1.37	1.32
2	C	389	FAD	C2A-N3A	3.14	1.37	1.32
2	C	389	FAD	C10-N1	3.25	1.41	1.35
2	A	389	FAD	C4-N3	3.28	1.39	1.33
2	C	389	FAD	C4-N3	3.31	1.39	1.33
2	D	389	FAD	C10-N1	3.44	1.41	1.35
2	C	389	FAD	C2A-N1A	3.57	1.40	1.33
3	C	392	MIY	C18-C5	3.57	1.56	1.53
2	D	389	FAD	C4-N3	3.61	1.39	1.33
3	A	391	MIY	C18-C5	3.85	1.56	1.53
2	B	389	FAD	C4-N3	4.03	1.40	1.33
2	B	389	FAD	C5X-N5	4.06	1.41	1.35
2	A	389	FAD	C4X-N5	4.13	1.39	1.33
2	B	389	FAD	C4X-N5	4.20	1.39	1.33
2	D	389	FAD	C4X-N5	4.22	1.39	1.33
2	C	389	FAD	C4X-N5	4.46	1.40	1.33
3	A	392	MIY	C18-C5	4.55	1.57	1.53

All (135) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	389	FAD	N3A-C2A-N1A	-15.30	117.18	128.89
2	A	389	FAD	N3A-C2A-N1A	-14.05	118.14	128.89
2	C	389	FAD	N3A-C2A-N1A	-13.72	118.39	128.89
2	B	389	FAD	N3A-C2A-N1A	-13.26	118.74	128.89
3	C	392	MIY	O6-C17-C16	-9.62	114.63	123.84
3	C	392	MIY	C20-N1-C4	-6.19	98.95	114.07
3	D	393	MIY	C11-C10-N7	-5.63	113.70	121.59
3	D	391	MIY	C20-N1-C4	-5.50	100.63	114.07
3	C	391	MIY	C20-N1-C4	-5.42	100.83	114.07
3	A	392	MIY	C5-C18-C1	-5.38	105.03	111.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	392	MIY	C21-C2-C1	-5.06	114.91	120.87
3	B	391	MIY	O6-C17-C16	-5.05	119.01	123.84
3	A	392	MIY	C7-C6-C5	-4.70	101.64	110.71
3	C	391	MIY	O6-C17-C16	-4.65	119.39	123.84
3	D	392	MIY	C20-N1-C4	-4.19	103.85	114.07
3	D	392	MIY	C5-C18-C1	-4.05	106.55	111.17
3	A	392	MIY	C1-C18-C17	-4.02	104.69	109.73
3	A	392	MIY	C20-N1-C4	-4.00	104.29	114.07
3	B	391	MIY	C20-N1-C4	-4.00	104.30	114.07
2	B	389	FAD	O5'-P-O1P	-3.83	94.74	109.62
3	A	391	MIY	C20-N1-C4	-3.82	104.73	114.07
3	A	392	MIY	O6-C17-C16	-3.79	120.22	123.84
2	B	389	FAD	C2B-C1B-N9A	-3.70	108.64	114.29
3	C	392	MIY	C1-C18-C17	-3.69	105.09	109.73
3	D	392	MIY	O8-C21-N2	-3.67	113.63	122.76
3	D	392	MIY	C11-C12-C13	-3.65	116.75	120.49
3	D	391	MIY	O8-C21-N2	-3.56	113.91	122.76
2	A	389	FAD	C4X-C4-N3	-3.56	118.72	123.59
2	D	389	FAD	C1B-N9A-C4A	-3.54	121.60	126.94
3	D	393	MIY	C20-N1-C4	-3.51	105.49	114.07
3	D	393	MIY	C13-C14-C15	-3.49	115.89	121.19
2	C	389	FAD	C1B-N9A-C4A	-3.46	121.72	126.94
3	D	392	MIY	C71-N7-C10	-3.44	104.47	115.18
3	A	391	MIY	O8-C21-N2	-3.43	114.23	122.76
2	B	389	FAD	C4X-C4-N3	-3.38	118.97	123.59
3	D	391	MIY	O6-C17-C16	-3.35	120.63	123.84
3	A	391	MIY	C7-C6-C5	-3.24	104.44	110.71
2	C	389	FAD	C4X-C10-N10	-3.24	118.61	120.52
2	D	389	FAD	C4X-C4-N3	-3.12	119.32	123.59
2	A	389	FAD	C2B-C1B-N9A	-3.10	109.56	114.29
3	D	393	MIY	C1-C18-C17	-3.09	105.84	109.73
