Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:41 PM GMT

PDB ID	:	4A6N
Title	:	STRUCTURE OF THE TETRACYCLINE DEGRADING MONOOXYGENASE TETX IN COMPLEX WITH TIGECYCLINE
Authors	:	Volkers, G.; Palm, G.J.; Weiss, M.S.; Hinrichs, W.
Deposited on	:	2011-11-07
Resolution	:	2.30 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:

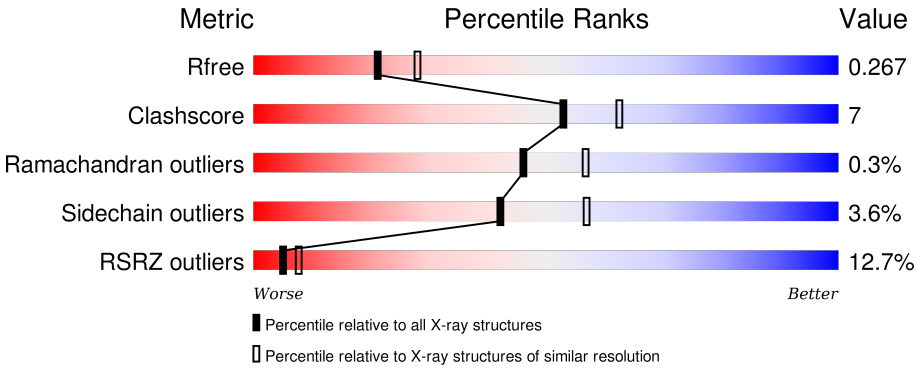
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	8% 79% 13% • 8%
2	B	398	11% 78% 13% • 8%
2	C	398	15% 78% 13% • 8%
2	D	398	13% 80% 11% • 8%

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
4	T1C	B	392	-	-	-	X
4	T1C	C	392	-	-	-	X
4	T1C	D	392	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 12141 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	1827	490	557	12			

There are 21 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
A	272	LYS	GLU	CONFLICT	UNP Q93L51

- Molecule 2 is a protein called TETX2 PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	368	Total	C	N	O	S	0	0	0
			2883	1826	489	556	12			
2	C	367	Total	C	N	O	S	0	0	0
			2868	1817	485	554	12			
2	D	367	Total	C	N	O	S	0	0	0
			2859	1812	485	550	12			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-9	MET	-	EXPRESSION TAG	UNP Q93L51
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

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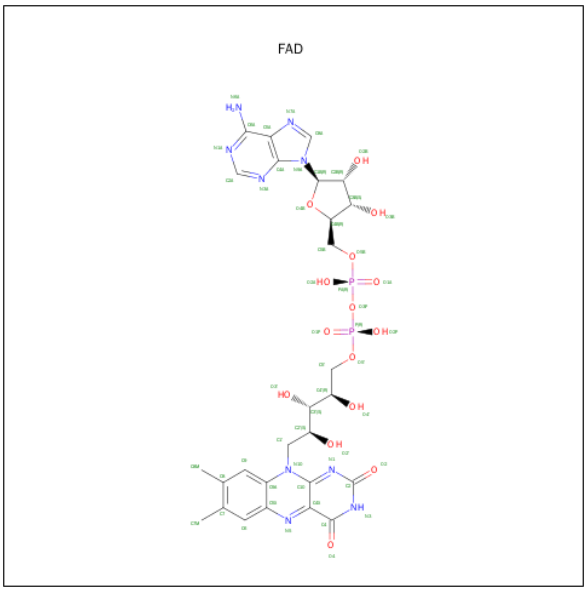
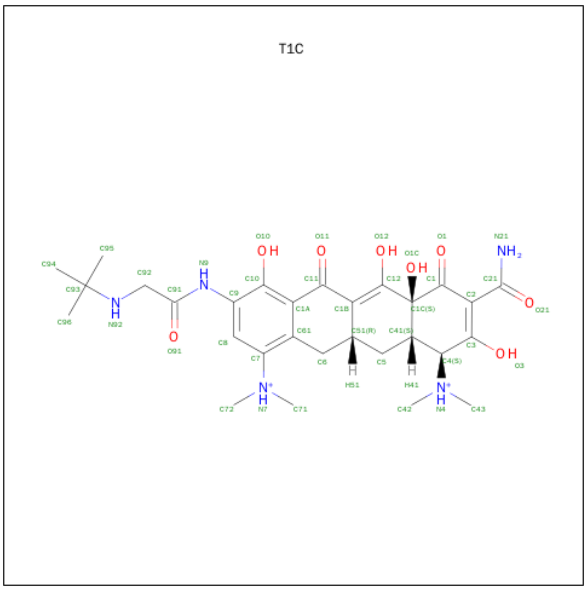
Chain	Residue	Modelled	Actual	Comment	Reference
C	4	LEU	-	EXPRESSION TAG	UNP Q93L51
C	5	VAL	-	EXPRESSION TAG	UNP Q93L51
C	6	PRO	-	EXPRESSION TAG	UNP Q93L51
C	7	ARG	-	EXPRESSION TAG	UNP Q93L51
C	8	GLY	-	EXPRESSION TAG	UNP Q93L51
C	9	SER	-	EXPRESSION TAG	UNP Q93L51
C	10	HIS	-	EXPRESSION TAG	UNP Q93L51
D	-9	MET	-	EXPRESSION TAG	UNP Q93L51
D	-8	GLY	-	EXPRESSION TAG	UNP Q93L51
D	-7	SER	-	EXPRESSION TAG	UNP Q93L51
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 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



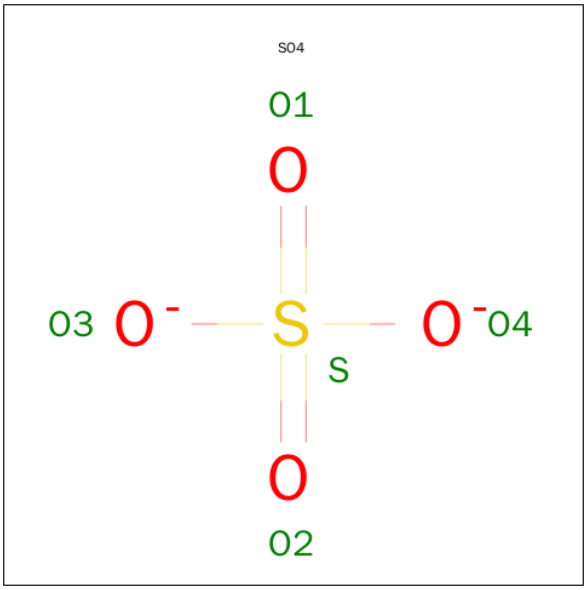
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 4 is TIGECYCLINE (three-letter code: T1C) (formula: $C_{29}H_{41}N_5O_8$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 42 29 5 8	0	0
4	B	1	Total C N O 42 29 5 8	0	0
4	C	1	Total C N O 42 29 5 8	0	0
4	D	1	Total C N O 42 29 5 8	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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

- Molecule 6 is water.

