Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 03:20 PM GMT

PDB ID	:	4C5O
Title	:	Flavin monooxygenase from Stenotrophomonas maltophilia. Q193R H194T mutant
Authors	:	Jensen, C.N.; Ali, S.T.; Allen, M.J.; Grogan, G.
Deposited on	:	2013-09-13
Resolution	:	2.60 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 (i) symbol.

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

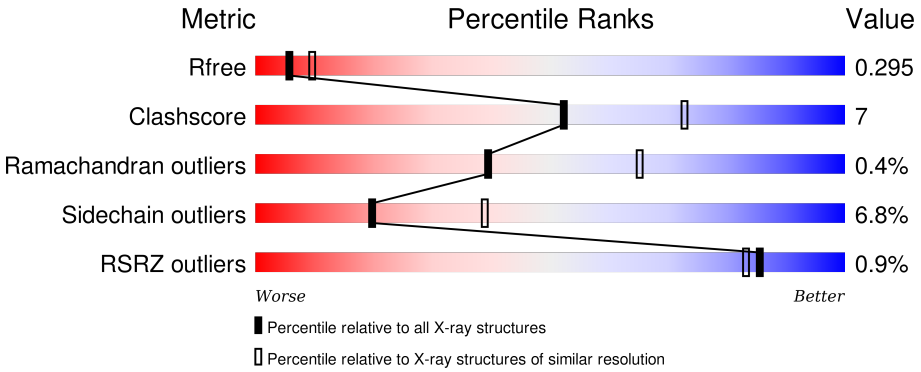
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.60 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	357	5% 78% 12% • 8%
1	B	357	% 77% 14% •• 8%
1	C	357	78% 13% • 8%
1	D	357	76% 16% • 7%
1	E	357	79% 13% 8%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	357	79% 12% •• 8%
1	G	357	77% 14% •• 8%
1	H	357	78% 14% •• 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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	A	1355	-	-	-	X
3	SO4	B	1355	-	-	-	X
3	SO4	B	1357	-	-	-	X
3	SO4	C	1355	-	-	-	X
3	SO4	C	1356	-	-	-	X
3	SO4	D	1355	-	-	-	X
3	SO4	D	1356	-	-	-	X
3	SO4	E	1355	-	-	-	X
3	SO4	F	1357	-	-	X	X
3	SO4	H	1355	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 20137 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 FLAVIN MONOOXYGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	327	Total	C	N	O	S	0	0	0
			2256	1444	392	414	6			
1	B	330	Total	C	N	O	S	0	0	0
			2388	1533	414	434	7			
1	C	330	Total	C	N	O	S	0	0	0
			2475	1588	436	443	8			
1	D	333	Total	C	N	O	S	0	0	0
			2495	1599	438	451	7			
1	E	330	Total	C	N	O	S	0	0	0
			2448	1574	429	437	8			
1	F	330	Total	C	N	O	S	0	0	0
			2436	1567	422	440	7			
1	G	330	Total	C	N	O	S	0	0	0
			2450	1575	432	436	7			
1	H	331	Total	C	N	O	S	0	0	0
			2494	1597	441	448	8			

There are 16 discrepancies between the modelled and reference sequences:

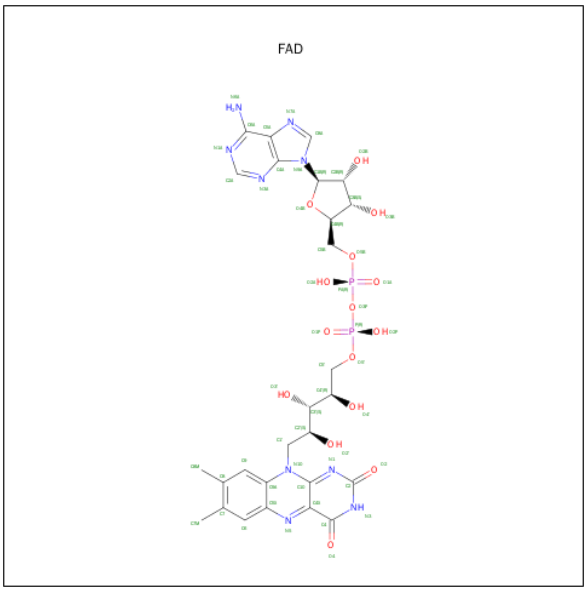
Chain	Residue	Modelled	Actual	Comment	Reference
A	193	ARG	GLN	ENGINEERED MUTATION	UNP B2FRL2
A	194	THR	HIS	ENGINEERED MUTATION	UNP B2FRL2
B	193	ARG	GLN	ENGINEERED MUTATION	UNP B2FRL2
B	194	THR	HIS	ENGINEERED MUTATION	UNP B2FRL2
C	193	ARG	GLN	ENGINEERED MUTATION	UNP B2FRL2
C	194	THR	HIS	ENGINEERED MUTATION	UNP B2FRL2
D	193	ARG	GLN	ENGINEERED MUTATION	UNP B2FRL2
D	194	THR	HIS	ENGINEERED MUTATION	UNP B2FRL2
E	193	ARG	GLN	ENGINEERED MUTATION	UNP B2FRL2
E	194	THR	HIS	ENGINEERED MUTATION	UNP B2FRL2
F	193	ARG	GLN	ENGINEERED MUTATION	UNP B2FRL2
F	194	THR	HIS	ENGINEERED MUTATION	UNP B2FRL2
G	193	ARG	GLN	ENGINEERED MUTATION	UNP B2FRL2

Continued on next page...

Continued from previous page...

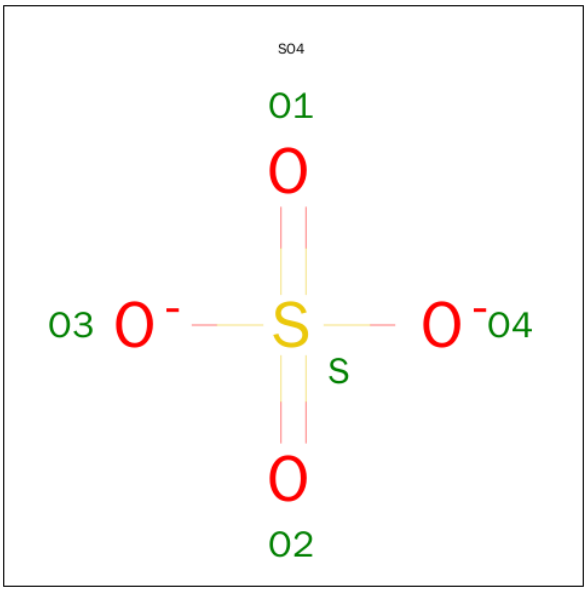
Chain	Residue	Modelled	Actual	Comment	Reference
G	194	THR	HIS	ENGINEERED MUTATION	UNP B2FRL2
H	193	ARG	GLN	ENGINEERED MUTATION	UNP B2FRL2
H	194	THR	HIS	ENGINEERED MUTATION	UNP B2FRL2

- 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		
2	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	F	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	G	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	H	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 O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0
3	G	1	Total O S 5 4 1	0	0
3	G	1	Total O S 5 4 1	0	0
3	G	1	Total O S 5 4 1	0	0
3	G	1	Total O S 5 4 1	0	0
3	H	1	Total O S 5 4 1	0	0
3	H	1	Total O S 5 4 1	0	0
3	H	1	Total O S 5 4 1	0	0
3	H	1	Total O S 5 4 1	0	0

- Molecule 4 is water.

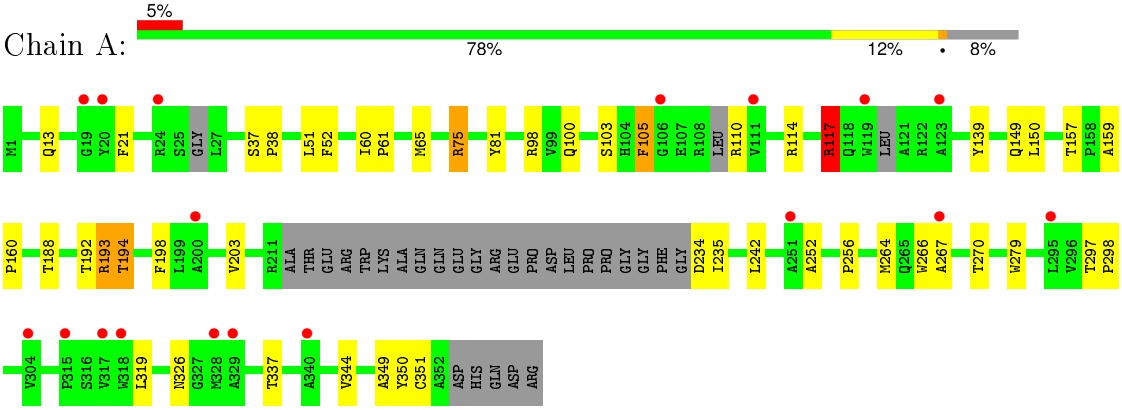
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	5	Total O 5 5	0	0
4	B	4	Total O 4 4	0	0
4	C	18	Total O 18 18	0	0
4	D	12	Total O 12 12	0	0
4	E	13	Total O 13 13	0	0
4	F	18	Total O 18 18	0	0
4	G	15	Total O 15 15	0	0
4	H	21	Total O 21 21	0	0

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.