3	C	391	MIY	O8-C21-N2	-3.05	115.18	122.76
3	D	391	MIY	C7-C6-C5	-3.00	104.92	110.71
3	D	393	MIY	C11-C10-C9	-2.99	116.61	120.47
3	C	391	MIY	C6-C7-C16	-2.98	104.25	109.56
3	D	392	MIY	C6-C5-C4	-2.98	106.97	111.47
3	D	393	MIY	O8-C21-N2	-2.94	115.45	122.76
2	A	389	FAD	C1B-N9A-C4A	-2.94	122.50	126.94
2	C	389	FAD	C4X-C4-N3	-2.91	119.61	123.59
3	A	392	MIY	C21-C2-C1	-2.89	117.47	120.87
3	D	392	MIY	O6-C17-C16	-2.87	121.09	123.84
3	B	391	MIY	C7-C6-C5	-2.83	105.25	110.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	391	MIY	O6-C17-C16	-2.81	121.15	123.84
3	B	391	MIY	O8-C21-N2	-2.78	115.85	122.76
3	D	392	MIY	C1-C18-C17	-2.78	106.24	109.73
3	B	391	MIY	C6-C7-C16	-2.76	104.64	109.56
3	C	391	MIY	C7-C6-C5	-2.76	105.39	110.71
2	B	389	FAD	C4X-C10-N10	-2.66	118.95	120.52
3	B	391	MIY	C71-N7-CN7	-2.61	107.33	115.96
2	B	389	FAD	C1B-N9A-C4A	-2.58	123.04	126.94
3	C	392	MIY	C5-C18-C1	-2.58	108.23	111.17
2	C	389	FAD	O5'-P-O1P	-2.57	99.66	109.62
2	C	389	FAD	C4-C4X-C10	-2.55	118.31	119.94
3	D	393	MIY	C15-C16-C17	-2.54	116.77	118.93
3	C	392	MIY	O8-C21-N2	-2.51	116.53	122.76
3	A	391	MIY	C6-C7-C16	-2.48	105.15	109.56
3	A	391	MIY	O7-C18-C17	-2.46	105.44	109.85
3	A	392	MIY	O8-C21-N2	-2.41	116.78	122.76
3	A	391	MIY	C21-C2-C1	-2.40	118.05	120.87
3	B	391	MIY	C1-C18-C17	-2.35	106.77	109.73
3	D	391	MIY	C6-C7-C16	-2.35	105.38	109.56
2	C	389	FAD	O3B-C3B-C4B	-2.34	104.03	111.05
3	D	391	MIY	C6-C5-C4	-2.34	107.94	111.47
3	A	391	MIY	C71-N7-CN7	-2.31	108.34	115.96
3	C	391	MIY	C13-C14-C15	-2.23	117.81	121.19
2	A	389	FAD	P-O3P-PA	-2.21	126.52	132.73
3	B	391	MIY	C21-C2-C1	-2.20	118.28	120.87
3	D	391	MIY	O7-C18-C17	-2.19	105.93	109.85
3	C	392	MIY	C9-C10-N7	-2.16	117.11	118.94
3	C	392	MIY	CN7-N7-C10	-2.15	108.49	115.18
3	C	391	MIY	C71-N7-CN7	-2.14	108.91	115.96
2	B	389	FAD	O5B-C5B-C4B	-2.11	101.33	109.12
2	A	389	FAD	O3P-P-O5'	-2.07	97.44	102.94
3	D	393	MIY	C6-C7-C16	-2.07	105.88	109.56
2	D	389	FAD	O4'-C4'-C5'	-2.06	105.69	110.19
3	D	392	MIY	C11-C10-N7	-2.04	118.73	121.59
3	C	391	MIY	C12-C13-C14	-2.01	117.57	120.21
2	C	389	FAD	C9A-C5X-N5	-2.00	119.39	122.36
3	A	392	MIY	C8-C9-C14	2.03	121.76	117.77
2	C	389	FAD	C8M-C8-C7	2.03	125.20	120.73
3	C	391	MIY	O6-C17-C18	2.07	116.81	113.50
2	A	389	FAD	C2A-N1A-C6A	2.08	122.49	118.77
2	D	389	FAD	O2'-C2'-C3'	2.12	114.35	109.02
2	C	389	FAD	O4B-C4B-C3B	2.15	109.48	105.15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	391	MIY	O7-C18-C5	2.17	112.91	110.17
3	D	391	MIY	O7-C18-C5	2.21	112.95	110.17
3	D	393	MIY	O1-C1-C18	2.23	123.38	118.72