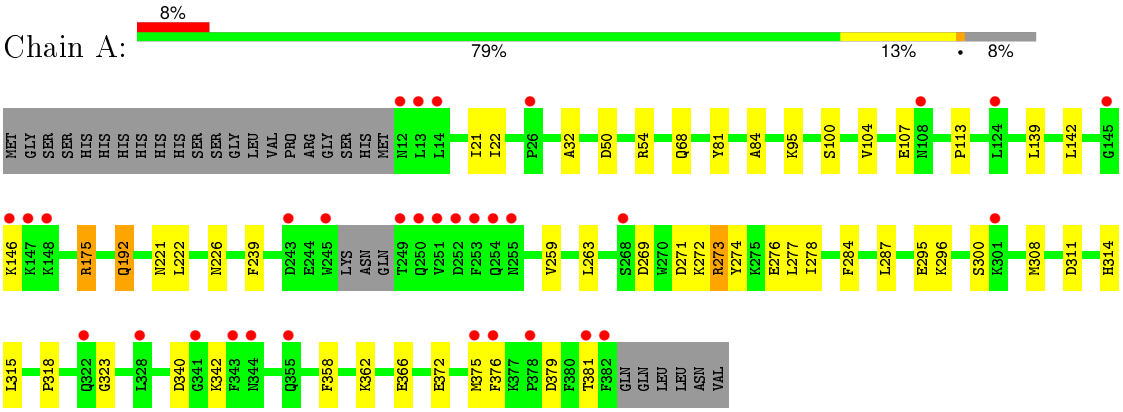
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	61	Total O 61 61	0	0
6	B	68	Total O 68 68	0	0
6	C	35	Total O 35 35	0	0
6	D	46	Total O 46 46	0	0

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.

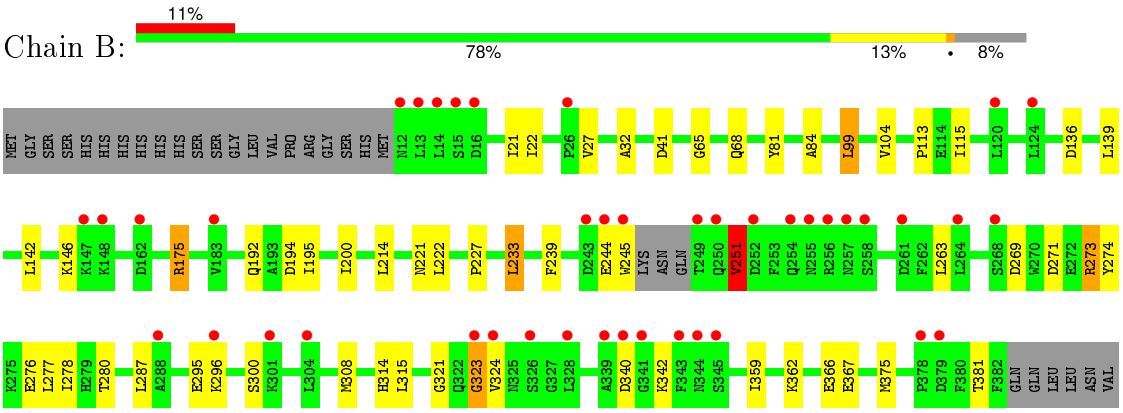
- Molecule 1: TETX2 PROTEIN

Chain A:



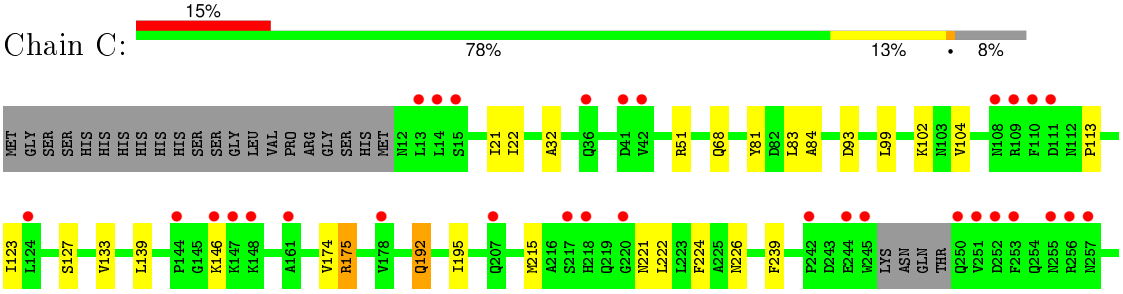
- Molecule 2: TETX2 PROTEIN

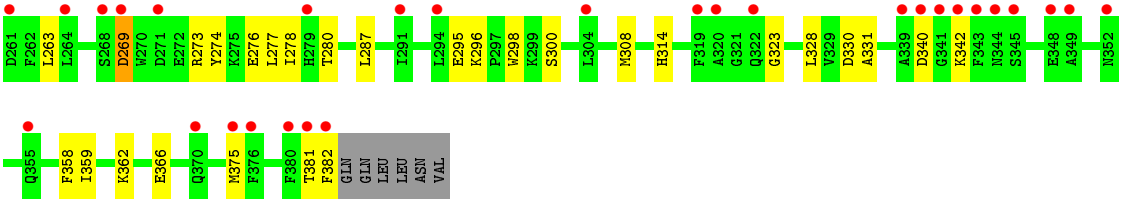
Chain B:



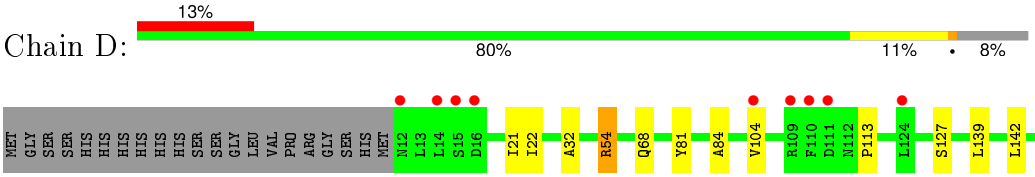
- Molecule 2: TETX2 PROTEIN

Chain C:





- Molecule 2: TETX2 PROTEIN



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	68.88Å 80.79Å 87.65Å 110.84° 89.84° 93.63°	Depositor
Resolution (Å)	81.90 – 2.30 40.95 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.0 (81.90-2.30) 84.0 (40.95-2.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.08 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.6.0116	Depositor
R, R_{free}	0.218 , 0.260 0.227 , 0.267	Depositor DCC
R_{free} test set	3769 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	43.0	Xtriage
Anisotropy	0.334	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 57.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 75166 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	12141	wwPDB-VP
Average B, all atoms (Å^2)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.33% 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: SO4, FAD, T1C

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	0.85	0/2944	0.89	5/3987 (0.1%)
2	B	0.84	0/2941	0.90	7/3983 (0.2%)
2	C	0.70	1/2926 (0.0%)	0.80	3/3965 (0.1%)
2	D	0.70	0/2917	0.80	4/3954 (0.1%)
All	All	0.78	1/11728 (0.0%)	0.85	19/15889 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	298	TRP	CD2-CE2	5.54	1.48	1.41

