



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:33 AM GMT

PDB ID : 3P4S  
Title : Crystal structure of Menaquinol:fumarate oxidoreductase in complex with a 3-nitropropionate adduct  
Authors : Tomasiak, T.M.; Archuleta, T.L.; Andrell, J.; Luna-Chavez, C.; Davis, T.A.; Sarwar, M.; Ham, A.J.; McDonald, W.H.; Yankowskaya, V.; Stern, H.A.; Johnston, J.N.; Maklashina, E.; Cecchini, G.; Iverson, T.M.  
Deposited on : 2010-10-07  
Resolution : 3.10 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](mailto: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 ⓘ](#)) 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

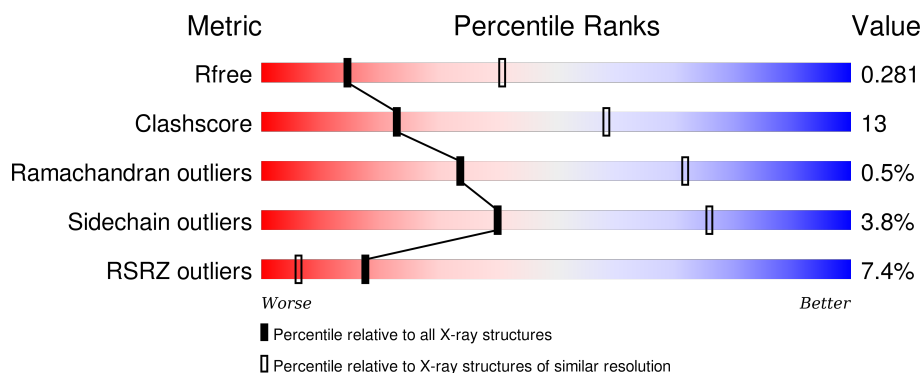
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	577	<div> <div>21%</div> <div>82%17%</div> </div>
1	M	577	<div> <div>21%</div> <div>59%38%</div> </div>
2	B	243	<div> <div>%</div> <div>83%16%</div> </div>
2	N	243	<div> <div>10%</div> <div>74%25%</div> </div>
3	C	130	<div> <div></div> <div>85%14%</div> </div>

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
3	O	130	
4	D	119	
4	P	119	

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
5	FAD	A	601	-	-	-	X
5	FAD	M	601	-	-	-	X
6	3NP	A	602	-	-	-	X
7	FES	N	244	-	-	X	-
8	F3S	B	245	-	-	X	-
8	F3S	N	245	-	-	X	-
9	SF4	B	246	-	-	X	-
9	SF4	N	246	-	-	X	-

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 16792 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 Fumarate reductase flavoprotein subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	577	Total	C	N	O	S	0	0	0
			4449	2775	802	841	31			
1	M	577	Total	C	N	O	S	0	0	0
			4449	2775	802	841	31			

- Molecule 2 is a protein called Fumarate reductase iron-sulfur subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	243	Total	C	N	O	S	0	0	0
			1888	1189	323	357	19			
2	N	243	Total	C	N	O	S	0	0	0
			1888	1189	323	357	19			

- Molecule 3 is a protein called Fumarate reductase subunit C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	130	Total	C	N	O	S	0	0	0
			1058	720	166	169	3			
3	O	130	Total	C	N	O	S	0	0	0
			1058	720	166	169	3			

- Molecule 4 is a protein called Fumarate reductase subunit D.

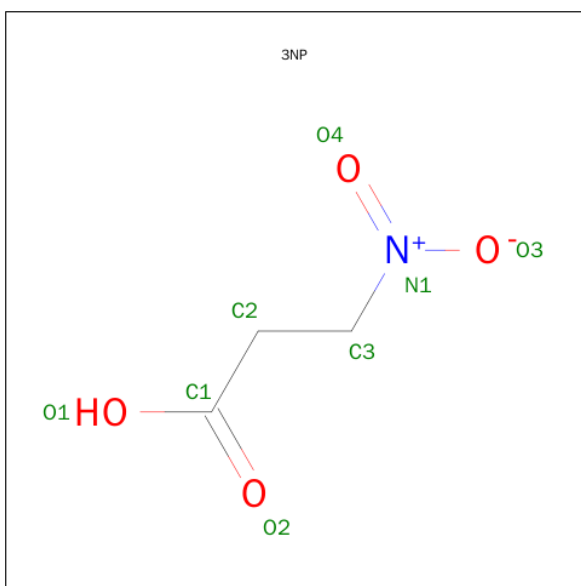
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	119	Total	C	N	O	S	0	0	0
			926	626	151	142	7			
4	P	119	Total	C	N	O	S	0	0	0
			926	626	151	142	7			

- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C<sub>27</sub>H<sub>33</sub>N<sub>9</sub>O<sub>15</sub>P<sub>2</sub>).