3	B	391	MIY	O6-C17-C18	2.32	117.20	113.50
2	D	389	FAD	O4'-C4'-C3'	2.33	114.87	109.02
3	D	393	MIY	C12-C11-C10	2.38	124.51	119.29
3	D	393	MIY	C19-N1-C4	2.41	119.97	114.07
2	A	389	FAD	O4'-C4'-C3'	2.42	115.09	109.02
3	A	392	MIY	O1-C1-C18	2.43	123.80	118.72
2	B	389	FAD	O3P-P-O5'	2.45	109.43	102.94
3	D	393	MIY	C2-C21-N2	2.49	124.07	119.27
2	C	389	FAD	C2A-N1A-C6A	2.51	123.25	118.77
3	C	392	MIY	C2-C21-N2	2.56	124.20	119.27
2	C	389	FAD	C4X-N5-C5X	2.63	119.79	116.76
2	A	389	FAD	C1'-N10-C9A	2.65	121.83	118.86
3	C	392	MIY	C8-C9-C14	2.71	123.10	117.77
3	D	392	MIY	C2-C21-N2	2.76	124.59	119.27
3	B	391	MIY	O7-C18-C5	2.83	113.74	110.17
3	C	391	MIY	C13-C14-C9	2.88	122.77	119.21
3	C	392	MIY	C6-C5-C4	2.89	115.84	111.47
3	D	391	MIY	C2-C21-N2	2.90	124.87	119.27
2	C	389	FAD	O4'-C4'-C3'	2.94	116.41	109.02
3	D	393	MIY	C13-C14-C9	2.96	122.87	119.21
3	A	392	MIY	C2-C21-N2	3.02	125.09	119.27
2	B	389	FAD	C5X-C9A-N10	3.08	119.96	117.62
3	A	392	MIY	O6-C17-C18	3.14	118.50	113.50
2	C	389	FAD	O3P-P-O5'	3.61	112.52	102.94
3	C	392	MIY	C19-N1-C4	3.69	123.10	114.07
2	D	389	FAD	C5X-C9A-N10	4.17	120.79	117.62
2	C	389	FAD	C5X-C9A-N10	4.70	121.19	117.62
2	D	389	FAD	O3P-P-O5'	4.79	115.64	102.94
3	C	392	MIY	O6-C17-C18	5.00	121.47	113.50
3	A	392	MIY	O7-C18-C5	5.01	116.49	110.17
2	A	389	FAD	C5X-C9A-N10	5.17	121.55	117.62
3	D	392	MIY	C18-C5-C4	5.29	118.83	111.73
3	D	392	MIY	O7-C18-C5	5.48	117.08	110.17
2	D	389	FAD	C4-N3-C2	6.26	120.66	115.25
2	A	389	FAD	C4-N3-C2	6.26	120.66	115.25
2	C	389	FAD	C4-N3-C2	6.38	120.76	115.25
2	B	389	FAD	C4-N3-C2	6.96	121.26	115.25
3	D	393	MIY	C9-C10-N7	12.51	129.57	118.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	389	FAD	4	0
3	A	391	MIY	2	0
3	A	392	MIY	1	0
2	B	389	FAD	3	0
3	B	391	MIY	2	0
2	C	389	FAD	2	0
3	C	391	MIY	1	0
3	C	392	MIY	6	0
2	D	389	FAD	3	0
3	D	392	MIY	2	0
3	D	393	MIY	5	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	368/398 (92%)	0.26	13 (3%)	48	50	33, 47, 77, 124	0
1	B	368/398 (92%)	0.46	21 (5%)	27	29	32, 48, 80, 124	0
1	C	367/398 (92%)	0.49	30 (8%)	14	15	36, 53, 85, 119	0
1	D	367/398 (92%)	0.45	24 (6%)	22	24	33, 52, 84, 118	0
All	All	1470/1592 (92%)	0.41	88 (5%)	25	27	32, 50, 83, 124	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	341	GLY	7.6
1	A	249	THR	7.1
1	D	251	VAL	5.9
1	C	251	VAL	5.4
1	C	340	ASP	4.7
1	B	249	THR	4.6
1	B	251	VAL	4.6
1	A	378	PRO	4.5
1	C	341	GLY	4.5
1	B	378	PRO	4.4
1	C	379	ASP	4.3
1	B	340	ASP	4.2
1	B	243	ASP	4.2
1	D	252	ASP	4.0
1	A	377	LYS	4.0