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	175	ARG	NE-CZ-NH1	8.96	124.78	120.30
2	B	251	VAL	CG1-CB-CG2	8.76	124.92	110.90
2	B	175	ARG	NE-CZ-NH1	8.12	124.36	120.30
2	C	175	ARG	NE-CZ-NH1	7.27	123.94	120.30
2	D	175	ARG	NE-CZ-NH1	7.17	123.88	120.30
2	B	175	ARG	NE-CZ-NH2	-6.92	116.84	120.30
2	D	175	ARG	NE-CZ-NH2	-6.27	117.16	120.30
2	D	287	LEU	CB-CG-CD2	6.08	121.33	111.00
1	A	175	ARG	NE-CZ-NH2	-6.07	117.26	120.30
1	A	50	ASP	CB-CG-OD1	5.90	123.61	118.30
2	B	99	LEU	CB-CG-CD2	5.79	120.85	111.00
1	A	311	ASP	CB-CG-OD2	-5.74	113.14	118.30
2	C	175	ARG	NE-CZ-NH2	-5.45	117.58	120.30
2	B	41	ASP	CB-CG-OD1	5.43	123.19	118.30
2	D	54	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	A	311	ASP	CB-CG-OD1	5.23	123.01	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	93	ASP	CB-CG-OD1	5.11	122.90	118.30
2	B	194	ASP	CB-CG-OD1	5.04	122.83	118.30
2	B	136	ASP	CB-CG-OD1	5.03	122.82	118.30

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	2886	0	2807	32	0
2	B	2883	0	2797	36	0
2	C	2868	0	2771	31	0
2	D	2859	0	2761	33	0
3	A	53	0	31	4	0
3	B	53	0	31	8	0
3	C	53	0	31	1	0
3	D	53	0	31	2	0
4	A	42	0	39	10	0
4	B	42	0	39	7	0
4	C	42	0	40	5	0
4	D	42	0	38	15	0
5	A	10	0	0	0	0
5	B	20	0	0	0	0
5	C	10	0	0	0	0
5	D	15	0	0	0	0
6	A	61	0	0	0	0
6	B	68	0	0	2	0
6	C	35	0	0	4	0
6	D	46	0	0	5	0
All	All	12141	0	11416	154	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 7.