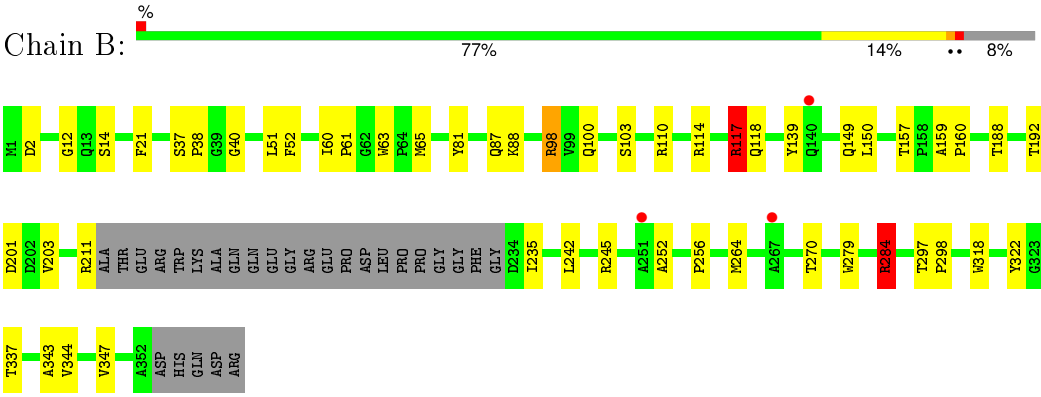
- Molecule 1: FLAVIN MONOOXYGENASE

Chain A:



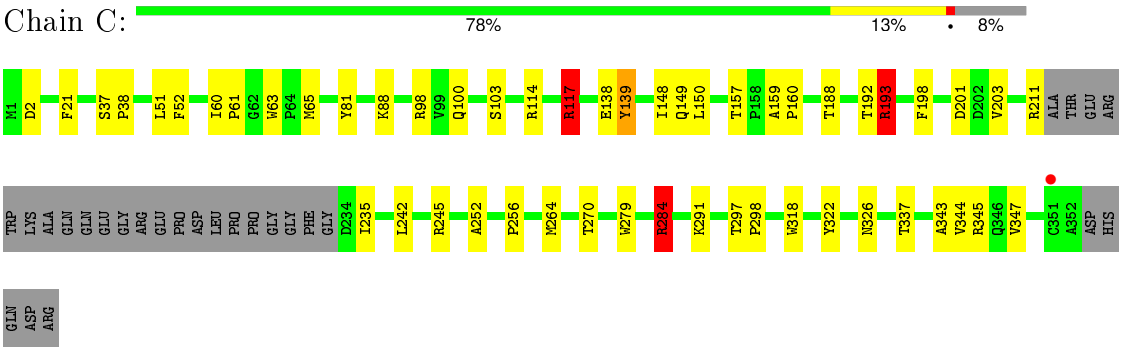
- Molecule 1: FLAVIN MONOOXYGENASE

Chain B:



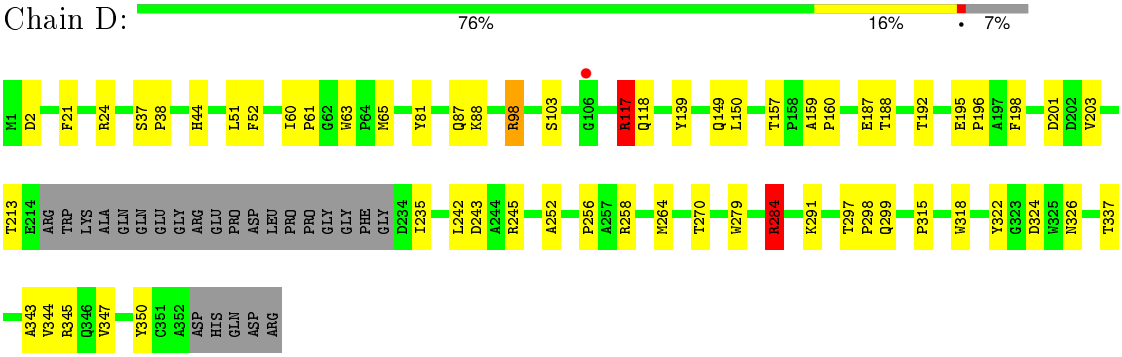
- Molecule 1: FLAVIN MONOOXYGENASE

Chain C:



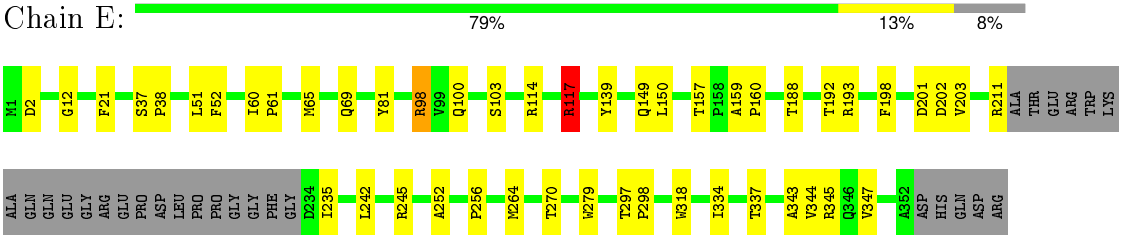
• Molecule 1: FLAVIN MONOOXYGENASE

Chain D:



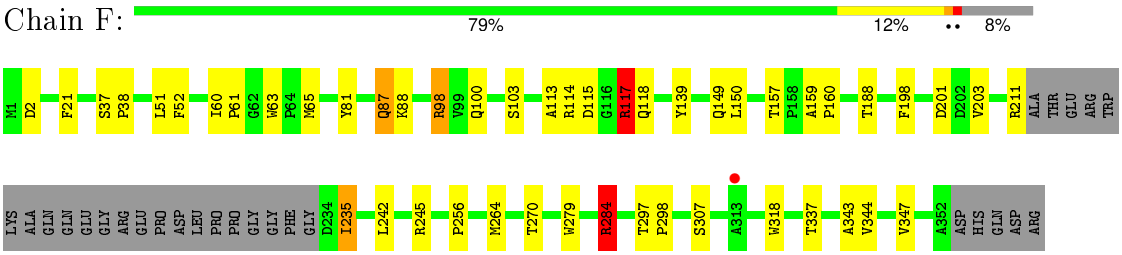
• Molecule 1: FLAVIN MONOOXYGENASE

Chain E:



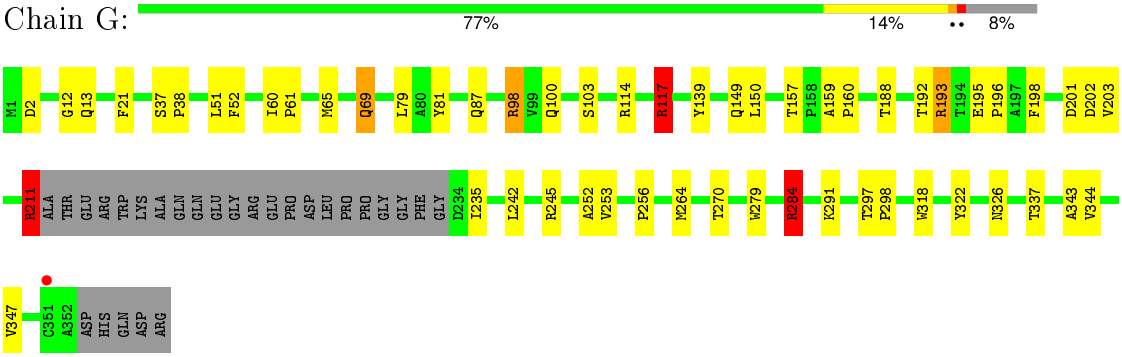
• Molecule 1: FLAVIN MONOOXYGENASE

Chain F:



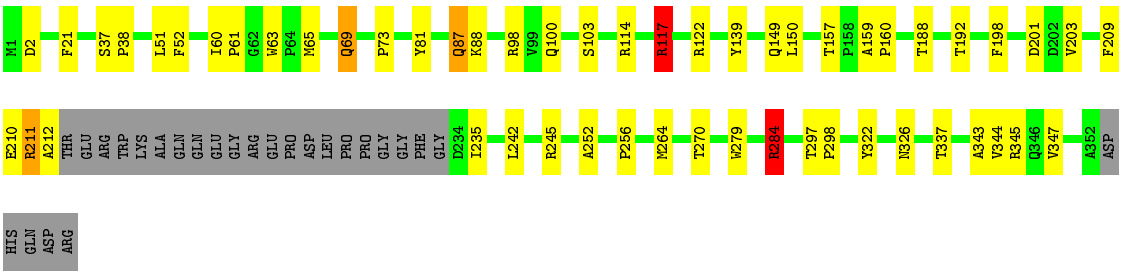
• Molecule 1: FLAVIN MONOOXYGENASE

Chain G:



• Molecule 1: FLAVIN MONOOXYGENASE

Chain H:


M1 D2 F21 S37 P38 L51 F52 I60 P61 G62 W63 P64 M65 Q69 P73 Y81 Q87 K88 R98 V99 Q100 S103 R114 R117 R122 Y139 Q149 L150 T157 P158 A159 P160 T188 T192 F198 D201 D202 V203 F209
E210 R211 A212 THR GLU ARG TRP LYS ALA GLN GLN GLU GLY ARG GLU PRO ASP LEU PRO PRO GLY GLY PHE GLY D234 I235 L242 R245 A252 P256 M264 T270 W279 R284 T297 P298 Y322 N326 T337 A343 V344 R345 Q346 V347 A352 ASP
HIS GLN ASP ARG

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	170.54Å 170.54Å 101.76Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	147.69 – 2.60 49.23 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.2 (147.69-2.60) 97.6 (49.23-2.40)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.78 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0033	Depositor
R, R_{free}	0.255 , 0.295 0.258 , 0.295	Depositor DCC
R_{free} test set	5030 reflections (5.35%)	DCC
Wilson B-factor (Å^2)	46.4	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 9.3	EDS
Estimated twinning fraction	0.039 for -h,-k,l 0.057 for h,-h-k,-l 0.044 for -k,-h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	0 of 126991 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	20137	wwPDB-VP
Average B, all atoms (Å^2)	53.0	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 71.77 % 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 2.4807e-06.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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

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	0.59	0/2318	0.77	7/3187 (0.2%)
1	B	0.60	0/2457	0.78	6/3377 (0.2%)
1	C	0.64	0/2546	0.77	6/3483 (0.2%)
1	D	0.65	0/2566	0.79	3/3512 (0.1%)
1	E	0.65	0/2519	0.74	1/3451 (0.0%)
1	F	0.65	0/2507	0.77	4/3439 (0.1%)
1	G	0.64	0/2521	0.77	4/3454 (0.1%)
1	H	0.67	0/2565	0.78	3/3508 (0.1%)
All	All	0.64	0/19999	0.77	34/27411 (0.1%)