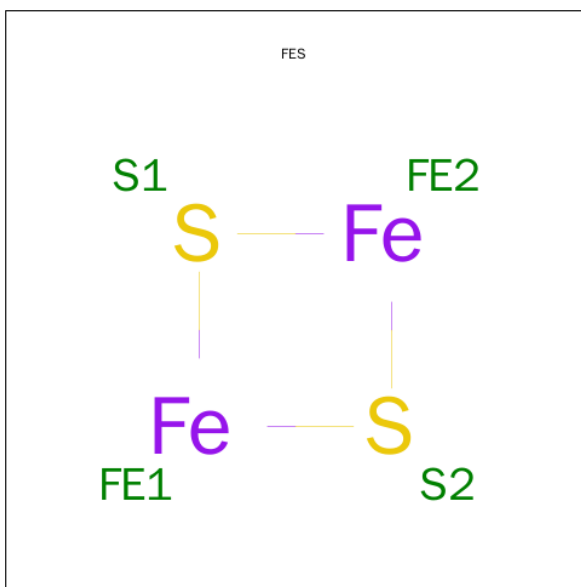
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0
			53	27	9	15	2	
5	M	1	Total	C	N	O	P	0
			53	27	9	15	2	

- Molecule 6 is 3-NITROPROPANOIC ACID (three-letter code: 3NP) (formula:  $C_3H_5NO_4$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			6	3	1	2		

- Molecule 7 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula:  $Fe_2S_2$ ).



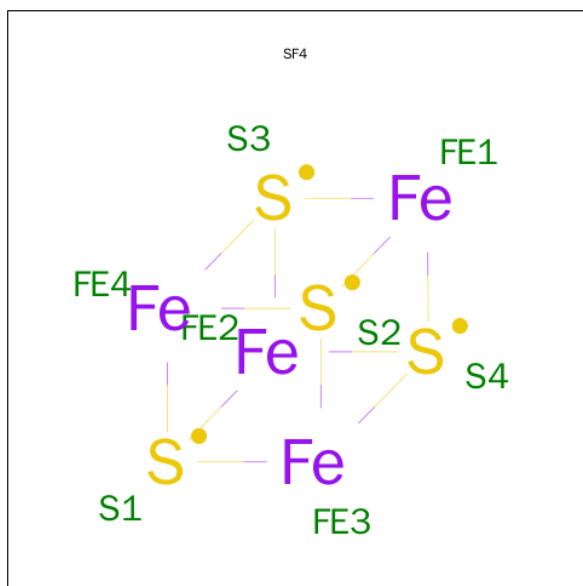
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	Fe	S	0	0
			4	2	2		
7	N	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 8 is FE3-S4 CLUSTER (three-letter code: F3S) (formula:  $\text{Fe}_3\text{S}_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	Fe	S	0	0
			7	3	4		
8	N	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 9 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).

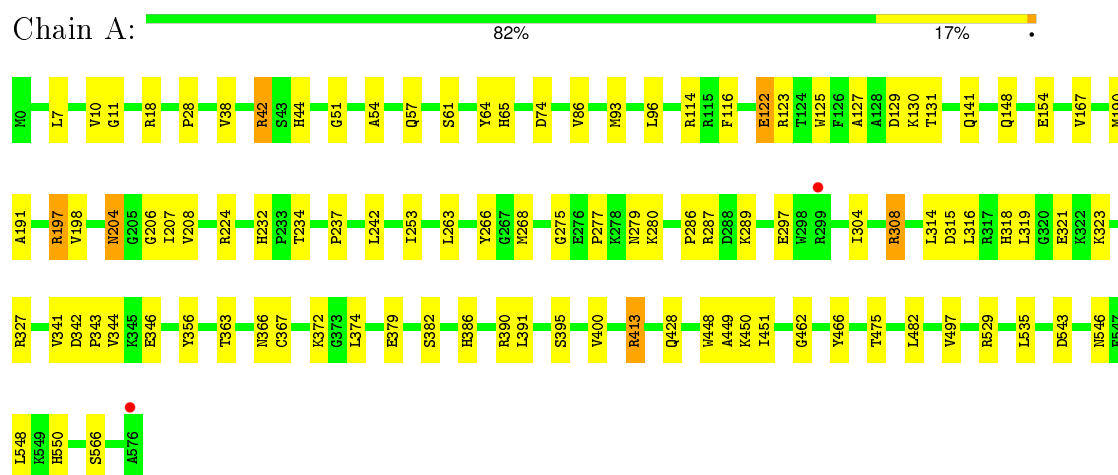


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	Fe	S	0	0
			8	4	4		
9	N	1	Total	Fe	S	0	0
			8	4	4		