All (154) 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)
3:A:389:FAD:HM73	4:A:392:T1C:H421	1.35	1.06
2:C:269:ASP:HB2	6:C:2030:HOH:O	1.59	1.02
2:D:279:HIS:CE1	6:D:2037:HOH:O	2.13	0.98
4:D:392:T1C:H62C	4:D:392:T1C:C72	2.03	0.87
4:D:392:T1C:O3	4:D:392:T1C:H422	1.81	0.81
4:D:392:T1C:H62C	4:D:392:T1C:H722	1.62	0.80
3:A:389:FAD:C7M	4:A:392:T1C:H421	2.19	0.72
3:B:389:FAD:H6	4:B:392:T1C:H433	1.71	0.72
2:D:146:LYS:HG3	6:D:2021:HOH:O	1.90	0.71
4:D:392:T1C:C72	4:D:392:T1C:C6	2.69	0.70
2:B:263:LEU:HB3	2:B:278:ILE:HD13	1.75	0.69
4:A:392:T1C:H712	4:A:392:T1C:C6	2.25	0.66
3:B:389:FAD:HM73	4:B:392:T1C:H431	1.77	0.65
2:C:133:VAL:O	6:C:2016:HOH:O	2.14	0.65
4:D:392:T1C:H62C	4:D:392:T1C:H723	1.79	0.64
2:D:263:LEU:HB3	2:D:278:ILE:HD13	1.77	0.64
4:D:392:T1C:H723	4:D:392:T1C:C6	2.28	0.64
2:C:263:LEU:HB3	2:C:278:ILE:HD13	1.81	0.61
2:B:323:GLY:HA3	3:B:389:FAD:H1'2	1.82	0.60
4:B:392:T1C:O11	4:B:392:T1C:O12	2.12	0.60
2:D:21:ILE:HD12	2:D:32:ALA:HB2	1.82	0.60
3:B:389:FAD:H6	4:B:392:T1C:C43	2.32	0.60
2:D:146:LYS:CG	6:D:2021:HOH:O	2.48	0.60
2:D:318:PRO:HG2	4:D:392:T1C:H431	1.84	0.59
1:A:263:LEU:HB3	1:A:278:ILE:HD13	1.85	0.59
4:C:392:T1C:H432	4:C:392:T1C:O3	2.01	0.59
2:B:324:VAL:HG12	3:B:389:FAD:O2	2.06	0.56
2:D:375:MET:SD	4:D:392:T1C:H721	2.46	0.56
3:B:389:FAD:C6	4:B:392:T1C:C43	2.84	0.56
4:A:392:T1C:O3	4:A:392:T1C:C42	2.54	0.56
2:D:84:ALA:HB1	2:D:113:PRO:HB2	1.86	0.55
2:C:362:LYS:O	2:C:366:GLU:HG2	2.06	0.55
1:A:95:LYS:NZ	2:B:367:GLU:HA	2.22	0.54
2:C:68:GLN:NE2	2:C:81:TYR:OH	2.39	0.54
2:D:68:GLN:NE2	2:D:81:TYR:OH	2.41	0.53
2:D:22:ILE:HD13	2:D:22:ILE:N	2.24	0.53
2:C:84:ALA:HB1	2:C:113:PRO:HB2	1.90	0.53
2:D:362:LYS:O	2:D:366:GLU:HG2	2.09	0.52
2:B:323:GLY:N	6:B:2061:HOH:O	2.18	0.52
1:A:362:LYS:O	1:A:366:GLU:HG2	2.10	0.52
2:B:68:GLN:NE2	2:B:81:TYR:OH	2.42	0.52
2:D:222:LEU:CD2	2:D:375:MET:HE3	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:GLU:HG2	2:C:359:ILE:HD13	1.92	0.51
2:C:221:ASN:HD22	2:C:239:PHE:HB3	1.76	0.51
2:D:279:HIS:HE1	6:D:2037:HOH:O	1.71	0.51
2:B:362:LYS:O	2:B:366:GLU:HG2	2.11	0.50
1:A:379:ASP:HB3	2:B:65:GLY:HA3	1.94	0.50
2:C:382:PHE:C	6:C:2035:HOH:O	2.49	0.50
2:B:221:ASN:HD22	2:B:239:PHE:HB3	1.77	0.50
2:D:22:ILE:HG13	2:D:139:LEU:HD22	1.94	0.49
1:A:318:PRO:HG2	4:A:392:T1C:H431	1.93	0.49
2:D:318:PRO:HG2	4:D:392:T1C:C43	2.42	0.49
1:A:100:SER:HB2	2:B:359:ILE:HG12	1.95	0.49
1:A:84:ALA:HB1	1:A:113:PRO:HB2	1.94	0.49
2:C:224:PHE:HB2	4:C:392:T1C:O3	2.12	0.48
2:B:245:TRP:CZ2	2:B:251:VAL:HG13	2.49	0.48
2:C:21:ILE:HD12	2:C:32:ALA:HB2	1.95	0.48
2:C:195:ILE:HD12	2:C:277:LEU:HD12	1.96	0.48
1:A:22:ILE:N	1:A:22:ILE:HD13	2.29	0.47
2:B:139:LEU:HD21	2:B:142:LEU:HD13	1.94	0.47
2:C:222:LEU:CD2	2:C:375:MET:HE3	2.43	0.47
1:A:68:GLN:NE2	1:A:81:TYR:OH	2.47	0.47
1:A:274:TYR:O	1:A:277:LEU:HB3	2.14	0.47
1:A:21:ILE:HD12	1:A:32:ALA:HB2	1.96	0.47
2:B:295:GLU:HG3	2:B:296:LYS:HG2	1.97	0.47
2:C:295:GLU:HG3	2:C:296:LYS:HG2	1.97	0.47
2:D:295:GLU:HG3	2:D:296:LYS:HG2	1.97	0.47
1:A:95:LYS:NZ	2:B:367:GLU:HG3	2.29	0.47
1:A:372:GLU:O	1:A:376:PHE:HD2	1.97	0.47
2:B:84:ALA:HB1	2:B:113:PRO:HB2	1.97	0.46
2:C:328:LEU:O	2:C:331:ALA:HB3	2.15	0.46
3:B:389:FAD:HM73	4:B:392:T1C:C43	2.44	0.46
4:C:392:T1C:H41	4:C:392:T1C:H423	1.73	0.46
4:D:392:T1C:O3	4:D:392:T1C:C42	2.56	0.46
2:B:27:VAL:HG23	3:B:389:FAD:P	2.55	0.46
2:B:274:TYR:O	2:B:277:LEU:HB3	2.16	0.46
2:B:21:ILE:HD12	2:B:32:ALA:HB2	1.98	0.46
2:D:195:ILE:HD13	2:D:280:THR:CG2	2.46	0.46
1:A:221:ASN:HD22	1:A:239:PHE:HB3	1.81	0.46
1:A:22:ILE:HG13	1:A:139:LEU:HD22	1.99	0.46
2:D:196:HIS:CE1	6:D:2034:HOH:O	2.68	0.46
2:D:358:PHE:O	2:D:362:LYS:HB2	2.17	0.45
1:A:314:HIS:O	1:A:315:LEU:C	2.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:MET:SD	4:A:392:T1C:H721	2.56	0.45
2:C:226:ASN:C	2:C:226:ASN:OD1	2.55	0.45
2:B:340:ASP:HB2	2:B:342:LYS:HB2	1.97	0.45
2:D:221:ASN:HD22	2:D:239:PHE:HB3	1.82	0.45
4:D:392:T1C:H922	4:D:392:T1C:H951	1.80	0.45
2:D:139:LEU:HD23	2:D:174:VAL:HG11	1.99	0.45
1:A:295:GLU:HG3	1:A:296:LYS:HG2	1.99	0.45
2:B:321:GLY:HA2	6:B:2060:HOH:O	2.16	0.45
1:A:379:ASP:CB	2:B:65:GLY:HA3	2.47	0.45
2:C:195:ILE:HD13	2:C:280:THR:CG2	2.47	0.45
2:C:274:TYR:O	2:C:277:LEU:HB3	2.17	0.44
4:D:392:T1C:O10	4:D:392:T1C:O11	2.31	0.44
2:B:227:PRO:HA	2:B:233:LEU:HD12	2.00	0.44
2:D:340:ASP:HB2	2:D:342:LYS:HB2	1.99	0.44
2:B:22:ILE:HG13	2:B:139:LEU:HD22	1.99	0.44
1:A:222:LEU:CD2	1:A:375:MET:HE2	2.47	0.44
2:C:358:PHE:O	2:C:362:LYS:HB2	2.18	0.44
3:D:389:FAD:H2'	3:D:389:FAD:N1	2.32	0.44
4:D:392:T1C:O11	4:D:392:T1C:O12	2.32	0.44
4:A:392:T1C:H62C	4:A:392:T1C:H712	1.99	0.44
2:C:139:LEU:HD23	2:C:174:VAL:HG11	1.99	0.44
2:D:139:LEU:HD21	2:D:142:LEU:HD13	1.99	0.44
1:A:142:LEU:HA	1:A:142:LEU:HD12	1.87	0.43
2:D:226:ASN:OD1	2:D:226:ASN:C	2.56	0.43
2:D:375:MET:SD	4:D:392:T1C:C72	3.07	0.43
2:D:274:TYR:O	2:D:277:LEU:HB3	2.17	0.43
1:A:340:ASP:HB2	1:A:342:LYS:HB2	1.99	0.43
2:B:222:LEU:CD2	2:B:375:MET:HE3	2.47	0.43
1:A:192:GLN:NE2	3:A:389:FAD:HM72	2.34	0.43
2:B:214:LEU:HD23	2:B:214:LEU:C	2.39	0.43
2:B:175:ARG:HG2	2:B:308:MET:SD	2.59	0.42
4:B:392:T1C:H423	4:B:392:T1C:H41	1.74	0.42
2:C:340:ASP:HB2	2:C:342:LYS:HB2	2.00	0.42
2:C:314:HIS:NE2	2:C:330:ASP:OD2	2.44	0.42
1:A:226:ASN:C	1:A:226:ASN:OD1	2.58	0.42
3:A:389:FAD:H9	3:A:389:FAD:H1'1	1.76	0.42
2:B:340:ASP:CB	2:B:342:LYS:HB2	2.49	0.42
2:D:175:ARG:HG2	2:D:308:MET:SD	2.60	0.42
2:C:382:PHE:CE1	4:C:392:T1C:H711	2.55	0.42
1:A:139:LEU:HD21	1:A:142:LEU:HD13	2.01	0.42
1:A:340:ASP:CB	1:A:342:LYS:HB2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:83:LEU:HD22	2:C:123:ILE:HD11	2.02	0.41
4:A:392:T1C:O12	4:A:392:T1C:O11	2.37	0.41
2:C:51:ARG:HG2	6:C:2005:HOH:O	2.20	0.41
2:B:195:ILE:HD13	2:B:280:THR:CG2	2.51	0.41
2:C:215:MET:SD	4:C:392:T1C:H712	2.60	0.41
4:A:392:T1C:C71	4:A:392:T1C:C6	2.95	0.41
2:B:221:ASN:ND2	2:B:239:PHE:HB3	2.36	0.41
2:D:192:GLN:NE2	3:D:389:FAD:HM72	2.35	0.41
2:D:195:ILE:HD12	2:D:277:LEU:HD12	2.03	0.41
2:C:22:ILE:HG13	2:C:139:LEU:HD22	2.03	0.41
2:C:192:GLN:NE2	3:C:389:FAD:HM72	2.36	0.41
4:A:392:T1C:H423	4:A:392:T1C:O3	2.20	0.41
2:D:340:ASP:CB	2:D:342:LYS:HB2	2.50	0.41
1:A:54:ARG:CZ	2:D:54:ARG:CZ	2.98	0.41
2:C:195:ILE:CD1	2:C:277:LEU:HD12	2.50	0.41
2:B:142:LEU:HD12	2:B:142:LEU:HA	1.89	0.41
2:B:115:ILE:O	2:B:115:ILE:HG23	2.20	0.41
2:B:200:ILE:HA	2:B:200:ILE:HD13	1.82	0.41
2:D:224:PHE:CD2	4:D:392:T1C:H51C	2.55	0.41
2:C:22:ILE:N	2:C:22:ILE:HD13	2.36	0.40
1:A:259:VAL:HG11	1:A:284:PHE:CG	2.57	0.40
2:B:271:ASP:OD2	2:B:273:ARG:HD3	2.21	0.40
1:A:358:PHE:O	1:A:362:LYS:HB2	2.20	0.40
2:B:22:ILE:N	2:B:22:ILE:HD13	2.35	0.40
2:D:302:ARG:HA	2:D:303:PRO:HD3	1.99	0.40
1:A:271:ASP:OD2	1:A:273:ARG:HD3	2.22	0.40
1:A:175:ARG:HG2	1:A:308:MET:SD	2.62	0.40
2:C:175:ARG:HG2	2:C:308:MET:SD	2.61	0.40
2:B:244:GLU:CD	2:B:244:GLU:H	2.24	0.40
2:B:314:HIS:O	2:B:315:LEU:C	2.60	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%)	351 (96%)	12 (3%)	1 (0%)	46	57
2	B	364/398 (92%)	350 (96%)	13 (4%)	1 (0%)	46	57
2	C	363/398 (91%)	348 (96%)	14 (4%)	1 (0%)	46	57
2	D	363/398 (91%)	348 (96%)	14 (4%)	1 (0%)	46	57
All	All	1454/1592 (91%)	1397 (96%)	53 (4%)	4 (0%)	46	57