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	211	ARG	N-CA-C	8.91	135.06	111.00
1	H	117	ARG	NE-CZ-NH1	8.48	124.54	120.30
1	C	284	ARG	NE-CZ-NH1	8.34	124.47	120.30
1	D	284	ARG	NE-CZ-NH1	8.33	124.47	120.30
1	G	117	ARG	NE-CZ-NH1	8.12	124.36	120.30
1	H	284	ARG	NE-CZ-NH1	8.01	124.31	120.30
1	B	117	ARG	NE-CZ-NH1	7.89	124.25	120.30
1	C	193	ARG	NE-CZ-NH1	7.89	124.25	120.30
1	A	117	ARG	NE-CZ-NH1	7.74	124.17	120.30
1	F	117	ARG	NE-CZ-NH1	7.65	124.13	120.30
1	B	193	ARG	CA-CB-CG	7.61	130.13	113.40
1	D	117	ARG	NE-CZ-NH1	7.49	124.05	120.30
1	B	284	ARG	NE-CZ-NH1	7.48	124.04	120.30
1	F	284	ARG	NE-CZ-NH1	7.34	123.97	120.30
1	E	117	ARG	NE-CZ-NH1	7.29	123.95	120.30
1	G	284	ARG	NE-CZ-NH1	6.96	123.78	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	193	ARG	N-CA-C	-6.75	92.78	111.00
1	C	117	ARG	NE-CZ-NH1	6.71	123.66	120.30
1	B	193	ARG	CB-CG-CD	-6.68	94.23	111.60
1	A	105	PHE	CB-CG-CD1	6.21	125.15	120.80
1	A	105	PHE	CB-CG-CD2	-5.90	116.67	120.80
1	C	284	ARG	NE-CZ-NH2	-5.81	117.39	120.30
1	A	75	ARG	NE-CZ-NH2	-5.75	117.42	120.30
1	C	193	ARG	NE-CZ-NH2	-5.65	117.48	120.30
1	B	193	ARG	N-CA-CB	-5.58	100.56	110.60
1	B	284	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	A	110	ARG	CA-CB-CG	5.46	125.40	113.40
1	F	118	GLN	N-CA-CB	-5.37	100.93	110.60
1	H	69	GLN	CB-CA-C	5.28	120.97	110.40
1	F	284	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	G	69	GLN	CB-CA-C	5.20	120.81	110.40
1	D	258	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	A	75	ARG	NE-CZ-NH1	5.13	122.87	120.30
1	C	193	ARG	CD-NE-CZ	5.11	130.75	123.60