1	B	341	GLY	4.0
1	C	380	PHE	3.9
1	B	13	LEU	3.9
1	C	257	ASN	3.8
1	B	250	GLN	3.7
1	A	376	PHE	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	379	ASP	3.6
1	D	340	ASP	3.6
1	D	245	TRP	3.6
1	C	245	TRP	3.5
1	D	250	GLN	3.5
1	D	12	ASN	3.5
1	C	242	PRO	3.4
1	C	244	GLU	3.4
1	B	379	ASP	3.4
1	C	14	LEU	3.3
1	C	250	GLN	3.2
1	D	342	LYS	3.2
1	C	382	PHE	3.2
1	D	300	SER	3.1
1	C	345	SER	3.1
1	C	243	ASP	3.1
1	D	262	PHE	3.0
1	C	252	ASP	3.0
1	D	339	ALA	3.0
1	C	15	SER	3.0
1	A	251	VAL	3.0
1	D	15	SER	2.9
1	D	296	LYS	2.9
1	C	261	ASP	2.8
1	C	109	ARG	2.8
1	C	255	ASN	2.8
1	B	258	SER	2.8
1	C	264	LEU	2.8
1	B	344	ASN	2.7
1	D	257	ASN	2.7
1	D	378	PRO	2.7
1	D	242	PRO	2.7
1	D	109	ARG	2.7
1	D	297	PRO	2.7
1	C	13	LEU	2.6
1	C	296	LYS	2.6
1	B	264	LEU	2.6
1	C	99	LEU	2.6
1	A	250	GLN	2.6
1	A	243	ASP	2.6
1	B	381	THR	2.5
1	D	255	ASN	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	382	PHE	2.5
1	C	262	PHE	2.5
1	B	12	ASN	2.5
1	D	268	SER	2.5
1	C	268	SER	2.4
1	D	14	LEU	2.4
1	A	252	ASP	2.4
1	D	380	PHE	2.4
1	B	252	ASP	2.4
1	D	343	PHE	2.4
1	B	342	LYS	2.4
1	A	381	THR	2.3
1	D	264	LEU	2.3
1	C	258	SER	2.3
1	C	259	VAL	2.2
1	A	258	SER	2.2
1	B	262	PHE	2.2
1	C	253	PHE	2.2
1	C	378	PRO	2.2
1	A	261	ASP	2.2
1	C	344	ASN	2.2
1	A	380	PHE	2.1
1	B	268	SER	2.1
1	B	254	GLN	2.1
1	B	323	GLY	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 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	FAD	D	389	53/53	0.97	0.12	0.11	33,42,56,62	0
2	FAD	A	389	53/53	0.97	0.12	-0.01	29,38,52,67	0
2	FAD	C	389	53/53	0.96	0.12	-0.12	33,42,60,68	0
3	MIY	B	391	33/33	0.92	0.13	-0.38	32,47,62,71	0
2	FAD	B	389	53/53	0.96	0.14	-0.46	31,40,55,59	0
3	MIY	C	391	33/33	0.94	0.11	-0.46	41,50,58,63	0
3	MIY	D	393	33/33	0.92	0.12	-0.64	42,50,54,60	0
3	MIY	D	391	33/33	0.95	0.11	-0.78	38,55,64,71	0
3	MIY	C	392	33/33	0.93	0.10	-1.12	42,52,55,62	0
3	MIY	A	391	33/33	0.95	0.10	-1.13	32,43,57,59	0
3	MIY	D	392	33/33	0.93	0.12	-1.38	38,45,54,69	0
3	MIY	A	392	33/33	0.94	0.11	-1.53	42,50,55,56	0
4	SO4	B	1384	5/5	0.96	0.25	-	80,81,83,96	0
4	SO4	B	1383	5/5	0.96	0.09	-	92,94,101,104	0
4	SO4	C	1385	5/5	0.90	0.11	-	101,102,111,113	0
4	SO4	A	1383	5/5	0.97	0.20	-	86,88,91,92	0
4	SO4	D	1383	5/5	0.89	0.19	-	72,93,95,102	0
4	SO4	C	1384	5/5	0.97	0.20	-	79,80,84,87	0
4	SO4	C	1383	5/5	0.85	0.18	-	81,85,105,109	0
4	SO4	D	1384	5/5	0.96	0.24	-	65,70,80,83	0
4	SO4	D	1385	5/5	0.78	0.21	-	81,86,93,98	5
4	SO4	B	1385	5/5	0.69	0.32	-	74,87,92,95	5

6.5 Other polymers

There are no such residues in this entry.