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	323	GLY
1	A	323	GLY
2	D	323	GLY
2	C	323	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%)	302 (97%)	10 (3%)	46	62
2	B	310/345 (90%)	298 (96%)	12 (4%)	39	53
2	C	307/345 (89%)	295 (96%)	12 (4%)	39	53
2	D	305/345 (88%)	295 (97%)	10 (3%)	45	61
All	All	1234/1380 (89%)	1190 (96%)	44 (4%)	42	57

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	104	VAL
1	A	146	LYS
1	A	192	GLN
1	A	269	ASP

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Mol	Chain	Res	Type
1	A	272	LYS
1	A	273	ARG
1	A	276	GLU
1	A	287	LEU
1	A	300	SER
1	A	381	THR
2	B	99	LEU
2	B	104	VAL
2	B	146	LYS
2	B	192	GLN
2	B	233	LEU
2	B	251	VAL
2	B	269	ASP
2	B	273	ARG
2	B	276	GLU
2	B	287	LEU
2	B	300	SER
2	B	381	THR
2	C	99	LEU
2	C	102	LYS
2	C	104	VAL
2	C	127	SER
2	C	146	LYS
2	C	192	GLN
2	C	269	ASP
2	C	273	ARG
2	C	276	GLU
2	C	287	LEU
2	C	300	SER
2	C	381	THR
2	D	104	VAL
2	D	127	SER
2	D	146	LYS
2	D	192	GLN
2	D	269	ASP
2	D	273	ARG
2	D	276	GLU
2	D	287	LEU
2	D	300	SER
2	D	381	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	A	68	GLN
1	A	130	ASN
1	A	190	ASN
1	A	221	ASN
1	A	371	ASN
2	B	38	ASN
2	B	68	GLN
2	B	130	ASN
2	B	190	ASN
2	B	192	GLN
2	B	221	ASN
2	B	250	GLN
2	B	371	ASN
2	C	38	ASN
2	C	68	GLN
2	C	130	ASN
2	C	190	ASN
2	C	221	ASN
2	C	371	ASN
2	D	38	ASN
2	D	68	GLN
2	D	130	ASN
2	D	190	ASN
2	D	192	GLN
2	D	207	GLN
2	D	221	ASN
2	D	371	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

19 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	$\#\|Z\| > 2$
5	SO4	A	1383	-	4,4,4	0.43	0	6,6,6	0.44	0
5	SO4	A	1384	-	4,4,4	0.74	0	6,6,6	0.43	0
3	FAD	A	389	-	48,58,58	1.56	9 (18%)	54,89,89	2.59	13 (24%)
4	T1C	A	392	-	44,45,45	2.06	12 (27%)	48,72,72	1.94	13 (27%)
5	SO4	B	1383	-	4,4,4	0.47	0	6,6,6	0.24	0
5	SO4	B	1384	-	4,4,4	0.45	0	6,6,6	0.26	0
5	SO4	B	1385	-	4,4,4	0.53	0	6,6,6	0.25	0
5	SO4	B	1386	-	4,4,4	0.57	0	6,6,6	0.22	0
3	FAD	B	389	-	48,58,58	1.47	8 (16%)	54,89,89	2.77	11 (20%)
4	T1C	B	392	-	44,45,45	2.05	12 (27%)	48,72,72	2.43	17 (35%)
5	SO4	C	1383	-	4,4,4	0.73	0	6,6,6	0.22	0
5	SO4	C	1384	-	4,4,4	0.62	0	6,6,6	0.31	0
3	FAD	C	389	-	48,58,58	1.48	7 (14%)	54,89,89	2.96	17 (31%)
4	T1C	C	392	-	44,45,45	1.93	9 (20%)	48,72,72	1.93	9 (18%)
5	SO4	D	1383	-	4,4,4	0.42	0	6,6,6	0.16	0
5	SO4	D	1384	-	4,4,4	0.44	0	6,6,6	0.28	0
5	SO4	D	1385	-	4,4,4	0.57	0	6,6,6	0.47	0
3	FAD	D	389	-	48,58,58	1.68	11 (22%)	54,89,89	2.90	18 (33%)
4	T1C	D	392	-	44,45,45	1.93	10 (22%)	48,72,72	2.20	13 (27%)

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
5	SO4	A	1383	-	-	0/0/0/0	0/0/0/0
5	SO4	A	1384	-	-	0/0/0/0	0/0/0/0
3	FAD	A	389	-	-	0/30/50/50	0/6/6/6
4	T1C	A	392	-	-	0/22/80/80	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	SO4	B	1383	-	-	0/0/0/0	0/0/0/0
5	SO4	B	1384	-	-	0/0/0/0	0/0/0/0
5	SO4	B	1385	-	-	0/0/0/0	0/0/0/0
5	SO4	B	1386	-	-	0/0/0/0	0/0/0/0
3	FAD	B	389	-	-	0/30/50/50	0/6/6/6
4	T1C	B	392	-	-	0/22/80/80	0/4/4/4
5	SO4	C	1383	-	-	0/0/0/0	0/0/0/0
5	SO4	C	1384	-	-	0/0/0/0	0/0/0/0
3	FAD	C	389	-	-	0/30/50/50	0/6/6/6
4	T1C	C	392	-	-	0/22/80/80	0/4/4/4
5	SO4	D	1383	-	-	0/0/0/0	0/0/0/0
5	SO4	D	1384	-	-	0/0/0/0	0/0/0/0
5	SO4	D	1385	-	-	0/0/0/0	0/0/0/0
3	FAD	D	389	-	-	0/30/50/50	0/6/6/6
4	T1C	D	392	-	-	0/22/80/80	0/4/4/4