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	2256	0	2032	29	0
1	B	2388	0	2265	34	0
1	C	2475	0	2413	31	0
1	D	2495	0	2425	35	0
1	E	2448	0	2370	27	0
1	F	2436	0	2339	30	0
1	G	2450	0	2375	35	0
1	H	2494	0	2434	39	0
2	A	53	0	31	4	0
2	B	53	0	31	4	0
2	C	53	0	31	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	53	0	31	1	0
2	E	53	0	31	2	0
2	F	53	0	31	0	0
2	G	53	0	31	3	0
2	H	53	0	31	2	0
3	A	15	0	0	1	0
3	B	20	0	0	2	0
3	C	25	0	0	1	0
3	D	30	0	0	3	0
3	E	15	0	0	2	0
3	F	20	0	0	3	0
3	G	20	0	0	2	0
3	H	20	0	0	1	0
4	A	5	0	0	1	0
4	B	4	0	0	1	0
4	C	18	0	0	0	0
4	D	12	0	0	1	0
4	E	13	0	0	0	0
4	F	18	0	0	1	0
4	G	15	0	0	0	0
4	H	21	0	0	0	0
All	All	20137	0	18901	259	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 (259) 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:H:210:GLU:C	1:H:212:ALA:HB3	1.59	1.22
1:H:210:GLU:O	1:H:212:ALA:HB3	1.52	1.10
1:A:266:TRP:O	1:D:315:PRO:HG2	1.68	0.92
1:H:210:GLU:C	1:H:212:ALA:CB	2.40	0.89
1:D:117:ARG:HG3	1:D:117:ARG:HH11	1.39	0.86
1:H:117:ARG:HH11	1:H:117:ARG:HG3	1.41	0.85
1:B:117:ARG:HH11	1:B:117:ARG:HG3	1.42	0.85
1:F:117:ARG:HH11	1:F:117:ARG:HG3	1.40	0.85
1:F:87:GLN:HE22	1:G:202:ASP:HB3	1.43	0.84
1:H:211:ARG:N	1:H:212:ALA:HB3	1.94	0.82
1:G:117:ARG:HG3	1:G:117:ARG:HH11	1.42	0.82
1:C:117:ARG:HH11	1:C:117:ARG:HG3	1.45	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:117:ARG:HG3	1:E:117:ARG:HH11	1.45	0.81
1:A:267:ALA:O	1:D:315:PRO:HD2	1.81	0.81
1:A:117:ARG:HH11	1:A:117:ARG:HG3	1.45	0.80
1:A:193:ARG:O	1:A:194:THR:OG1	2.01	0.78
1:H:198:PHE:CE1	1:H:235:ILE:HD11	2.21	0.75
1:D:198:PHE:CE1	1:D:235:ILE:HD11	2.23	0.74
1:H:211:ARG:CA	1:H:212:ALA:HB3	2.16	0.73
1:H:210:GLU:O	1:H:212:ALA:CB	2.33	0.73
1:B:193:ARG:HB3	1:B:193:ARG:CZ	2.09	0.72
1:A:157:THR:HG22	1:A:159:ALA:H	1.55	0.72
1:B:198:PHE:CE1	1:B:235:ILE:HD11	2.24	0.71
1:F:198:PHE:CE1	1:F:235:ILE:HD11	2.25	0.71
1:A:198:PHE:CE1	1:A:235:ILE:HD11	2.26	0.71
1:G:198:PHE:CE1	1:G:235:ILE:HD11	2.25	0.70
1:C:198:PHE:CE1	1:C:235:ILE:HD11	2.27	0.70
1:E:198:PHE:CE1	1:E:235:ILE:HD11	2.27	0.69
1:A:60:ILE:HB	1:A:61:PRO:HD2	1.76	0.68
1:D:284:ARG:HG2	1:D:284:ARG:HH11	1.59	0.68
1:B:60:ILE:HB	1:B:61:PRO:HD2	1.75	0.68
1:D:60:ILE:HB	1:D:61:PRO:HD2	1.76	0.67
1:C:60:ILE:HB	1:C:61:PRO:HD2	1.76	0.67
1:H:284:ARG:HH11	1:H:284:ARG:HG2	1.59	0.67
1:E:60:ILE:HB	1:E:61:PRO:HD2	1.76	0.66
1:C:157:THR:HG22	1:C:159:ALA:H	1.60	0.66
1:H:209:PHE:O	1:H:212:ALA:HB2	1.96	0.66
1:B:284:ARG:HH11	1:B:284:ARG:HG2	1.60	0.66
1:G:60:ILE:HB	1:G:61:PRO:HD2	1.77	0.65
1:H:60:ILE:HB	1:H:61:PRO:HD2	1.77	0.65
1:E:157:THR:HG22	1:E:159:ALA:H	1.62	0.64
1:F:284:ARG:HG2	1:F:284:ARG:HH11	1.62	0.64
1:F:60:ILE:HB	1:F:61:PRO:HD2	1.78	0.64
1:G:284:ARG:HH11	1:G:284:ARG:HG2	1.63	0.63
1:H:149:GLN:HE21	1:H:279:TRP:HE1	1.47	0.62
1:C:149:GLN:HE21	1:C:279:TRP:HE1	1.47	0.62
1:D:157:THR:HG22	1:D:159:ALA:H	1.64	0.62
1:E:149:GLN:HE21	1:E:279:TRP:HE1	1.49	0.61
1:D:149:GLN:HE21	1:D:279:TRP:HE1	1.48	0.61
1:A:319:LEU:CB	1:A:326:ASN:HD21	2.14	0.61
1:B:149:GLN:HE21	1:B:279:TRP:HE1	1.49	0.61
1:G:149:GLN:HE21	1:G:279:TRP:HE1	1.49	0.61
1:D:117:ARG:NH1	1:D:117:ARG:HG3	2.13	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:193:ARG:HH11	1:C:193:ARG:HG2	1.65	0.61
1:H:211:ARG:HA	1:H:212:ALA:HB3	1.83	0.61
1:F:157:THR:HG22	1:F:159:ALA:H	1.66	0.60
1:G:157:THR:HG22	1:G:159:ALA:H	1.66	0.60
1:A:149:GLN:HE21	1:A:279:TRP:HE1	1.49	0.60
1:B:14:SER:HB2	4:B:2001:HOH:O	2.02	0.60
1:B:157:THR:HG22	1:B:159:ALA:H	1.67	0.59
1:C:284:ARG:HG2	1:C:284:ARG:HH11	1.66	0.59
1:F:149:GLN:HE21	1:F:279:TRP:HE1	1.50	0.59
1:A:13:GLN:NE2	2:A:1353:FAD:H4'	2.16	0.59
1:C:148:ILE:HA	3:C:1356:SO4:O1	2.03	0.58
1:D:324:ASP:N	3:D:1358:SO4:O4	2.36	0.58
1:B:284:ARG:HH11	1:B:284:ARG:CG	2.17	0.58
1:F:307:SER:O	4:F:2018:HOH:O	2.17	0.58
1:E:117:ARG:HG3	1:E:117:ARG:NH1	2.18	0.57
1:A:319:LEU:HB3	1:A:326:ASN:HD21	1.70	0.57
1:H:284:ARG:HH11	1:H:284:ARG:CG	2.18	0.56
1:H:157:THR:HG22	1:H:159:ALA:H	1.70	0.56
1:G:201:ASP:OD2	1:G:245:ARG:NH2	2.38	0.56
1:H:201:ASP:OD2	1:H:245:ARG:NH2	2.38	0.56
1:F:284:ARG:CG	1:F:284:ARG:HH11	2.18	0.56
1:C:201:ASP:OD2	1:C:245:ARG:NH2	2.39	0.56
1:F:113:ALA:HB1	3:F:1357:SO4:O4	2.06	0.55
1:B:324:ASP:N	3:B:1357:SO4:O3	2.39	0.55
1:D:60:ILE:HB	1:D:61:PRO:CD	2.37	0.55
1:C:284:ARG:HH11	1:C:284:ARG:CG	2.20	0.55
1:G:245:ARG:HH11	1:G:245:ARG:HG2	1.72	0.55
1:E:69:GLN:HG2	1:G:79:LEU:HD13	1.89	0.55
1:F:87:GLN:NE2	1:G:202:ASP:HB3	2.18	0.55
1:G:284:ARG:HH11	1:G:284:ARG:CG	2.20	0.55
1:B:201:ASP:OD2	1:B:245:ARG:NH2	2.40	0.55
1:F:245:ARG:HH11	1:F:245:ARG:HG2	1.72	0.54
1:D:284:ARG:CG	1:D:284:ARG:HH11	2.20	0.54
1:E:202:ASP:HB3	1:H:87:GLN:HE22	1.71	0.54
1:E:192:THR:OG1	3:E:1356:SO4:O3	2.23	0.54
1:C:60:ILE:HB	1:C:61:PRO:CD	2.38	0.54
1:E:201:ASP:OD2	1:E:245:ARG:NH2	2.41	0.54
1:D:201:ASP:OD2	1:D:245:ARG:NH2	2.41	0.53
1:H:211:ARG:CA	1:H:212:ALA:CB	2.86	0.53
1:F:201:ASP:OD2	1:F:245:ARG:NH2	2.41	0.53
1:H:60:ILE:HB	1:H:61:PRO:CD	2.38	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:60:ILE:HB	1:E:61:PRO:CD	2.38	0.53
1:A:13:GLN:CD	2:A:1353:FAD:H4'	2.28	0.53
1:A:234:ASP:N	4:A:2005:HOH:O	2.42	0.53
1:D:245:ARG:HH11	1:D:245:ARG:HG2	1.72	0.53
1:A:349:ALA:O	1:A:351:CYS:N	2.42	0.53
1:E:98:ARG:NH1	3:E:1354:SO4:O3	2.32	0.53
1:A:60:ILE:HB	1:A:61:PRO:CD	2.38	0.52
1:B:245:ARG:HG2	1:B:245:ARG:HH11	1.74	0.52
1:H:284:ARG:NH1	1:H:284:ARG:HG2	2.25	0.52
1:C:117:ARG:NH1	1:C:117:ARG:HG3	2.19	0.52
1:B:60:ILE:HB	1:B:61:PRO:CD	2.37	0.52
1:F:159:ALA:HB3	1:F:160:PRO:HD3	1.92	0.52
1:F:60:ILE:HB	1:F:61:PRO:CD	2.40	0.52
1:H:245:ARG:HG2	1:H:245:ARG:HH11	1.73	0.52
1:G:60:ILE:HB	1:G:61:PRO:CD	2.39	0.52
1:C:148:ILE:HD11	1:D:118:GLN:CD	2.30	0.51
1:G:98:ARG:HD2	3:G:1354:SO4:O3	2.10	0.51
1:C:193:ARG:HH11	1:C:193:ARG:CG	2.22	0.51
1:C:245:ARG:HG2	1:C:245:ARG:HH11	1.75	0.51
1:B:63:TRP:HB2	1:B:88:LYS:HE3	1.92	0.51
1:B:117:ARG:NH1	1:B:117:ARG:HG3	2.16	0.51
1:G:12:GLY:HA3	2:G:1353:FAD:H52A	1.93	0.50
1:H:63:TRP:HB2	1:H:88:LYS:HE3	1.93	0.50
1:B:193:ARG:CB	1:B:193:ARG:CZ	2.86	0.50
1:D:63:TRP:HB2	1:D:88:LYS:HE3	1.94	0.50
1:D:159:ALA:HB3	1:D:160:PRO:HD3	1.94	0.50
1:E:245:ARG:HG2	1:E:245:ARG:HH11	1.76	0.50
1:C:37:SER:HB3	1:C:38:PRO:HD2	1.94	0.50
1:B:98:ARG:HD2	3:B:1354:SO4:O3	2.11	0.50
1:G:37:SER:HB3	1:G:38:PRO:HD2	1.93	0.50
1:H:37:SER:HB3	1:H:38:PRO:HD2	1.95	0.49
1:E:202:ASP:HB3	1:H:87:GLN:NE2	2.27	0.49
1:D:37:SER:HB3	1:D:38:PRO:HD2	1.94	0.48
1:A:159:ALA:HB3	1:A:160:PRO:HD3	1.96	0.48
1:E:37:SER:HB3	1:E:38:PRO:HD2	1.94	0.48
1:F:37:SER:HB3	1:F:38:PRO:HD2	1.95	0.48
1:A:37:SER:HB3	1:A:38:PRO:HD2	1.95	0.48
1:F:117:ARG:NH1	1:F:117:ARG:HG3	2.15	0.48
1:H:211:ARG:N	1:H:212:ALA:CB	2.72	0.48
1:G:211:ARG:N	1:G:211:ARG:HD3	2.29	0.48
1:B:110:ARG:HE	1:B:118:GLN:NE2	2.11	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:343:ALA:O	1:B:347:VAL:HG13	2.14	0.48
1:F:117:ARG:HH11	1:F:117:ARG:CG	2.21	0.47
1:H:117:ARG:NH1	1:H:117:ARG:HG3	2.15	0.47
1:F:63:TRP:HB2	1:F:88:LYS:HE3	1.95	0.47
1:A:117:ARG:HG3	1:A:117:ARG:NH1	2.18	0.47
2:A:1353:FAD:H1'1	2:A:1353:FAD:H9	1.72	0.47
1:E:343:ALA:O	1:E:347:VAL:HG13	2.15	0.47
1:H:297:THR:HB	1:H:298:PRO:HD2	1.96	0.47
1:E:297:THR:HB	1:E:298:PRO:HD2	1.97	0.47
1:B:159:ALA:HB3	1:B:160:PRO:HD3	1.97	0.47
1:G:297:THR:HB	1:G:298:PRO:HD2	1.96	0.47
1:B:297:THR:HB	1:B:298:PRO:HD2	1.96	0.47
1:C:63:TRP:HB2	1:C:88:LYS:HE3	1.95	0.47
1:E:12:GLY:HA3	2:E:1353:FAD:H52A	1.97	0.47
1:F:343:ALA:O	1:F:347:VAL:HG13	2.15	0.47
1:A:61:PRO:HG3	1:A:337:THR:HG23	1.97	0.47
1:E:159:ALA:HB3	1:E:160:PRO:HD3	1.98	0.46
1:B:65:MET:HG3	1:B:81:TYR:CD2	2.50	0.46
1:D:65:MET:HG3	1:D:81:TYR:CD2	2.51	0.46
1:B:117:ARG:HH11	1:B:117:ARG:CG	2.22	0.46
1:H:343:ALA:O	1:H:347:VAL:HG13	2.15	0.46
1:F:297:THR:HB	1:F:298:PRO:HD2	1.98	0.46
1:G:117:ARG:HG3	1:G:117:ARG:NH1	2.16	0.46
1:F:284:ARG:HG2	1:F:284:ARG:NH1	2.29	0.46
1:D:44:HIS:O	3:D:1355:SO4:O3	2.33	0.46
1:A:267:ALA:HB2	1:D:350:TYR:OH	2.15	0.46
1:B:37:SER:HB3	1:B:38:PRO:HD2	1.96	0.46
1:C:322:TYR:H	1:C:326:ASN:HD22	1.64	0.46
1:D:343:ALA:O	1:D:347:VAL:HG13	2.15	0.46
1:F:21:PHE:HB2	1:F:344:VAL:HG21	1.98	0.46
2:E:1353:FAD:O2'	2:E:1353:FAD:N1	2.39	0.46
1:B:40:GLY:HA2	2:B:1353:FAD:O3B	2.15	0.46
1:D:284:ARG:HG2	1:D:284:ARG:NH1	2.23	0.46
1:A:114:ARG:NH1	3:A:1354:SO4:O3	2.43	0.46
1:D:61:PRO:HG3	1:D:337:THR:HG23	1.98	0.46
1:G:343:ALA:O	1:G:347:VAL:HG13	2.16	0.46
1:E:61:PRO:HG3	1:E:337:THR:HG23	1.98	0.45
1:B:12:GLY:HA3	2:B:1353:FAD:H52A	1.97	0.45
1:A:297:THR:HB	1:A:298:PRO:HD2	1.98	0.45
1:A:65:MET:HG3	1:A:81:TYR:CD2	2.51	0.45
1:G:318:TRP:CD2	1:G:347:VAL:HG12	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:61:PRO:HG3	1:F:337:THR:HG23	1.98	0.45
1:G:61:PRO:HG3	1:G:337:THR:HG23	1.98	0.45
1:C:297:THR:HB	1:C:298:PRO:HD2	1.99	0.45
1:E:21:PHE:HB2	1:E:344:VAL:HG21	1.99	0.45
1:G:117:ARG:CG	1:G:117:ARG:HH11	2.22	0.45
1:B:284:ARG:NH1	1:B:284:ARG:HG2	2.27	0.45
1:C:343:ALA:O	1:C:347:VAL:HG13	2.16	0.45
1:F:115:ASP:HB3	3:F:1357:SO4:O2	2.17	0.45
1:H:322:TYR:H	1:H:326:ASN:HD22	1.65	0.45
1:H:159:ALA:HB3	1:H:160:PRO:HD3	1.98	0.45
1:H:61:PRO:HG3	1:H:337:THR:HG23	1.98	0.45
1:D:318:TRP:CD2	1:D:347:VAL:HG12	2.52	0.45
1:D:297:THR:HB	1:D:298:PRO:HD2	1.99	0.45
1:G:256:PRO:HG3	1:G:264:MET:SD	2.57	0.45
1:A:267:ALA:CB	1:D:350:TYR:OH	2.65	0.45
1:D:117:ARG:CG	1:D:117:ARG:HH11	2.21	0.45
1:C:61:PRO:HG3	1:C:337:THR:HG23	1.97	0.45
1:A:21:PHE:HB2	1:A:344:VAL:HG21	1.99	0.45
1:H:65:MET:HG3	1:H:81:TYR:CD2	2.52	0.44
1:D:21:PHE:HB2	1:D:344:VAL:HG21	2.00	0.44
1:A:256:PRO:HG3	1:A:264:MET:SD	2.57	0.44
1:G:65:MET:HG3	1:G:81:TYR:CD2	2.53	0.44
1:F:256:PRO:HG3	1:F:264:MET:SD	2.57	0.44
1:C:284:ARG:NH1	1:C:284:ARG:HG2	2.32	0.44
1:G:322:TYR:H	1:G:326:ASN:HD22	1.64	0.44
2:G:1353:FAD:H9	2:G:1353:FAD:H1'1	1.84	0.44
1:A:319:LEU:HB2	1:A:326:ASN:HD21	1.81	0.44
1:F:318:TRP:CD2	1:F:347:VAL:HG12	2.53	0.44
1:D:322:TYR:H	1:D:326:ASN:HD22	1.65	0.44
1:G:21:PHE:HB2	1:G:344:VAL:HG21	2.00	0.44
1:C:159:ALA:HB3	1:C:160:PRO:HD3	1.99	0.44
1:B:192:THR:HG22	1:B:252:ALA:HB1	1.99	0.44
1:D:195:GLU:HA	1:D:196:PRO:HD3	1.91	0.44
1:B:21:PHE:HB2	1:B:344:VAL:HG21	2.00	0.44
1:E:117:ARG:HH11	1:E:117:ARG:CG	2.24	0.44
1:H:192:THR:HG22	1:H:252:ALA:HB1	1.99	0.44
1:D:98:ARG:NH1	3:D:1354:SO4:O3	2.51	0.43
1:C:192:THR:HG22	1:C:252:ALA:HB1	2.00	0.43
1:E:256:PRO:HG3	1:E:264:MET:SD	2.59	0.43
1:G:193:ARG:HB2	1:G:193:ARG:HH11	1.83	0.43
2:B:1353:FAD:N1	2:B:1353:FAD:O2'	2.46	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:PRO:HG3	1:B:264:MET:SD	2.59	0.43
2:D:1353:FAD:H51A	4:D:2002:HOH:O	2.18	0.43
1:H:21:PHE:HB2	1:H:344:VAL:HG21	1.99	0.43
1:C:21:PHE:HB2	1:C:344:VAL:HG21	2.00	0.43
1:G:100:GLN:HG3	1:G:114:ARG:HA	2.01	0.43
1:E:65:MET:HG3	1:E:81:TYR:CD2	2.54	0.43
1:E:192:THR:HG22	1:E:252:ALA:HB1	2.00	0.43
1:H:65:MET:HE1	1:H:73:PRO:HG3	2.01	0.43
1:B:61:PRO:HG3	1:B:337:THR:HG23	2.00	0.42
1:D:192:THR:HG22	1:D:252:ALA:HB1	2.01	0.42
2:H:1353:FAD:O2'	2:H:1353:FAD:N1	2.49	0.42
1:D:256:PRO:HG3	1:D:264:MET:SD	2.60	0.42
2:H:1353:FAD:H2'	2:H:1353:FAD:H5'2	1.87	0.42
1:A:192:THR:HG22	1:A:252:ALA:HB1	2.00	0.42
1:G:159:ALA:HB3	1:G:160:PRO:HD3	2.02	0.42
1:C:318:TRP:CD2	1:C:347:VAL:HG12	2.55	0.42
1:H:256:PRO:HG3	1:H:264:MET:SD	2.59	0.42
2:A:1353:FAD:N1	2:A:1353:FAD:O2'	2.42	0.42
1:C:100:GLN:HG3	1:C:114:ARG:HA	2.01	0.42
1:B:322:TYR:H	1:B:326:ASN:HD22	1.66	0.42
1:H:192:THR:OG1	3:H:1357:SO4:O3	2.36	0.42
1:B:100:GLN:HG3	1:B:114:ARG:HA	2.02	0.42
1:C:256:PRO:HG3	1:C:264:MET:SD	2.60	0.42
1:C:65:MET:HG3	1:C:81:TYR:CD2	2.54	0.42
1:F:98:ARG:HD2	3:F:1354:SO4:O3	2.20	0.42
1:H:117:ARG:HH11	1:H:117:ARG:CG	2.23	0.41
1:B:318:TRP:CD2	1:B:347:VAL:HG12	2.56	0.41
1:G:284:ARG:HG2	1:G:284:ARG:NH1	2.31	0.41
1:G:13:GLN:OE1	2:G:1353:FAD:H4'	2.20	0.41
1:G:192:THR:HG22	1:G:252:ALA:HB1	2.02	0.41
1:G:193:ARG:NH1	3:G:1356:SO4:O4	2.53	0.41
1:C:117:ARG:HH11	1:C:117:ARG:CG	2.25	0.41
1:E:100:GLN:HG3	1:E:114:ARG:HA	2.03	0.41
2:B:1353:FAD:H1'1	2:B:1353:FAD:H9	1.74	0.41
1:C:138:GLU:O	1:C:139:TYR:O	2.39	0.41
1:F:65:MET:HG3	1:F:81:TYR:CD2	2.56	0.40
1:D:245:ARG:NH1	1:D:245:ARG:HG2	2.36	0.40
1:E:318:TRP:CD2	1:E:347:VAL:HG12	2.57	0.40
1:A:100:GLN:HG3	1:A:114:ARG:HA	2.03	0.40
1:F:100:GLN:HG3	1:F:114:ARG:HA	2.04	0.40
1:G:195:GLU:HA	1:G:196:PRO:HD3	1.97	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:100:GLN:HG3	1:H:114:ARG:HA	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	317/357 (89%)	296 (93%)	18 (6%)	3 (1%)	21	42
1	B	326/357 (91%)	309 (95%)	16 (5%)	1 (0%)	46	72
1	C	326/357 (91%)	310 (95%)	15 (5%)	1 (0%)	46	72
1	D	329/357 (92%)	316 (96%)	12 (4%)	1 (0%)	46	72
1	E	326/357 (91%)	311 (95%)	14 (4%)	1 (0%)	46	72
1	F	326/357 (91%)	311 (95%)	14 (4%)	1 (0%)	46	72
1	G	326/357 (91%)	312 (96%)	13 (4%)	1 (0%)	46	72
1	H	327/357 (92%)	312 (95%)	14 (4%)	1 (0%)	46	72
All	All	2603/2856 (91%)	2477 (95%)	116 (4%)	10 (0%)	39	65