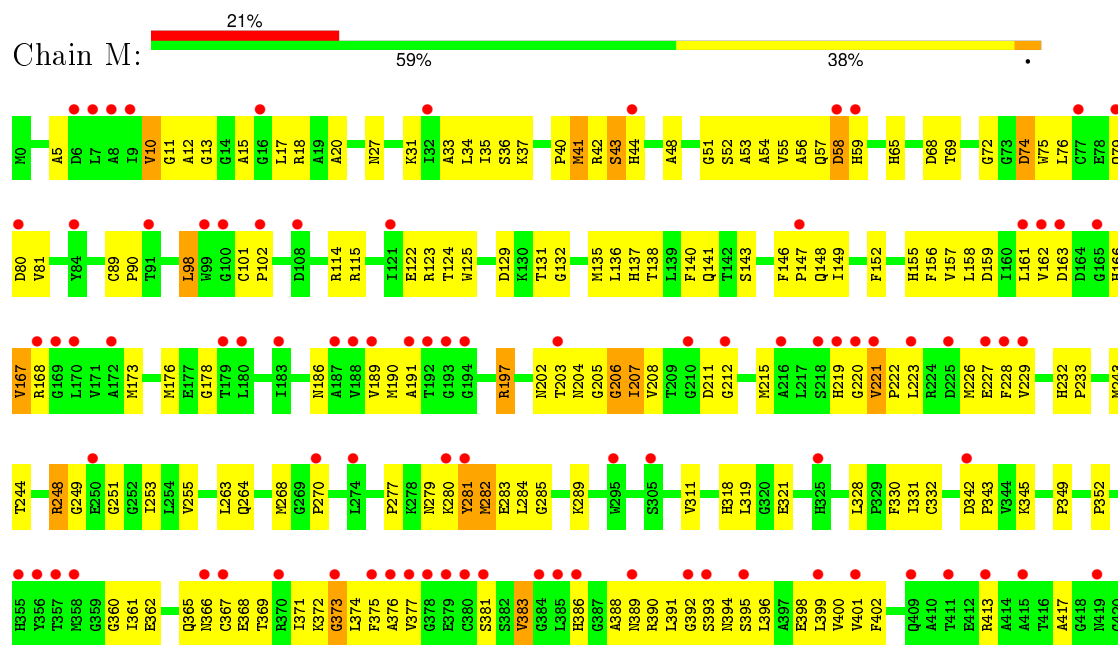
### 3 Residue-property plots

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.

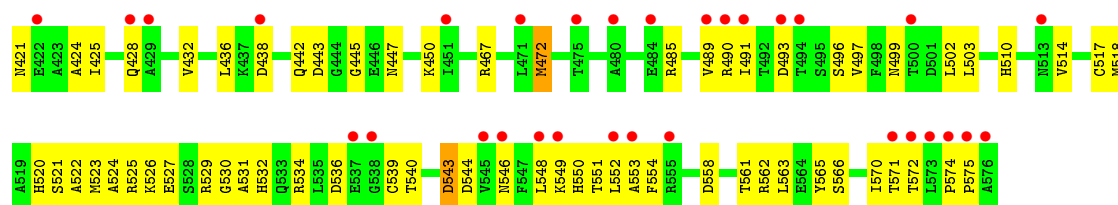
#### • Molecule 1: Fumarate reductase flavoprotein subunit



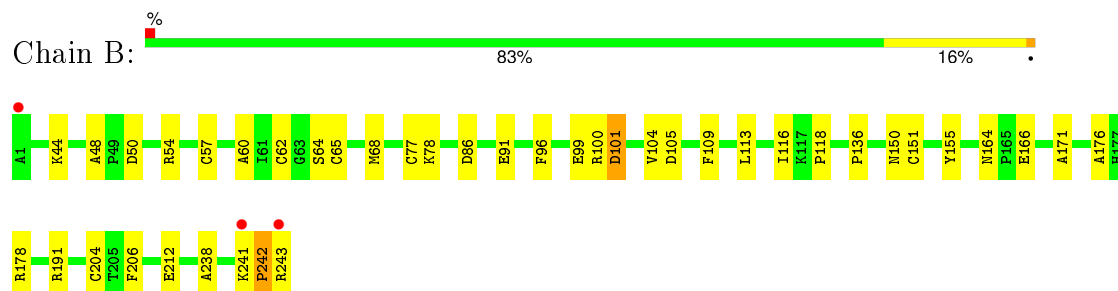
#### • Molecule 1: Fumarate reductase flavoprotein subunit



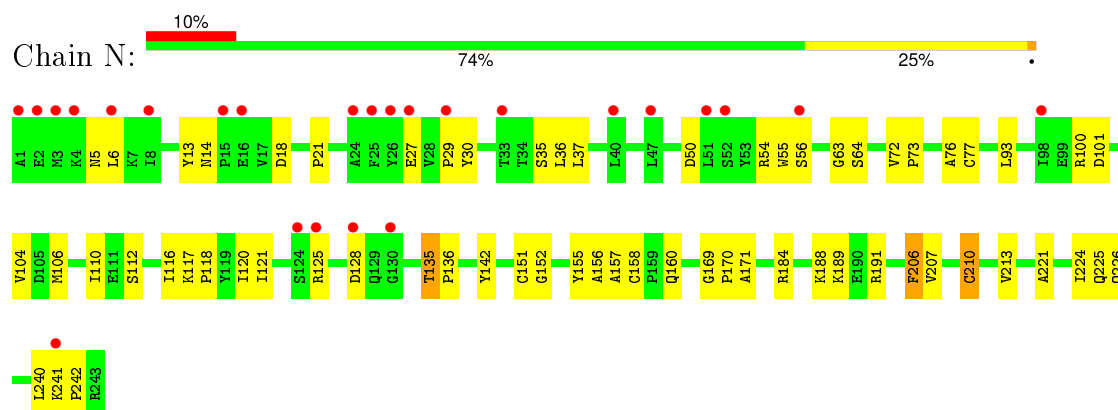




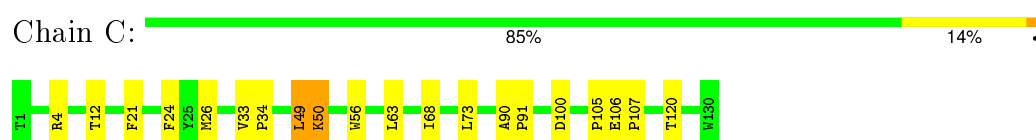
• Molecule 2: Fumarate reductase iron-sulfur subunit