All (78) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	392	T1C	C1C-C41	-5.03	1.48	1.53
3	A	389	FAD	C6-C5X	-3.86	1.35	1.41
4	B	392	T1C	C1C-C41	-3.48	1.50	1.53
4	C	392	T1C	C7-N7	-3.14	1.34	1.42
3	B	389	FAD	C10-N10	-3.10	1.35	1.39
4	C	392	T1C	C9-N9	-3.07	1.35	1.41
3	A	389	FAD	C10-N10	-3.03	1.35	1.39
4	B	392	T1C	C1B-C11	-2.97	1.40	1.47
3	B	389	FAD	C6-C5X	-2.95	1.37	1.41
4	D	392	T1C	C9-N9	-2.90	1.36	1.41
4	C	392	T1C	C1B-C11	-2.79	1.40	1.47
4	A	392	T1C	C9-N9	-2.79	1.36	1.41
3	B	389	FAD	PA-O1A	-2.76	1.41	1.51
4	B	392	T1C	C9-N9	-2.73	1.36	1.41
4	D	392	T1C	C7-N7	-2.66	1.35	1.42
4	C	392	T1C	C1A-C11	-2.65	1.39	1.46
4	A	392	T1C	C7-N7	-2.60	1.35	1.42
4	D	392	T1C	C1B-C11	-2.57	1.41	1.47
3	A	389	FAD	C1'-N10	-2.57	1.45	1.48
4	B	392	T1C	C7-N7	-2.49	1.35	1.42
3	D	389	FAD	C6-C5X	-2.46	1.38	1.41
4	D	392	T1C	C1A-C11	-2.37	1.40	1.46
4	A	392	T1C	C1B-C11	-2.33	1.41	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	389	FAD	O4B-C4B	-2.24	1.39	1.45
3	A	389	FAD	C4'-C3'	-2.20	1.49	1.53
3	C	389	FAD	C4'-C3'	-2.13	1.49	1.53
3	D	389	FAD	C4'-C3'	-2.11	1.49	1.53
4	A	392	T1C	C2-C1	-2.02	1.40	1.45
4	B	392	T1C	C1A-C11	-2.00	1.41	1.46
3	D	389	FAD	C2A-N3A	2.00	1.35	1.32
3	C	389	FAD	C2A-N3A	2.00	1.35	1.32
4	A	392	T1C	C4-C3	2.02	1.55	1.51
3	D	389	FAD	C4-C4X	2.03	1.45	1.41
4	D	392	T1C	C7-C61	2.15	1.43	1.40
3	B	389	FAD	C1'-N10	2.18	1.50	1.48
4	A	392	T1C	C1C-C1	2.27	1.58	1.55
3	D	389	FAD	C9A-N10	2.27	1.41	1.38
3	B	389	FAD	C5A-C4A	2.28	1.45	1.40
3	D	389	FAD	C8A-N7A	2.37	1.39	1.34
4	D	392	T1C	C1B-C12	2.48	1.39	1.36
4	B	392	T1C	O1C-C1C	2.49	1.46	1.42
4	B	392	T1C	C4-C3	2.50	1.56	1.51
4	A	392	T1C	C1B-C12	2.58	1.39	1.36
3	A	389	FAD	C4X-C10	2.64	1.46	1.41
4	C	392	T1C	C1B-C12	2.73	1.39	1.36
3	C	389	FAD	C4-C4X	2.74	1.46	1.41
3	A	389	FAD	C4X-N5	2.76	1.37	1.33
3	C	389	FAD	C8A-N7A	2.77	1.39	1.34
4	C	392	T1C	C6-C61	2.82	1.56	1.51
3	A	389	FAD	O4'-C4'	2.92	1.49	1.43
3	B	389	FAD	C8A-N7A	3.02	1.40	1.34
4	B	392	T1C	C51-C1B	3.06	1.54	1.51
3	A	389	FAD	C8-C7	3.18	1.49	1.41
3	D	389	FAD	C8-C7	3.29	1.49	1.41
3	B	389	FAD	C9A-C5X	3.40	1.49	1.42
4	A	392	T1C	C6-C61	3.42	1.57	1.51
4	B	392	T1C	C41-C4	3.47	1.58	1.54
4	A	392	T1C	C41-C4	3.47	1.58	1.54
4	A	392	T1C	C1C-C12	3.48	1.55	1.52
3	D	389	FAD	C5A-C4A	3.52	1.48	1.40
4	D	392	T1C	C6-C61	3.52	1.57	1.51
4	B	392	T1C	C6-C61	3.52	1.57	1.51
3	D	389	FAD	C9A-C5X	3.69	1.50	1.42
3	C	389	FAD	C9A-C5X	3.90	1.50	1.42
3	C	389	FAD	C8-C7	3.91	1.51	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	392	T1C	C1C-C12	3.92	1.55	1.52
3	A	389	FAD	C9A-C5X	4.04	1.50	1.42
4	D	392	T1C	C1C-C12	4.25	1.56	1.52
3	C	389	FAD	C4X-C10	4.27	1.49	1.41
3	D	389	FAD	O4B-C1B	4.43	1.46	1.41
4	C	392	T1C	C41-C4	4.84	1.60	1.54
3	D	389	FAD	C4X-C10	4.97	1.50	1.41
4	D	392	T1C	C41-C4	5.11	1.60	1.54
4	B	392	T1C	C1C-C12	5.88	1.57	1.52
4	D	392	T1C	C2-C21	6.22	1.59	1.47
4	B	392	T1C	C2-C21	6.28	1.59	1.47
4	C	392	T1C	C2-C21	6.47	1.59	1.47
4	A	392	T1C	C2-C21	7.52	1.61	1.47