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	139	TYR
1	A	350	TYR
1	B	139	TYR
1	C	139	TYR
1	D	139	TYR
1	E	139	TYR
1	F	139	TYR
1	G	139	TYR
1	H	139	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	194	THR

5.3.2 Protein sidechains

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	193/272 (71%)	181 (94%)	12 (6%)	23	45
1	B	225/272 (83%)	211 (94%)	14 (6%)	23	45
1	C	244/272 (90%)	228 (93%)	16 (7%)	21	40
1	D	246/272 (90%)	226 (92%)	20 (8%)	15	28
1	E	238/272 (88%)	223 (94%)	15 (6%)	22	44
1	F	235/272 (86%)	220 (94%)	15 (6%)	22	43
1	G	237/272 (87%)	219 (92%)	18 (8%)	16	32
1	H	247/272 (91%)	230 (93%)	17 (7%)	19	38
All	All	1865/2176 (86%)	1738 (93%)	127 (7%)	20	39

All (127) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	LEU
1	A	52	PHE
1	A	75	ARG
1	A	98	ARG
1	A	103	SER
1	A	105	PHE
1	A	117	ARG
1	A	150	LEU
1	A	188	THR
1	A	203	VAL
1	A	242	LEU
1	A	270	THR
1	B	2	ASP
1	B	51	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	52	PHE
1	B	87	GLN
1	B	98	ARG
1	B	103	SER
1	B	117	ARG
1	B	150	LEU
1	B	188	THR
1	B	203	VAL
1	B	211	ARG
1	B	242	LEU
1	B	270	THR
1	B	284	ARG
1	C	2	ASP
1	C	51	LEU
1	C	52	PHE
1	C	98	ARG
1	C	103	SER
1	C	117	ARG
1	C	150	LEU
1	C	188	THR
1	C	193	ARG
1	C	203	VAL
1	C	211	ARG
1	C	242	LEU
1	C	270	THR
1	C	284	ARG
1	C	291	LYS
1	C	345	ARG
1	D	2	ASP
1	D	24	ARG
1	D	51	LEU
1	D	52	PHE
1	D	87	GLN
1	D	98	ARG
1	D	103	SER
1	D	117	ARG
1	D	150	LEU
1	D	187	GLU
1	D	188	THR
1	D	203	VAL
1	D	213	THR
1	D	242	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	243	ASP
1	D	270	THR
1	D	284	ARG
1	D	291	LYS
1	D	299	GLN
1	D	345	ARG
1	E	2	ASP
1	E	51	LEU
1	E	52	PHE
1	E	98	ARG
1	E	103	SER
1	E	117	ARG
1	E	150	LEU
1	E	188	THR
1	E	193	ARG
1	E	203	VAL
1	E	211	ARG
1	E	242	LEU
1	E	270	THR
1	E	334	ILE
1	E	345	ARG
1	F	2	ASP
1	F	51	LEU
1	F	52	PHE
1	F	87	GLN
1	F	98	ARG
1	F	103	SER
1	F	117	ARG
1	F	150	LEU
1	F	188	THR
1	F	203	VAL
1	F	211	ARG
1	F	235	ILE
1	F	242	LEU
1	F	270	THR
1	F	284	ARG
1	G	2	ASP
1	G	51	LEU
1	G	52	PHE
1	G	69	GLN
1	G	87	GLN
1	G	98	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	103	SER
1	G	117	ARG
1	G	150	LEU
1	G	188	THR
1	G	193	ARG
1	G	203	VAL
1	G	211	ARG
1	G	242	LEU
1	G	253	VAL
1	G	270	THR
1	G	284	ARG
1	G	291	LYS
1	H	2	ASP
1	H	51	LEU
1	H	52	PHE
1	H	69	GLN
1	H	87	GLN
1	H	98	ARG
1	H	103	SER
1	H	117	ARG
1	H	122	ARG
1	H	150	LEU
1	H	188	THR
1	H	203	VAL
1	H	211	ARG
1	H	242	LEU
1	H	270	THR
1	H	284	ARG
1	H	345	ARG