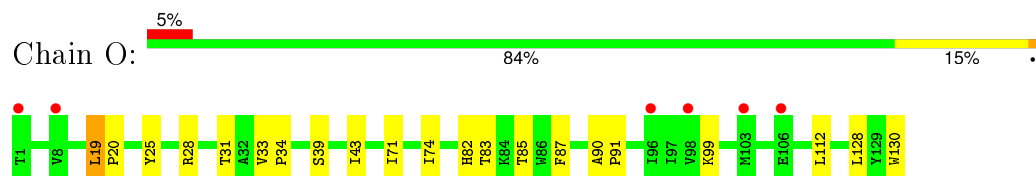
• Molecule 2: Fumarate reductase iron-sulfur subunit



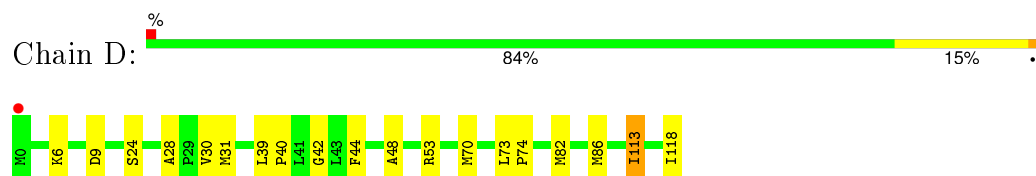
• Molecule 3: Fumarate reductase subunit C




• Molecule 3: Fumarate reductase subunit C



• Molecule 4: Fumarate reductase subunit D



## ● Molecule 4: Fumarate reductase subunit D

Chain P:  % 78% 20% .



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	98.06Å 139.01Å 276.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.10 39.99 – 3.10	Depositor EDS
% Data completeness (in resolution range)	93.5 (40.00-3.10) 92.8 (39.99-3.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.68 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.255 , 0.279 0.254 , 0.281	Depositor DCC
$R_{free}$ test set	1254 reflections (1.98%)	DCC
Wilson B-factor (Å <sup>2</sup> )	73.8	Xtriage
Anisotropy	0.130	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 33.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 68923 reflections	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	16792	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, F3S, FES, 3NP, 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	0.33	0/4541	0.51	2/6139 (0.0%)
1	M	0.35	0/4541	0.53	0/6139
2	B	0.37	0/1931	0.50	0/2617
2	N	0.35	0/1931	0.49	0/2617
3	C	0.34	0/1094	0.44	0/1496
3	O	0.36	0/1094	0.43	0/1496
4	D	0.34	0/956	0.45	0/1303
4	P	0.35	0/956	0.48	0/1303
All	All	0.35	0/17044	0.50	2/23110 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	287	ARG	NE-CZ-NH1	8.67	124.63	120.30
1	A	287	ARG	NH1-CZ-NH2	-5.02	113.88	119.40

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	4449	0	4333	76	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	M	4449	0	4335	238	0
2	B	1888	0	1839	41	0
2	N	1888	0	1839	55	0
3	C	1058	0	1108	12	0
3	O	1058	0	1108	21	0
4	D	926	0	971	11	0
4	P	926	0	971	18	0
5	A	53	0	31	5	0
5	M	53	0	31	20	0
6	A	6	0	2	0	0
7	B	4	0	0	0	0
7	N	4	0	0	2	0
8	B	7	0	0	3	0
8	N	7	0	0	5	0
9	B	8	0	0	4	0
9	N	8	0	0	3	0
All	All	16792	0	16568	449	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 13.

All (449) 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:M:44:HIS:NE2	5:M:601:FAD:HM82	1.50	1.24
1:M:211:ASP:OD1	1:M:510:HIS:CD2	2.04	1.11
2:B:151:CYS:SG	9:B:246:SF4:FE1	1.46	1.06
1:M:115:ARG:HG2	1:M:122:GLU:HB3	1.38	1.03
1:M:219:HIS:HD2	1:M:371:ILE:HD13	1.18	1.02
1:M:227:GLU:HB2	1:M:522:ALA:HB2	1.42	1.02
1:M:219:HIS:CD2	1:M:371:ILE:HD13	1.98	0.98
1:M:129:ASP:OD2	1:M:330:PHE:HB2	1.62	0.98
1:M:44:HIS:NE2	5:M:601:FAD:C8M	2.26	0.98
1:M:158:LEU:HD13	1:M:436:LEU:HG	1.51	0.93
1:M:394:ASN:HB3	5:M:601:FAD:O2	1.67	0.93
2:N:210:CYS:SG	8:N:245:F3S:FE3	1.60	0.92
2:N:5:ASN:HA	2:N:30:TYR:CD2	2.05	0.92
2:B:151:CYS:HG	9:B:246:SF4:FE1	0.74	0.91
2:B:136:PRO:HB2	3:C:100:ASP:OD2	1.71	0.89
1:M:15:ALA:HB2	1:M:399:LEU:HD22	1.55	0.88
2:N:210:CYS:HG	8:N:245:F3S:FE3	0.61	0.88