All (111) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	389	FAD	C4-C4X-C10	-11.35	112.67	119.94
3	C	389	FAD	N3A-C2A-N1A	-8.99	122.01	128.89
3	D	389	FAD	N3A-C2A-N1A	-8.78	122.17	128.89
3	C	389	FAD	C4-C4X-C10	-7.65	115.04	119.94
4	B	392	T1C	O12-C12-C1B	-7.48	116.68	123.84
4	C	392	T1C	O12-C12-C1B	-7.39	116.77	123.84
4	D	392	T1C	O12-C12-C1B	-7.15	117.00	123.84
3	A	389	FAD	C4-C4X-C10	-6.74	115.62	119.94
3	B	389	FAD	N3A-C2A-N1A	-6.57	123.86	128.89
3	A	389	FAD	N3A-C2A-N1A	-6.34	124.04	128.89
3	D	389	FAD	C4X-C4-N3	-5.97	115.43	123.59
3	D	389	FAD	C4-C4X-C10	-5.36	116.51	119.94
3	C	389	FAD	C2B-C1B-N9A	-5.34	106.13	114.29
3	C	389	FAD	C1B-N9A-C4A	-5.21	119.08	126.94
3	A	389	FAD	C4X-C4-N3	-5.20	116.48	123.59
3	C	389	FAD	C4X-C4-N3	-5.09	116.63	123.59
4	B	392	T1C	C42-N4-C4	-4.79	102.37	114.07
3	D	389	FAD	C1B-N9A-C4A	-4.72	119.81	126.94
4	B	392	T1C	O1C-C1C-C41	-4.60	104.38	110.17
4	A	392	T1C	C43-N4-C4	-4.54	102.98	114.07
4	D	392	T1C	C8-C7-N7	-4.37	113.95	120.54
4	A	392	T1C	O12-C12-C1B	-4.05	119.96	123.84
3	C	389	FAD	O3'-C3'-C4'	-3.90	98.93	108.75
3	A	389	FAD	C4X-C10-N10	-3.77	118.30	120.52
4	A	392	T1C	O1-C1-C2	-3.76	115.89	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	392	T1C	O1C-C1C-C12	-3.67	103.27	109.85
4	B	392	T1C	C21-C2-C1	-3.62	116.61	120.87
4	C	392	T1C	C42-N4-C4	-3.44	105.67	114.07
4	C	392	T1C	O1-C1-C2	-3.39	116.64	123.59
3	D	389	FAD	C2B-C1B-N9A	-3.35	109.17	114.29
3	C	389	FAD	C4X-C10-N10	-3.33	118.56	120.52
3	D	389	FAD	O3'-C3'-C4'	-3.30	100.42	108.75
3	B	389	FAD	C4X-C10-N10	-3.29	118.58	120.52
3	A	389	FAD	C2B-C1B-N9A	-3.28	109.29	114.29
4	B	392	T1C	O11-C11-C1B	-3.23	115.92	120.73
3	A	389	FAD	O4B-C1B-N9A	-3.18	101.45	108.10
4	A	392	T1C	C21-C2-C1	-3.18	117.13	120.87
3	A	389	FAD	C1B-N9A-C4A	-3.18	122.15	126.94
4	D	392	T1C	O1-C1-C2	-3.17	117.09	123.59
3	A	389	FAD	O3B-C3B-C2B	-3.14	101.61	111.83
3	D	389	FAD	C4A-C5A-N7A	-3.10	106.62	109.48
3	B	389	FAD	O5B-C5B-C4B	-2.94	98.27	109.12
3	C	389	FAD	C4A-C5A-N7A	-2.91	106.81	109.48
3	B	389	FAD	C4X-C4-N3	-2.84	119.71	123.59
4	B	392	T1C	O1C-C1C-C12	-2.75	104.91	109.85
3	D	389	FAD	C4X-C10-N10	-2.75	118.90	120.52
4	B	392	T1C	O1C-C1C-C1	-2.73	100.09	106.80
4	A	392	T1C	O11-C11-C1B	-2.69	116.73	120.73
4	B	392	T1C	C11-C1B-C12	-2.68	116.64	118.93
4	B	392	T1C	C1C-C12-C1B	-2.65	119.77	122.95
3	B	389	FAD	C2B-C1B-N9A	-2.62	110.29	114.29
4	D	392	T1C	O1C-C1C-C12	-2.53	105.31	109.85
3	D	389	FAD	O3B-C3B-C2B	-2.53	103.60	111.83
4	D	392	T1C	O1C-C1C-C41	-2.50	107.02	110.17
3	D	389	FAD	P-O3P-PA	-2.49	125.73	132.73
3	A	389	FAD	P-O3P-PA	-2.43	125.91	132.73
4	C	392	T1C	C1-C1C-C12	-2.41	106.70	109.73
3	C	389	FAD	P-O3P-PA	-2.37	126.08	132.73
4	C	392	T1C	O1C-C1C-C12	-2.36	105.62	109.85
4	D	392	T1C	O11-C11-C1A	-2.24	117.82	122.01
4	A	392	T1C	C61-C7-N7	-2.19	117.09	118.94
4	D	392	T1C	C43-N4-C4	-2.16	108.81	114.07
4	D	392	T1C	C42-N4-C4	-2.12	108.91	114.07
4	C	392	T1C	O11-C11-C1A	-2.06	118.15	122.01
4	A	392	T1C	O1C-C1C-C41	-2.03	107.61	110.17
4	B	392	T1C	C72-N7-C71	-2.01	109.31	115.96
4	B	392	T1C	C1A-C11-C1B	2.03	121.89	118.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	392	T1C	C5-C41-C4	2.11	114.66	111.47
3	D	389	FAD	C2B-C3B-C4B	2.15	107.03	102.61
3	C	389	FAD	C6-C5X-N5	2.16	121.74	118.96
3	B	389	FAD	O2P-P-O1P	2.16	124.22	112.53
4	B	392	T1C	C5-C51-C1B	2.18	113.43	109.56
3	A	389	FAD	C5X-C9A-N10	2.26	119.34	117.62
4	C	392	T1C	C1A-C11-C1B	2.39	122.45	118.68
3	A	389	FAD	C6-C5X-N5	2.44	122.11	118.96
3	A	389	FAD	O3P-P-O5'	2.55	109.71	102.94
3	C	389	FAD	O3P-P-O5'	2.65	109.97	102.94
3	D	389	FAD	C2A-N1A-C6A	2.66	123.51	118.77
4	A	392	T1C	C1A-C11-C1B	2.68	122.92	118.68
4	B	392	T1C	C1-C1C-C12	2.73	113.15	109.73
3	D	389	FAD	O4'-C4'-C5'	2.74	116.16	110.19
4	A	392	T1C	O12-C12-C1C	2.75	117.88	113.50
4	D	392	T1C	C1A-C11-C1B	2.76	123.04	118.68
3	C	389	FAD	O3P-PA-O5B	2.87	110.55	102.94
3	C	389	FAD	O5'-P-O1P	2.89	120.85	109.62
3	D	389	FAD	C4-C4X-N5	3.09	122.47	118.72
3	C	389	FAD	C1'-N10-C9A	3.15	122.40	118.86
3	C	389	FAD	C4X-N5-C5X	3.20	120.44	116.76
4	D	392	T1C	O12-C12-C1C	3.22	118.64	113.50
4	B	392	T1C	C5-C41-C4	3.27	116.42	111.47
3	D	389	FAD	O3P-P-O5'	3.30	111.69	102.94
3	D	389	FAD	C4X-N5-C5X	3.33	120.59	116.76
3	B	389	FAD	O3P-PA-O5B	3.36	111.85	102.94
3	C	389	FAD	C4-C4X-N5	3.50	122.97	118.72
4	A	392	T1C	C1-C1C-C12	3.67	114.34	109.73
4	B	392	T1C	C1C-C1-C2	3.71	122.08	116.13
4	C	392	T1C	O12-C12-C1C	3.75	119.48	113.50
4	A	392	T1C	C5-C41-C4	3.80	117.22	111.47
3	B	389	FAD	C1'-N10-C9A	4.05	123.41	118.86
4	A	392	T1C	C1C-C1-C2	4.37	123.13	116.13
4	B	392	T1C	C41-C1C-C1	4.46	116.24	111.17
3	D	389	FAD	C1'-N10-C9A	4.53	123.95	118.86
4	D	392	T1C	C1C-C1-C2	5.16	124.40	116.13
3	B	389	FAD	C5X-C9A-N10	5.35	121.68	117.62
4	C	392	T1C	C1C-C1-C2	6.06	125.83	116.13
4	B	392	T1C	O12-C12-C1C	6.30	123.55	113.50
4	D	392	T1C	C61-C7-N7	7.40	125.23	118.94
3	B	389	FAD	C4-N3-C2	9.78	123.70	115.25
3	C	389	FAD	C4-N3-C2	10.41	124.25	115.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	389	FAD	C4-N3-C2	10.90	124.67	115.25
3	D	389	FAD	C4-N3-C2	11.23	124.95	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 45 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	389	FAD	4	0
4	A	392	T1C	10	0
3	B	389	FAD	8	0
4	B	392	T1C	7	0
3	C	389	FAD	1	0
4	C	392	T1C	5	0
3	D	389	FAD	2	0
4	D	392	T1C	15	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%)	0.74	32 (8%) 13 18	43, 62, 96, 142	0
2	B	368/398 (92%)	0.86	42 (11%) 7 10	45, 63, 95, 130	0
2	C	367/398 (92%)	1.01	60 (16%) 2 4	53, 75, 111, 156	0
2	D	367/398 (92%)	0.95	53 (14%) 3 5	50, 75, 115, 144	0
All	All	1470/1592 (92%)	0.89	187 (12%) 5 8	43, 69, 108, 156	0

All (187) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	340	ASP	9.1
2	B	249	THR	7.5
1	A	249	THR	7.1
1	A	343	PHE	6.5
2	C	380	PHE	6.5
2	B	343	PHE	6.1
2	D	245	TRP	6.1
2	C	343	PHE	5.5
2	B	12	ASN	5.5
2	B	341	GLY	5.3
1	A	145	GLY	5.3
2	D	380	PHE	5.2
1	A	378	PRO	5.1
2	D	378	PRO	4.8
2	D	110	PHE	4.8
2	C	252	ASP	4.7
2	B	250	GLN	4.7
2	C	220	GLY	4.7
2	D	343	PHE	4.7
2	D	339	ALA	4.7
2	C	341	GLY	4.7