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	149	GLN
1	A	326	ASN
1	B	118	GLN
1	B	149	GLN
1	B	301	GLN
1	B	326	ASN
1	C	118	GLN
1	C	149	GLN
1	C	301	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	326	ASN
1	D	118	GLN
1	D	149	GLN
1	D	299	GLN
1	D	301	GLN
1	D	326	ASN
1	E	118	GLN
1	E	149	GLN
1	E	301	GLN
1	E	326	ASN
1	F	87	GLN
1	F	149	GLN
1	F	301	GLN
1	F	326	ASN
1	G	149	GLN
1	G	301	GLN
1	G	326	ASN
1	H	87	GLN
1	H	118	GLN
1	H	149	GLN
1	H	299	GLN
1	H	301	GLN
1	H	326	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

41 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	$\#\|Z\| > 2$
2	FAD	A	1353	-	48,58,58	1.83	9 (18%)	54,89,89	2.00	13 (24%)
3	SO4	A	1354	-	4,4,4	0.41	0	6,6,6	0.84	0
3	SO4	A	1355	-	4,4,4	0.54	0	6,6,6	0.16	0
3	SO4	A	1356	-	4,4,4	0.66	0	6,6,6	0.61	0
2	FAD	B	1353	-	48,58,58	1.73	12 (25%)	54,89,89	2.71	17 (31%)
3	SO4	B	1354	-	4,4,4	0.44	0	6,6,6	0.54	0
3	SO4	B	1355	-	4,4,4	0.63	0	6,6,6	0.32	0
3	SO4	B	1356	-	4,4,4	0.66	0	6,6,6	0.61	0
3	SO4	B	1357	-	4,4,4	0.41	0	6,6,6	0.18	0
2	FAD	C	1353	-	48,58,58	1.72	7 (14%)	54,89,89	2.44	17 (31%)
3	SO4	C	1354	-	4,4,4	0.53	0	6,6,6	0.45	0
3	SO4	C	1355	-	4,4,4	0.51	0	6,6,6	0.27	0
3	SO4	C	1356	-	4,4,4	0.42	0	6,6,6	0.27	0
3	SO4	C	1357	-	4,4,4	0.65	0	6,6,6	0.57	0
3	SO4	C	1358	-	4,4,4	0.59	0	6,6,6	0.38	0
2	FAD	D	1353	-	48,58,58	1.50	8 (16%)	54,89,89	2.81	22 (40%)
3	SO4	D	1354	-	4,4,4	0.57	0	6,6,6	0.38	0
3	SO4	D	1355	-	4,4,4	0.66	0	6,6,6	0.21	0
3	SO4	D	1356	-	4,4,4	0.57	0	6,6,6	0.15	0
3	SO4	D	1357	-	4,4,4	0.81	0	6,6,6	0.33	0
3	SO4	D	1358	-	4,4,4	0.42	0	6,6,6	0.18	0
3	SO4	D	1359	-	4,4,4	0.33	0	6,6,6	0.84	0
2	FAD	E	1353	-	48,58,58	1.77	12 (25%)	54,89,89	2.68	12 (22%)
3	SO4	E	1354	-	4,4,4	0.92	0	6,6,6	0.49	0
3	SO4	E	1355	-	4,4,4	0.74	0	6,6,6	0.53	0
3	SO4	E	1356	-	4,4,4	0.76	0	6,6,6	0.97	0
2	FAD	F	1353	-	48,58,58	1.72	11 (22%)	54,89,89	2.61	19 (35%)
3	SO4	F	1354	-	4,4,4	0.43	0	6,6,6	0.69	0
3	SO4	F	1355	-	4,4,4	0.46	0	6,6,6	0.48	0
3	SO4	F	1356	-	4,4,4	0.61	0	6,6,6	0.55	0
3	SO4	F	1357	-	4,4,4	0.57	0	6,6,6	0.67	0
2	FAD	G	1353	-	48,58,58	1.60	10 (20%)	54,89,89	2.50	15 (27%)
3	SO4	G	1354	-	4,4,4	0.27	0	6,6,6	0.24	0
3	SO4	G	1355	-	4,4,4	0.51	0	6,6,6	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	SO4	G	1356	-	4,4,4	0.74	0	6,6,6	0.68	0
3	SO4	G	1357	-	4,4,4	0.69	0	6,6,6	0.38	0
2	FAD	H	1353	-	48,58,58	1.78	11 (22%)	54,89,89	2.56	16 (29%)
3	SO4	H	1354	-	4,4,4	0.71	0	6,6,6	0.70	0
3	SO4	H	1355	-	4,4,4	0.53	0	6,6,6	0.37	0
3	SO4	H	1356	-	4,4,4	0.47	0	6,6,6	0.16	0
3	SO4	H	1357	-	4,4,4	0.42	0	6,6,6	0.95	1 (16%)

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	1353	-	-	0/30/50/50	0/6/6/6
3	SO4	A	1354	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1355	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1356	-	-	0/0/0/0	0/0/0/0
2	FAD	B	1353	-	-	0/30/50/50	0/6/6/6
3	SO4	B	1354	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1355	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1356	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1357	-	-	0/0/0/0	0/0/0/0
2	FAD	C	1353	-	-	0/30/50/50	0/6/6/6
3	SO4	C	1354	-	-	0/0/0/0	0/0/0/0
3	SO4	C	1355	-	-	0/0/0/0	0/0/0/0
3	SO4	C	1356	-	-	0/0/0/0	0/0/0/0
3	SO4	C	1357	-	-	0/0/0/0	0/0/0/0
3	SO4	C	1358	-	-	0/0/0/0	0/0/0/0
2	FAD	D	1353	-	-	0/30/50/50	0/6/6/6
3	SO4	D	1354	-	-	0/0/0/0	0/0/0/0
3	SO4	D	1355	-	-	0/0/0/0	0/0/0/0
3	SO4	D	1356	-	-	0/0/0/0	0/0/0/0
3	SO4	D	1357	-	-	0/0/0/0	0/0/0/0
3	SO4	D	1358	-	-	0/0/0/0	0/0/0/0
3	SO4	D	1359	-	-	0/0/0/0	0/0/0/0
2	FAD	E	1353	-	-	0/30/50/50	0/6/6/6
3	SO4	E	1354	-	-	0/0/0/0	0/0/0/0
3	SO4	E	1355	-	-	0/0/0/0	0/0/0/0
3	SO4	E	1356	-	-	0/0/0/0	0/0/0/0
2	FAD	F	1353	-	-	0/30/50/50	0/6/6/6
3	SO4	F	1354	-	-	0/0/0/0	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	F	1355	-	-	0/0/0/0	0/0/0/0
3	SO4	F	1356	-	-	0/0/0/0	0/0/0/0
3	SO4	F	1357	-	-	0/0/0/0	0/0/0/0
2	FAD	G	1353	-	-	0/30/50/50	0/6/6/6
3	SO4	G	1354	-	-	0/0/0/0	0/0/0/0
3	SO4	G	1355	-	-	0/0/0/0	0/0/0/0
3	SO4	G	1356	-	-	0/0/0/0	0/0/0/0
3	SO4	G	1357	-	-	0/0/0/0	0/0/0/0
2	FAD	H	1353	-	-	0/30/50/50	0/6/6/6
3	SO4	H	1354	-	-	0/0/0/0	0/0/0/0
3	SO4	H	1355	-	-	0/0/0/0	0/0/0/0
3	SO4	H	1356	-	-	0/0/0/0	0/0/0/0
3	SO4	H	1357	-	-	0/0/0/0	0/0/0/0