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:HIS:NE2	5:A:601:FAD:HM82	1.89	0.87
4:D:113:ILE:HG23	4:D:118:ILE:HD11	1.57	0.87
1:M:219:HIS:HD2	1:M:371:ILE:CD1	1.87	0.86
2:N:5:ASN:OD1	2:N:29:PRO:HA	1.75	0.86
2:B:96:PHE:HB3	2:B:104:VAL:CG1	2.07	0.85
1:M:211:ASP:OD1	1:M:510:HIS:HD2	1.60	0.84
1:M:53:ALA:H	1:M:394:ASN:HB2	1.44	0.83
2:B:204:CYS:SG	8:B:245:F3S:FE1	1.70	0.83
1:M:390:ARG:HD2	1:M:395:SER:HB2	1.60	0.83
1:M:11:GLY:HA2	5:M:601:FAD:H1B	1.60	0.82
1:A:286:PRO:HG2	1:A:289:LYS:HG3	1.61	0.82
1:A:390:ARG:HH11	1:A:395:SER:HB2	1.45	0.82
1:M:421:ASN:O	1:M:425:ILE:HG12	1.78	0.82
1:M:253:ILE:HA	1:M:283:GLU:HG2	1.61	0.81
1:M:202:ASN:ND2	1:M:204:ASN:HB2	1.96	0.81
1:M:221:VAL:CG2	1:M:371:ILE:HD12	2.11	0.81
2:N:35:SER:HB3	2:N:77:CYS:HA	1.62	0.81
1:M:12:ALA:HB3	5:M:601:FAD:O3B	1.80	0.80
2:N:5:ASN:HA	2:N:30:TYR:HD2	1.42	0.80
1:M:12:ALA:HB3	5:M:601:FAD:HO3A	1.47	0.80
1:M:129:ASP:HB2	1:M:328:LEU:HA	1.64	0.80
1:M:221:VAL:HG23	1:M:371:ILE:HD12	1.64	0.80
2:B:204:CYS:HG	8:B:245:F3S:FE1	0.53	0.79
1:M:12:ALA:CA	5:M:601:FAD:O3B	2.30	0.79
1:M:227:GLU:CB	1:M:522:ALA:HB2	2.13	0.79
1:M:12:ALA:N	5:M:601:FAD:O3B	2.15	0.79
1:M:205:GLY:HA3	2:N:56:SER:O	1.83	0.78
1:M:11:GLY:HA2	5:M:601:FAD:C1B	2.13	0.78
1:M:219:HIS:CD2	1:M:371:ILE:CD1	2.66	0.78
1:M:65:HIS:CD2	1:M:123:ARG:HD2	2.20	0.77
1:M:383:VAL:HG13	1:M:402:PHE:HE2	1.49	0.77
2:B:96:PHE:HB3	2:B:104:VAL:HG11	1.67	0.76
2:B:65:CYS:SG	2:B:77:CYS:HB2	2.25	0.76
1:M:372:LYS:O	1:M:413:ARG:HG2	1.84	0.76
3:O:87:PHE:CD1	3:O:112:LEU:HB3	2.21	0.75
1:M:211:ASP:HA	1:M:510:HIS:HB2	1.67	0.75
1:A:279:ASN:O	1:A:280:LYS:HG2	1.85	0.75
1:M:521:SER:OG	1:M:551:THR:HB	1.85	0.75
3:C:33:VAL:HB	3:C:34:PRO:HD3	1.69	0.75
1:M:227:GLU:HB2	1:M:522:ALA:CB	2.16	0.74
1:A:18:ARG:HG2	1:A:400:VAL:HA	1.70	0.74