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Mol	Chain	Res	Type	RSRZ
2	B	344	ASN	4.6
2	D	340	ASP	4.6
2	C	148	LYS	4.5
1	A	147	LYS	4.5
2	D	147	LYS	4.5
2	D	252	ASP	4.4
1	A	250	GLN	4.4
2	B	258	SER	4.3
2	D	322	GLN	4.3
2	C	245	TRP	4.2
2	B	252	ASP	4.2
2	B	13	LEU	4.2
2	C	110	PHE	4.2
2	C	268	SER	4.1
2	C	376	PHE	4.1
1	A	12	ASN	4.0
2	B	243	ASP	4.0
2	C	253	PHE	4.0
2	C	344	ASN	4.0
2	C	261	ASP	4.0
2	D	14	LEU	3.9
2	D	320	ALA	3.9
2	D	341	GLY	3.8
1	A	254	GLN	3.8
1	A	243	ASP	3.7
2	D	251	VAL	3.6
2	C	370	GLN	3.6
2	B	245	TRP	3.6
2	D	109	ARG	3.5
2	B	264	LEU	3.5
2	C	348	GLU	3.4
2	C	15	SER	3.4
2	D	254	GLN	3.4
2	B	345	SER	3.4
2	C	345	SER	3.4
2	D	255	ASN	3.4
2	C	217	SER	3.3
2	B	339	ALA	3.3
1	A	245	TRP	3.3
2	B	147	LYS	3.2
2	D	300	SER	3.2
2	D	16	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
2	C	257	ASN	3.1
2	C	147	LYS	3.1
2	C	256	ARG	3.1
2	D	15	SER	3.1
2	D	336	ASP	3.1
2	B	304	LEU	3.1
2	C	375	MET	3.1
2	C	264	LEU	3.0
2	D	218	HIS	3.0
2	D	345	SER	3.0
2	C	279	HIS	3.0
2	C	161	ALA	3.0
2	D	269	ASP	3.0
2	D	349	ALA	3.0
2	C	144	PRO	3.0
1	A	344	ASN	3.0
2	D	12	ASN	3.0
2	B	15	SER	3.0
2	C	251	VAL	2.9
1	A	341	GLY	2.9
1	A	301	LYS	2.9
2	D	243	ASP	2.9
1	A	146	LYS	2.9
2	B	255	ASN	2.9
2	D	268	SER	2.9
2	D	364	ALA	2.9
2	D	242	PRO	2.9
2	B	14	LEU	2.9
2	C	342	LYS	2.8
2	D	360	TYR	2.8
2	B	340	ASP	2.8
2	D	352	ASN	2.8
1	A	251	VAL	2.8
1	A	124	LEU	2.8
1	A	376	PHE	2.7
2	C	319	PHE	2.7
2	D	344	ASN	2.7
2	D	346	ILE	2.7
1	A	252	ASP	2.7
2	C	381	THR	2.7
1	A	355	GLN	2.7
2	C	250	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
2	C	339	ALA	2.7
2	C	42	VAL	2.7
2	B	257	ASN	2.7
2	C	36	GLN	2.7
2	B	261	ASP	2.7
1	A	13	LEU	2.7
2	C	14	LEU	2.6
2	B	254	GLN	2.6
2	C	111	ASP	2.6
1	A	14	LEU	2.6
1	A	148	LYS	2.6
1	A	268	SER	2.6
2	D	353	TYR	2.6
2	C	382	PHE	2.6
2	C	349	ALA	2.5
1	A	253	PHE	2.5
2	D	376	PHE	2.5
2	C	244	GLU	2.5
2	B	124	LEU	2.5
2	C	352	ASN	2.4
2	C	13	LEU	2.4
2	C	294	LEU	2.4
2	B	324	VAL	2.4
2	B	148	LYS	2.4
2	D	257	ASN	2.4
2	C	124	LEU	2.4
2	D	104	VAL	2.4
2	B	326	SER	2.4
2	D	148	LYS	2.4
2	D	253	PHE	2.4
2	B	183	VAL	2.3
2	C	178	VAL	2.3
2	D	146	LYS	2.3
2	C	322	GLN	2.3
2	B	16	ASP	2.3
2	B	288	ALA	2.3
2	B	120	LEU	2.3
2	C	271	ASP	2.3
2	C	255	ASN	2.3
2	C	242	PRO	2.3
2	C	291	ILE	2.3
2	C	304	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	379	ASP	2.3
2	B	328	LEU	2.3
2	D	381	THR	2.2
2	B	301	LYS	2.2
2	C	269	ASP	2.2
1	A	375	MET	2.2
2	D	162	ASP	2.2
1	A	322	GLN	2.2
2	C	207	GLN	2.2
2	B	378	PRO	2.2
1	A	381	THR	2.2
2	B	256	ARG	2.2
2	C	355	GLN	2.2
2	B	162	ASP	2.2
2	D	111	ASP	2.2
2	C	218	HIS	2.2
2	D	298	TRP	2.1
2	B	26	PRO	2.1
1	A	255	ASN	2.1
1	A	328	LEU	2.1
2	B	244	GLU	2.1
2	D	295	GLU	2.1
1	A	382	PHE	2.1
2	B	268	SER	2.1
2	C	41	ASP	2.1
1	A	26	PRO	2.1
2	D	178	VAL	2.1
2	D	294	LEU	2.1
2	C	108	ASN	2.1
2	D	271	ASP	2.1
2	D	188	THR	2.1
2	D	177	PHE	2.0
2	C	320	ALA	2.0
1	A	108	ASN	2.0
2	B	323	GLY	2.0
2	C	109	ARG	2.0
2	D	370	GLN	2.0
2	D	124	LEU	2.0
2	B	296	LYS	2.0
2	C	146	LYS	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. 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
4	T1C	C	392	42/42	0.67	0.35	2.96	77,120,163,175	0
4	T1C	B	392	42/42	0.79	0.23	2.46	61,90,115,117	0
4	T1C	D	392	42/42	0.78	0.31	2.43	91,115,142,151	0
4	T1C	A	392	42/42	0.83	0.22	0.89	61,85,102,117	0
3	FAD	B	389	53/53	0.92	0.19	0.20	33,45,58,72	0
3	FAD	C	389	53/53	0.94	0.14	-0.82	36,50,62,73	0
3	FAD	D	389	53/53	0.96	0.14	-0.83	39,50,61,69	0
3	FAD	A	389	53/53	0.96	0.14	-0.90	30,43,53,65	0
5	SO4	B	1386	5/5	0.94	0.23	-	80,96,107,108	0
5	SO4	B	1383	5/5	0.93	0.16	-	98,100,106,119	0
5	SO4	A	1384	5/5	0.38	0.24	-	109,115,142,145	0
5	SO4	C	1384	5/5	0.91	0.20	-	90,97,107,118	0
5	SO4	B	1385	5/5	0.89	0.12	-	105,109,124,129	0
5	SO4	D	1383	5/5	0.89	0.19	-	117,119,129,130	0
5	SO4	D	1385	5/5	0.94	0.23	-	90,93,100,108	0
5	SO4	B	1384	5/5	0.96	0.10	-	89,95,103,109	0
5	SO4	A	1383	5/5	0.96	0.12	-	94,96,104,108	0
5	SO4	C	1383	5/5	0.75	0.17	-	99,100,115,129	0
5	SO4	D	1384	5/5	0.98	0.08	-	88,88,92,98	0

6.5 Other polymers (i)

There are no such residues in this entry.