All (80) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1353	FAD	C1'-N10	-5.27	1.42	1.48
2	H	1353	FAD	C4'-C3'	-2.89	1.47	1.53
2	E	1353	FAD	C1'-N10	-2.85	1.45	1.48
2	B	1353	FAD	C1'-N10	-2.78	1.45	1.48
2	B	1353	FAD	C6-C5X	-2.74	1.37	1.41
2	G	1353	FAD	C5A-N7A	-2.64	1.30	1.39
2	D	1353	FAD	O5B-C5B	-2.62	1.34	1.44
2	E	1353	FAD	C5A-N7A	-2.53	1.30	1.39
2	E	1353	FAD	PA-O2A	-2.50	1.44	1.54
2	B	1353	FAD	O5B-C5B	-2.48	1.34	1.44
2	H	1353	FAD	O4B-C4B	-2.47	1.39	1.45
2	E	1353	FAD	C4'-C3'	-2.23	1.48	1.53
2	B	1353	FAD	C4'-C3'	-2.19	1.49	1.53
2	F	1353	FAD	O4-C4	2.00	1.29	1.24
2	G	1353	FAD	C5'-C4'	2.04	1.54	1.51
2	B	1353	FAD	C2A-N3A	2.05	1.35	1.32
2	F	1353	FAD	C2A-N3A	2.07	1.35	1.32
2	D	1353	FAD	C10-N10	2.19	1.41	1.39
2	E	1353	FAD	O4-C4	2.22	1.30	1.24
2	F	1353	FAD	C8-C7	2.25	1.47	1.41
2	G	1353	FAD	C5A-C4A	2.25	1.45	1.40
2	B	1353	FAD	O4B-C1B	2.29	1.44	1.41
2	G	1353	FAD	O4B-C1B	2.32	1.44	1.41
2	E	1353	FAD	C2A-N3A	2.33	1.36	1.32
2	H	1353	FAD	O4-C4	2.38	1.30	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1353	FAD	C4-C4X	2.43	1.46	1.41
2	A	1353	FAD	C9A-N10	2.43	1.42	1.38
2	A	1353	FAD	O4B-C1B	2.44	1.44	1.41
2	G	1353	FAD	C4X-N5	2.46	1.37	1.33
2	B	1353	FAD	O4-C4	2.47	1.30	1.24
2	C	1353	FAD	C8A-N7A	2.62	1.39	1.34
2	A	1353	FAD	C2A-N3A	2.69	1.36	1.32
2	F	1353	FAD	C9A-N10	2.73	1.42	1.38
2	E	1353	FAD	C9A-C5X	2.73	1.48	1.42
2	F	1353	FAD	C4-N3	2.76	1.38	1.33
2	F	1353	FAD	C8A-N7A	2.76	1.39	1.34
2	H	1353	FAD	C5A-C4A	2.78	1.46	1.40
2	E	1353	FAD	C5A-C4A	2.82	1.46	1.40
2	H	1353	FAD	C8-C7	2.84	1.48	1.41
2	H	1353	FAD	C4X-C10	2.92	1.46	1.41
2	H	1353	FAD	C9A-N10	2.94	1.42	1.38
2	D	1353	FAD	C8-C7	3.01	1.49	1.41
2	F	1353	FAD	C9A-C5X	3.02	1.48	1.42
2	D	1353	FAD	C5A-C4A	3.03	1.47	1.40
2	E	1353	FAD	C8-C7	3.09	1.49	1.41
2	G	1353	FAD	C9A-N10	3.10	1.43	1.38
2	H	1353	FAD	O4B-C1B	3.18	1.45	1.41
2	F	1353	FAD	C5A-C4A	3.21	1.47	1.40
2	D	1353	FAD	C9A-N10	3.23	1.43	1.38
2	B	1353	FAD	C8-C7	3.32	1.49	1.41
2	G	1353	FAD	C4X-C10	3.35	1.47	1.41
2	E	1353	FAD	C4-C4X	3.38	1.48	1.41
2	C	1353	FAD	C8-C7	3.40	1.50	1.41
2	A	1353	FAD	C5A-C4A	3.46	1.48	1.40
2	C	1353	FAD	O4B-C1B	3.47	1.45	1.41
2	D	1353	FAD	C4X-C10	3.52	1.47	1.41
2	A	1353	FAD	C10-N10	3.55	1.43	1.39
2	B	1353	FAD	C5A-C4A	3.59	1.48	1.40
2	E	1353	FAD	C4X-C10	3.60	1.47	1.41
2	A	1353	FAD	C8-C7	3.63	1.50	1.41
2	H	1353	FAD	C9A-C5X	3.68	1.50	1.42
2	F	1353	FAD	C4-C4X	3.76	1.48	1.41
2	B	1353	FAD	C9A-C5X	3.81	1.50	1.42
2	G	1353	FAD	C4-C4X	3.88	1.49	1.41
2	D	1353	FAD	C9A-C5X	3.90	1.50	1.42
2	C	1353	FAD	C9A-C5X	3.92	1.50	1.42
2	C	1353	FAD	C4X-C10	4.04	1.48	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1353	FAD	C4-C4X	4.13	1.49	1.41
2	C	1353	FAD	C5A-C4A	4.20	1.50	1.40
2	A	1353	FAD	C4X-C10	4.20	1.48	1.41
2	G	1353	FAD	C8-C7	4.29	1.52	1.41
2	G	1353	FAD	C9A-C5X	4.43	1.51	1.42
2	F	1353	FAD	C4X-C10	4.50	1.49	1.41
2	B	1353	FAD	C4X-C10	4.58	1.49	1.41
2	H	1353	FAD	C4-C4X	4.76	1.50	1.41
2	A	1353	FAD	C4-C4X	4.90	1.51	1.41
2	F	1353	FAD	O4B-C1B	5.21	1.47	1.41
2	C	1353	FAD	C4-C4X	5.25	1.51	1.41
2	A	1353	FAD	C9A-C5X	5.27	1.53	1.42
2	E	1353	FAD	O4B-C1B	5.48	1.48	1.41

All (132) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1353	FAD	N3A-C2A-N1A	-9.33	121.75	128.89
2	F	1353	FAD	C4B-O4B-C1B	-8.10	100.82	109.72
2	H	1353	FAD	C4B-O4B-C1B	-8.09	100.83	109.72
2	H	1353	FAD	N3A-C2A-N1A	-8.07	122.71	128.89
2	A	1353	FAD	N3A-C2A-N1A	-7.94	122.81	128.89
2	G	1353	FAD	N3A-C2A-N1A	-7.91	122.84	128.89
2	B	1353	FAD	N3A-C2A-N1A	-7.87	122.87	128.89
2	E	1353	FAD	N3A-C2A-N1A	-7.79	122.93	128.89
2	E	1353	FAD	C4B-O4B-C1B	-7.70	101.25	109.72
2	B	1353	FAD	C4B-O4B-C1B	-7.41	101.57	109.72
2	C	1353	FAD	N3A-C2A-N1A	-7.04	123.50	128.89
2	G	1353	FAD	C4-C4X-C10	-6.63	115.70	119.94
2	B	1353	FAD	C4X-C4-N3	-6.54	114.65	123.59
2	C	1353	FAD	C4B-O4B-C1B	-6.36	102.73	109.72
2	E	1353	FAD	C4X-C4-N3	-6.02	115.36	123.59
2	F	1353	FAD	N3A-C2A-N1A	-5.49	124.69	128.89
2	D	1353	FAD	C4B-O4B-C1B	-5.29	103.91	109.72
2	B	1353	FAD	C2B-C1B-N9A	-5.22	106.32	114.29
2	F	1353	FAD	C4X-C4-N3	-5.04	116.69	123.59
2	H	1353	FAD	C4X-C4-N3	-4.79	117.04	123.59
2	G	1353	FAD	C4B-O4B-C1B	-4.79	104.46	109.72
2	C	1353	FAD	C4X-C4-N3	-4.76	117.08	123.59
2	F	1353	FAD	C4-C4X-C10	-4.45	117.10	119.94
2	A	1353	FAD	O3P-P-O5'	-4.16	91.90	102.94
2	D	1353	FAD	P-O3P-PA	-3.94	121.68	132.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1353	FAD	C4X-C4-N3	-3.92	118.22	123.59
2	H	1353	FAD	C2B-C1B-N9A	-3.92	108.30	114.29
2	D	1353	FAD	C2B-C1B-N9A	-3.89	108.35	114.29
2	D	1353	FAD	C4-C4X-C10	-3.87	117.46	119.94
2	E	1353	FAD	C4A-C5A-N7A	-3.80	105.98	109.48
2	G	1353	FAD	P-O3P-PA	-3.63	122.54	132.73
2	D	1353	FAD	C1B-N9A-C4A	-3.31	121.95	126.94
2	C	1353	FAD	C4A-C5A-N7A	-3.21	106.53	109.48
2	F	1353	FAD	O3P-PA-O5B	-3.19	94.48	102.94
2	G	1353	FAD	O3'-C3'-C2'	-3.18	100.73	108.75
2	H	1353	FAD	P-O3P-PA	-3.13	123.93	132.73
2	G	1353	FAD	O3P-PA-O5B	-3.08	94.77	102.94
2	A	1353	FAD	C4-C4X-C10	-3.06	117.98	119.94
2	B	1353	FAD	O3P-PA-O5B	-3.01	94.95	102.94
2	F	1353	FAD	C4A-C5A-N7A	-2.95	106.77	109.48
2	A	1353	FAD	C4X-C4-N3	-2.85	119.69	123.59
2	F	1353	FAD	O2A-PA-O5B	-2.85	94.11	108.46
2	B	1353	FAD	O3'-C3'-C4'	-2.82	101.64	108.75
2	F	1353	FAD	P-O3P-PA	-2.80	124.87	132.73
2	G	1353	FAD	C2B-C1B-N9A	-2.75	110.10	114.29
2	B	1353	FAD	C1'-C2'-C3'	-2.74	101.98	109.82
2	C	1353	FAD	C4-C4X-C10	-2.72	118.20	119.94
2	D	1353	FAD	C1'-C2'-C3'	-2.66	102.21	109.82
2	A	1353	FAD	O5B-PA-O1A	-2.60	99.54	109.62
2	D	1353	FAD	O3B-C3B-C4B	-2.55	103.42	111.05
2	D	1353	FAD	C4A-C5A-N7A	-2.52	107.16	109.48
2	A	1353	FAD	C4A-C5A-N7A	-2.49	107.19	109.48
2	B	1353	FAD	C4A-C5A-N7A	-2.46	107.22	109.48
2	G	1353	FAD	C4X-C4-N3	-2.45	120.23	123.59
2	E	1353	FAD	O4'-C4'-C5'	-2.45	104.86	110.19
2	H	1353	FAD	O2A-PA-O5B	-2.41	96.29	108.46
2	H	1353	FAD	C4A-C5A-N7A	-2.40	107.27	109.48
2	D	1353	FAD	O3P-PA-O5B	-2.40	96.57	102.94
2	B	1353	FAD	O2'-C2'-C1'	-2.38	104.08	109.94
2	B	1353	FAD	P-O3P-PA	-2.36	126.10	132.73
2	E	1353	FAD	P-O3P-PA	-2.35	126.13	132.73
2	D	1353	FAD	O4'-C4'-C3'	-2.33	103.15	109.02
2	H	1353	FAD	C9A-C5X-N5	-2.26	119.02	122.36
2	A	1353	FAD	C4B-O4B-C1B	-2.22	107.28	109.72
2	A	1353	FAD	P-O3P-PA	-2.13	126.74	132.73
2	C	1353	FAD	O2'-C2'-C1'	-2.12	104.72	109.94
2	D	1353	FAD	O2'-C2'-C1'	-2.05	104.91	109.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1353	FAD	P-O3P-PA	-2.02	127.05	132.73
3	H	1357	SO4	O4-S-O3	-2.00	100.84	108.98
2	A	1353	FAD	C4-C4X-N5	2.00	121.15	118.72
2	F	1353	FAD	O5'-P-O1P	2.05	117.57	109.62
2	B	1353	FAD	O4B-C4B-C3B	2.05	109.29	105.15
2	D	1353	FAD	C6-C5X-C9A	2.09	121.73	118.98
2	C	1353	FAD	O5B-PA-O1A	2.11	117.80	109.62
2	F	1353	FAD	C4X-N5-C5X	2.11	119.19	116.76
2	F	1353	FAD	C5X-C9A-N10	2.13	119.23	117.62
2	H	1353	FAD	C4X-C10-N10	2.19	121.81	120.52
2	C	1353	FAD	C4X-N5-C5X	2.19	119.28	116.76
2	H	1353	FAD	O5B-C5B-C4B	2.22	117.31	109.12
2	E	1353	FAD	C1'-N10-C9A	2.23	121.36	118.86
2	D	1353	FAD	O2'-C2'-C3'	2.39	115.02	109.02
2	C	1353	FAD	C4-C4X-N5	2.43	121.67	118.72
2	F	1353	FAD	O2P-P-O3P	2.44	116.17	105.09
2	F	1353	FAD	O3'-C3'-C4'	2.51	115.08	108.75
2	B	1353	FAD	C4X-N5-C5X	2.52	119.66	116.76
2	B	1353	FAD	O4B-C4B-C5B	2.53	118.36	109.32
2	G	1353	FAD	O2P-P-O3P	2.55	116.67	105.09
2	F	1353	FAD	O2'-C2'-C3'	2.59	115.53	109.02
2	A	1353	FAD	O5B-C5B-C4B	2.65	118.89	109.12
2	H	1353	FAD	O2B-C2B-C3B	2.68	120.54	111.83
2	F	1353	FAD	O4B-C4B-C5B	2.70	118.98	109.32
2	G	1353	FAD	C4-C4X-N5	2.78	122.09	118.72
2	C	1353	FAD	C5X-C9A-N10	2.96	119.87	117.62
2	D	1353	FAD	C2A-N1A-C6A	2.96	124.06	118.77
2	G	1353	FAD	C4X-N5-C5X	3.08	120.31	116.76
2	H	1353	FAD	O2'-C2'-C3'	3.14	116.92	109.02
2	D	1353	FAD	O4B-C1B-N9A	3.16	114.71	108.10
2	A	1353	FAD	O2'-C2'-C3'	3.18	117.00	109.02
2	G	1353	FAD	O5B-PA-O1A	3.32	122.51	109.62
2	H	1353	FAD	O5B-PA-O1A	3.40	122.81	109.62
2	D	1353	FAD	O5B-PA-O1A	3.42	122.89	109.62
2	D	1353	FAD	O4B-C4B-C5B	3.52	121.90	109.32
2	F	1353	FAD	O5B-PA-O1A	3.54	123.35	109.62
2	E	1353	FAD	C5X-C9A-N10	3.55	120.31	117.62
2	G	1353	FAD	O4B-C1B-N9A	3.67	115.78	108.10
2	H	1353	FAD	C4-N3-C2	3.72	118.47	115.25
2	C	1353	FAD	O2'-C2'-C3'	3.85	118.69	109.02
2	B	1353	FAD	O5B-PA-O1A	3.87	124.62	109.62
2	A	1353	FAD	C4X-C10-N10	3.88	122.81	120.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1353	FAD	O4B-C1B-N9A	3.89	116.24	108.10
2	E	1353	FAD	O4B-C1B-N9A	3.91	116.29	108.10
2	C	1353	FAD	O4B-C1B-N9A	3.92	116.30	108.10
2	C	1353	FAD	O4B-C4B-C5B	3.96	123.47	109.32
2	F	1353	FAD	O4B-C1B-N9A	4.14	116.77	108.10
2	E	1353	FAD	O2'-C2'-C3'	4.16	119.47	109.02
2	A	1353	FAD	C4-N3-C2	4.31	118.97	115.25
2	H	1353	FAD	O4B-C1B-N9A	4.54	117.61	108.10
2	C	1353	FAD	C1'-N10-C9A	4.58	124.00	118.86
2	C	1353	FAD	C4X-C10-N10	4.67	123.27	120.52
2	E	1353	FAD	C4X-N5-C5X	4.96	122.46	116.76
2	D	1353	FAD	C5X-C9A-N10	5.02	121.44	117.62
2	F	1353	FAD	C1'-N10-C9A	5.17	124.67	118.86
2	G	1353	FAD	O2'-C2'-C3'	5.36	122.49	109.02
2	B	1353	FAD	O2'-C2'-C3'	5.39	122.58	109.02
2	C	1353	FAD	C4-N3-C2	5.55	120.04	115.25
2	G	1353	FAD	C4-N3-C2	6.14	120.55	115.25
2	D	1353	FAD	C1'-N10-C9A	6.58	126.25	118.86
2	H	1353	FAD	C4X-N5-C5X	6.63	124.39	116.76
2	D	1353	FAD	C4-N3-C2	7.13	121.41	115.25
2	B	1353	FAD	C4-N3-C2	7.31	121.56	115.25
2	F	1353	FAD	C4-N3-C2	7.72	121.92	115.25
2	E	1353	FAD	C4-N3-C2	8.95	122.98	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