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:151:CYS:HG	9:N:246:SF4:FE1	1.01	0.74
1:M:413:ARG:O	1:M:417:ALA:HB2	1.87	0.74
1:M:48:ALA:HB3	1:M:132:GLY:HA3	1.70	0.73
1:M:79:GLN:HB3	1:M:571:THR:HG22	1.69	0.73
2:N:210:CYS:SG	8:N:245:F3S:S1	2.87	0.73
1:M:57:GLN:O	1:M:58:ASP:HB2	1.86	0.72
1:M:168:ARG:HG3	1:M:425:ILE:HG13	1.71	0.72
1:M:53:ALA:HB3	1:M:394:ASN:H	1.55	0.72
3:O:83:THR:O	3:O:87:PHE:CD2	2.44	0.71
2:N:221:ALA:O	2:N:225:GLN:HG2	1.91	0.71
1:M:229:VAL:O	1:M:531:ALA:HB1	1.91	0.71
1:M:226:MET:HG3	1:M:517:CYS:HB3	1.72	0.71
1:M:191:ALA:HB2	1:M:377:VAL:HG13	1.71	0.71
1:A:390:ARG:HH11	1:A:395:SER:CB	2.03	0.71
3:O:83:THR:O	3:O:87:PHE:HD2	1.74	0.70
1:A:390:ARG:NH1	1:A:395:SER:CB	2.54	0.70
1:M:114:ARG:HH12	1:M:328:LEU:HD21	1.57	0.70
1:M:115:ARG:CG	1:M:122:GLU:HB3	2.18	0.69
3:O:33:VAL:HB	3:O:34:PRO:HD3	1.74	0.69
1:M:159:ASP:HB3	1:M:432:VAL:HG23	1.74	0.69
3:O:31:THR:HG21	3:O:82:HIS:HB2	1.74	0.69
1:A:390:ARG:NH1	1:A:395:SER:HB2	2.08	0.69
1:M:80:ASP:HB3	1:M:365:GLN:OE1	1.93	0.69
1:M:251:GLY:HA2	1:M:277:PRO:HG2	1.74	0.68
1:M:161:LEU:O	1:M:167:VAL:HG23	1.91	0.68
1:M:12:ALA:CB	5:M:601:FAD:O3B	2.40	0.68
1:M:163:ASP:HB2	1:M:425:ILE:HD11	1.75	0.68
1:M:114:ARG:O	1:M:124:THR:HB	1.93	0.68
1:M:55:VAL:HB	1:M:90:PRO:HG3	1.76	0.68
1:M:20:ALA:HB2	1:M:34:LEU:HD11	1.76	0.67
1:M:20:ALA:CB	1:M:34:LEU:HD11	2.24	0.67
2:N:37:LEU:HD22	2:N:77:CYS:HA	1.76	0.67
2:N:112:SER:O	2:N:116:ILE:HG12	1.95	0.67
1:M:42:ARG:O	1:M:43:SER:HB2	1.93	0.66
1:M:5:ALA:HA	1:M:31:LYS:HD2	1.76	0.66
7:N:244:FES:FE2	7:N:244:FES:S1	1.86	0.66
1:M:159:ASP:HB3	1:M:432:VAL:CG2	2.24	0.66
3:C:91:PRO:HB2	3:C:105:PRO:HB3	1.76	0.66
1:A:386:HIS:ND1	1:A:390:ARG:HG3	2.10	0.66
1:M:280:LYS:HA	1:M:285:GLY:HA2	1.76	0.65
2:B:96:PHE:CB	2:B:104:VAL:HG11	2.25	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:87:PHE:CE1	3:O:112:LEU:HB3	2.31	0.65
2:B:96:PHE:HB3	2:B:104:VAL:HG13	1.77	0.65
1:A:65:HIS:ND1	1:A:86:VAL:HG12	2.12	0.65
1:M:264:GLN:HE22	1:M:270:PRO:HA	1.61	0.65
1:A:242:LEU:HD22	5:A:601:FAD:HM73	1.79	0.64
1:A:44:HIS:NE2	5:A:601:FAD:C8M	2.59	0.64
2:N:151:CYS:SG	9:N:246:SF4:FE1	1.90	0.64
1:M:493:ASP:OD2	2:N:50:ASP:HA	1.98	0.64
3:O:87:PHE:CD1	3:O:112:LEU:CB	2.81	0.63
1:A:42:ARG:HG2	2:B:64:SER:HB3	1.80	0.63
1:M:543:ASP:HB3	1:M:546:ASN:HB2	1.80	0.62
1:M:227:GLU:HA	1:M:518:MET:O	1.99	0.62
2:N:14:ASN:H	2:N:18:ASP:HB2	1.64	0.62
1:M:68:ASP:O	1:M:391:LEU:CD2	2.47	0.62
2:B:151:CYS:SG	9:B:246:SF4:S2	2.97	0.62
1:M:140:PHE:O	1:M:143:SER:HB3	1.99	0.62
1:M:398:GLU:O	1:M:402:PHE:HB3	1.99	0.62
2:B:44:LYS:HA	2:B:48:ALA:O	2.00	0.62
4:P:6:LYS:H	4:P:6:LYS:HD3	1.64	0.62
1:M:208:VAL:O	1:M:208:VAL:HG12	1.99	0.61
1:M:526:LYS:HB3	1:M:539:CYS:SG	2.40	0.61
1:M:342:ASP:HB3	1:M:345:LYS:HB3	1.81	0.61
2:N:63:GLY:N	7:N:244:FES:S1	2.69	0.61
1:A:141:GLN:HB3	2:B:118:PRO:O	2.01	0.61
1:M:162:VAL:CG2	1:M:219:HIS:HE1	2.13	0.61
1:M:221:VAL:HG11	1:M:369:THR:HB	1.82	0.61
1:A:315:ASP:HB3	1:A:318:HIS:HE1	1.64	0.61
1:M:233:PRO:HG2	1:M:248:ARG:HH22	1.66	0.61
1:M:101:CYS:HB2	1:M:138:THR:HG21	1.83	0.60
3:O:87:PHE:HD1	3:O:112:LEU:CB	2.15	0.60
3:O:87:PHE:HD1	3:O:112:LEU:HB2	1.67	0.60
2:N:37:LEU:HD12	2:N:55:TRP:HB2	1.84	0.60
1:M:98:LEU:HD11	2:N:125:ARG:HD3	1.84	0.59
3:C:90:ALA:N	3:C:91:PRO:HD2	2.17	0.59
4:D:48:ALA:O	4:D:53:ARG:HD3	2.02	0.59
1:M:215:MET:HG3	1:M:510:HIS:CE1	2.37	0.59
1:A:129:ASP:OD1	1:A:130:LYS:HG2	2.01	0.59
1:A:51:GLY:HA2	1:A:131:THR:HG21	1.83	0.59
1:M:72:GLY:HA3	1:M:391:LEU:HD21	1.84	0.59
1:M:72:GLY:CA	1:M:391:LEU:HD21	2.33	0.59
1:M:51:GLY:O	5:M:601:FAD:N3	2.31	0.59

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:52:SER:O	1:M:125:TRP:HB2	2.03	0.58
1:A:390:ARG:NH1	1:A:395:SER:HB3	2.17	0.58
1:A:253:ILE:O	1:A:314:LEU:HA	2.03	0.58
1:A:167:VAL:HG21	1:A:374:LEU:HB2	1.85	0.58
1:M:54:ALA:O	1:M:123:ARG:O	2.22	0.58
2:B:155:TYR:HE1	2:B:171:ALA:HB3	1.68	0.58
1:M:211:ASP:HA	1:M:510:HIS:CB	2.33	0.58
1:M:162:VAL:HB	1:M:219:HIS:CE1	2.39	0.58
1:A:372:LYS:HE3	1:A:413:ARG:HD2	1.86	0.57
2:N:5:ASN:CA	2:N:30:TYR:CD2	2.86	0.57
1:M:166:HIS:NE2	1:M:373:GLY:CA	2.67	0.57
1:M:68:ASP:O	1:M:391:LEU:HD22	2.05	0.57
2:N:116:ILE:O	2:N:191:ARG:HG2	2.04	0.57
1:M:361:ILE:HB	1:M:376:ALA:HB3	1.85	0.57
4:P:64:ARG:HH21	4:P:116:VAL:HA	1.70	0.57
1:M:135:MET:HE1	1:M:396:LEU:HB3	1.87	0.56
1:M:178:GLY:HA3	1:M:496:SER:O	2.05	0.56
2:N:152:GLY:N	9:N:246:SF4:S4	2.72	0.56
1:M:311:VAL:HG11	1:M:349:PRO:HB3	1.85	0.56
2:B:241:LYS:N	2:B:242:PRO:HD2	2.20	0.56
1:M:31:LYS:HE2	1:M:33:ALA:HB2	1.86	0.56
1:M:226:MET:HB2	1:M:517:CYS:O	2.06	0.56
1:M:383:VAL:HG13	1:M:402:PHE:CE2	2.35	0.56
1:A:341:VAL:HA	1:A:346:GLU:OE2	2.06	0.56
1:M:12:ALA:C	5:M:601:FAD:O3B	2.44	0.55
2:N:158:CYS:HB2	8:N:245:F3S:S4	2.45	0.55
1:A:315:ASP:HB3	1:A:318:HIS:CE1	2.42	0.55
1:M:544:ASP:O	1:M:548:LEU:HB2	2.06	0.55
1:A:57:GLN:NE2	1:A:122:GLU:OE2	2.33	0.55
2:N:155:TYR:CE2	2:N:169:GLY:HA3	2.41	0.55
1:A:28:PRO:HA	1:A:148:GLN:HE21	1.70	0.55
1:M:263:LEU:HB2	1:M:282:MET:SD	2.47	0.55
1:M:232:HIS:O	1:M:352:PRO:HA	2.07	0.55
1:M:123:ARG:O	1:M:125:TRP:CD1	2.60	0.55
1:M:115:ARG:HG2	1:M:122:GLU:CB	2.25	0.54
1:A:197:ARG:HD2	1:A:206:GLY:HA2	1.89	0.54
1:M:211:ASP:O	1:M:510:HIS:CG	2.60	0.54
2:B:60:ALA:N	2:B:77:CYS:SG	2.81	0.54
1:M:268:MET:HE3	1:M:289:LYS:HB3	1.89	0.54
3:C:106:GLU:HB2	3:C:107:PRO:HD3	1.90	0.54
1:M:221:VAL:HG22	1:M:371:ILE:HD12	1.89	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:166:HIS:NE2	1:M:373:GLY:HA3	2.23	0.54
1:A:341:VAL:HG13	1:A:346:GLU:HG3	1.90	0.54
1:M:18:ARG:HG2	1:M:400:VAL:HA	1.88	0.54
2:B:116:ILE:HD11	2:B:118:PRO:HB3	1.88	0.54
1:A:224:ARG:NH2	1:A:382:SER:O	2.39	0.54
1:M:226:MET:CB	1:M:518:MET:HA	2.37	0.54
1:A:263:LEU:O	1:A:268:MET:HB2	2.08	0.54
1:M:443:ASP:HA	1:M:490:ARG:HG2	1.90	0.53
1:A:316:LEU:HA	1:A:319:LEU:HD23	1.91	0.53
1:M:166:HIS:CD2	1:M:373:GLY:HA3	2.43	0.53
1:A:253:ILE:HG12	1:A:318:HIS:CE1	2.44	0.53
1:M:467:ARG:O	1:M:534:ARG:HA	2.08	0.53
1:M:12:ALA:CB	5:M:601:FAD:HO3A	2.17	0.53
1:M:12:ALA:H	5:M:601:FAD:H1B	1.74	0.53
2:N:37:LEU:HD22	2:N:77:CYS:CA	2.39	0.53
1:M:57:GLN:O	1:M:58:ASP:CB	2.56	0.52
1:M:226:MET:HB3	1:M:518:MET:HA	1.90	0.52