20 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1353	FAD	4	0
3	A	1354	SO4	1	0
2	B	1353	FAD	4	0
3	B	1354	SO4	1	0
3	B	1357	SO4	1	0
3	C	1356	SO4	1	0
2	D	1353	FAD	1	0
3	D	1354	SO4	1	0
3	D	1355	SO4	1	0
3	D	1358	SO4	1	0
2	E	1353	FAD	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	1354	SO4	1	0
3	E	1356	SO4	1	0
3	F	1354	SO4	1	0
3	F	1357	SO4	2	0
2	G	1353	FAD	3	0
3	G	1354	SO4	1	0
3	G	1356	SO4	1	0
2	H	1353	FAD	2	0
3	H	1357	SO4	1	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	327/357 (91%)	0.19	18 (5%) 29 21	40, 79, 111, 127	0
1	B	330/357 (92%)	-0.27	3 (0%) 85 83	31, 65, 95, 135	0
1	C	330/357 (92%)	-0.52	1 (0%) 94 93	26, 45, 69, 86	0
1	D	333/357 (93%)	-0.49	1 (0%) 94 93	25, 46, 74, 94	0
1	E	330/357 (92%)	-0.53	0 100 100	22, 46, 70, 110	0
1	F	330/357 (92%)	-0.38	1 (0%) 94 93	29, 48, 74, 101	0
1	G	330/357 (92%)	-0.49	1 (0%) 94 93	24, 46, 77, 108	0
1	H	331/357 (92%)	-0.60	0 100 100	20, 40, 67, 96	0
All	All	2641/2856 (92%)	-0.39	25 (0%) 85 83	20, 49, 90, 135	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	318	TRP	7.4
1	A	251	ALA	6.4
1	A	304	VAL	4.7
1	A	267	ALA	3.8
1	B	267	ALA	3.6
1	G	351	CYS	3.6
1	A	123	ALA	3.5
1	A	20	TYR	3.5
1	A	119	TRP	3.2
1	A	329	ALA	3.2
1	F	313	ALA	2.9
1	A	340	ALA	2.8
1	A	295	LEU	2.5
1	A	317	VAL	2.5
1	A	315	PRO	2.3
1	D	106	GLY	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	351	CYS	2.2
1	B	140	GLN	2.2
1	A	328	MET	2.2
1	A	200	ALA	2.2
1	A	106	GLY	2.2
1	B	251	ALA	2.0
1	A	111	VAL	2.0
1	A	19	GLY	2.0
1	A	24	ARG	2.0

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

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

6.3 Carbohydrates (i)

There are no 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
3	SO4	D	1356	5/5	0.63	0.40	32.76	145,150,156,159	0
3	SO4	C	1355	5/5	0.83	0.60	30.88	98,122,126,127	0
3	SO4	B	1357	5/5	0.63	0.35	26.57	132,135,144,151	0
3	SO4	E	1355	5/5	0.82	0.31	18.55	93,94,105,111	0
3	SO4	A	1355	5/5	0.71	0.53	17.31	137,139,145,159	0
3	SO4	H	1355	5/5	0.87	0.26	9.79	105,117,124,131	0
3	SO4	B	1355	5/5	0.62	0.39	8.13	112,113,123,131	0
3	SO4	C	1356	5/5	0.95	0.38	6.22	106,114,117,127	0
3	SO4	F	1357	5/5	0.95	0.27	5.53	83,88,97,113	0
3	SO4	D	1355	5/5	0.89	0.20	3.95	86,89,99,100	0
3	SO4	B	1356	5/5	0.74	0.21	0.35	87,90,105,107	0
2	FAD	H	1353	53/53	0.97	0.12	0.01	18,25,30,32	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	SO4	D	1359	5/5	0.97	0.12	-0.17	50,56,58,64	0
2	FAD	F	1353	53/53	0.97	0.12	-0.28	23,29,33,43	0
3	SO4	H	1357	5/5	0.98	0.11	-0.41	42,47,51,54	0
2	FAD	D	1353	53/53	0.97	0.11	-0.49	22,28,36,44	0
2	FAD	E	1353	53/53	0.98	0.11	-0.51	21,26,33,36	0
2	FAD	C	1353	53/53	0.97	0.11	-0.63	23,29,37,38	0
2	FAD	G	1353	53/53	0.97	0.10	-0.78	24,30,34,39	0
2	FAD	A	1353	53/53	0.92	0.13	-0.89	33,48,57,59	0
3	SO4	G	1356	5/5	0.96	0.08	-0.96	54,56,67,75	0
2	FAD	B	1353	53/53	0.97	0.10	-0.97	25,31,39,44	0
3	SO4	E	1356	5/5	0.97	0.10	-1.35	42,50,51,55	0
3	SO4	F	1355	5/5	0.98	0.10	-1.35	46,56,58,68	0
3	SO4	C	1358	5/5	0.98	0.08	-2.02	59,60,68,70	0
3	SO4	A	1356	5/5	0.93	0.09	-2.35	57,66,83,83	0
3	SO4	D	1357	5/5	0.96	0.08	-2.69	58,60,68,69	0
3	SO4	C	1357	5/5	0.80	0.21	-	90,91,104,108	0
3	SO4	G	1357	5/5	0.93	0.11	-	66,73,80,83	0
3	SO4	H	1356	5/5	0.87	0.33	-	123,129,130,138	0
3	SO4	D	1354	5/5	0.99	0.07	-	36,40,49,50	0
3	SO4	F	1354	5/5	0.99	0.08	-	33,36,41,45	0
3	SO4	G	1355	5/5	0.73	0.44	-	132,142,147,158	0
3	SO4	C	1354	5/5	0.99	0.11	-	37,39,40,42	0
3	SO4	E	1354	5/5	0.98	0.12	-	36,42,44,45	0
3	SO4	H	1354	5/5	0.99	0.07	-	34,41,44,45	0
3	SO4	B	1354	5/5	0.98	0.09	-	48,49,59,63	0
3	SO4	G	1354	5/5	0.99	0.09	-	47,48,52,52	0
3	SO4	F	1356	5/5	0.89	0.23	-	76,83,93,111	0
3	SO4	A	1354	5/5	0.97	0.15	-	50,52,61,62	0
3	SO4	D	1358	5/5	0.73	0.34	-	137,141,153,154	0

6.5 Other polymers (i)

There are no such residues in this entry.