1:A:61:SER:HB3	1:A:64:TYR:CD1	2.44	0.52
3:C:120:THR:HG23	4:D:30:VAL:HB	1.91	0.52
1:M:36:SER:HA	5:M:601:FAD:N3A	2.24	0.52
2:N:210:CYS:SG	8:N:245:F3S:S4	3.07	0.52
2:N:206:PHE:CE1	2:N:225:GLN:HG3	2.44	0.52
2:B:65:CYS:SG	2:B:77:CYS:CB	2.97	0.52
1:M:445:GLY:H	1:M:490:ARG:HG3	1.74	0.52
1:M:222:PRO:HB3	1:M:552:LEU:HB3	1.89	0.52
1:M:553:ALA:HB1	1:M:561:THR:CG2	2.40	0.52
4:D:42:GLY:HA2	4:D:44:PHE:CE2	2.45	0.52
1:M:525:ARG:HG2	1:M:527:GLU:HG2	1.91	0.52
2:N:5:ASN:HB2	2:N:27:GLU:HG2	1.92	0.52
1:A:11:GLY:HA2	5:A:601:FAD:H1B	1.91	0.52
1:M:13:GLY:N	5:M:601:FAD:H4B	2.25	0.52
1:M:42:ARG:O	1:M:43:SER:CB	2.58	0.52
3:O:83:THR:HG23	3:O:87:PHE:CE2	2.44	0.52
2:N:35:SER:HB2	2:N:37:LEU:HD23	1.92	0.51
2:B:212:GLU:HG3	3:C:21:PHE:CE1	2.45	0.51
3:O:90:ALA:N	3:O:91:PRO:HD2	2.25	0.51
4:P:10:GLU:N	4:P:11:PRO:HD2	2.26	0.51
3:O:71:ILE:HA	3:O:74:ILE:HD12	1.93	0.51
1:M:72:GLY:H	1:M:391:LEU:HD21	1.75	0.51
1:M:524:ALA:CB	1:M:565:TYR:OH	2.59	0.51
1:M:53:ALA:N	1:M:394:ASN:HB2	2.21	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:166:HIS:NE2	1:M:373:GLY:HA2	2.25	0.50
4:P:39:LEU:HB3	4:P:40:PRO:HD3	1.91	0.50
1:A:266:TYR:OH	1:A:297:GLU:HG2	2.11	0.50
1:M:42:ARG:CZ	2:N:64:SER:HA	2.41	0.50
1:A:386:HIS:CE1	1:A:390:ARG:HG3	2.46	0.50
1:M:101:CYS:C	2:N:184:ARG:HH22	2.15	0.50
1:M:279:ASN:O	1:M:280:LYS:HG2	2.11	0.50
4:D:42:GLY:HA2	4:D:44:PHE:HE2	1.76	0.50
3:O:87:PHE:HE2	4:P:25:ALA:HB1	1.76	0.50
4:P:42:GLY:HA2	4:P:44:PHE:CE2	2.47	0.50
1:A:167:VAL:CG2	1:A:374:LEU:HB2	2.42	0.50
1:M:44:HIS:CE1	5:M:601:FAD:HM82	2.37	0.49
1:M:10:VAL:HG13	5:M:601:FAD:C2A	2.42	0.49
1:M:162:VAL:HG13	1:M:428:GLN:HE22	1.77	0.49
2:N:5:ASN:CA	2:N:30:TYR:CE2	2.96	0.49
1:M:69:THR:HA	1:M:391:LEU:HD22	1.94	0.49
1:M:249:GLY:HA2	1:M:284:LEU:HD21	1.93	0.49
1:M:123:ARG:O	1:M:125:TRP:HD1	1.94	0.49
1:A:232:HIS:CD2	1:A:234:THR:H	2.31	0.49
1:M:251:GLY:O	1:M:318:HIS:NE2	2.45	0.49
4:D:73:LEU:HB2	4:D:74:PRO:HD3	1.94	0.49
1:M:447:ASN:HB3	1:M:450:LYS:HG2	1.93	0.49
1:M:162:VAL:HB	1:M:219:HIS:HE1	1.76	0.49
4:P:60:SER:O	4:P:64:ARG:HG3	2.13	0.49
1:M:76:LEU:HD12	1:M:529:ARG:HD3	1.93	0.49
1:M:52:SER:HA	1:M:394:ASN:HB2	1.94	0.49
2:B:151:CYS:SG	9:B:246:SF4:S4	3.10	0.49
2:N:5:ASN:CG	2:N:29:PRO:HA	2.31	0.49
1:A:204:ASN:HD22	1:A:204:ASN:N	2.11	0.49
1:M:372:LYS:O	1:M:413:ARG:CG	2.59	0.49
1:M:268:MET:CE	1:M:289:LYS:HB3	2.42	0.49
2:N:13:TYR:HB2	2:N:21:PRO:HB3	1.93	0.49
1:A:122:GLU:CD	1:A:122:GLU:H	2.16	0.49
1:A:466:TYR:CD2	1:A:535:LEU:HD21	2.48	0.49
1:M:41:MET:HA	1:M:136:LEU:HD11	1.95	0.49
2:N:36:LEU:HB3	2:N:76:ALA:HB1	1.95	0.49
1:M:383:VAL:CG1	1:M:402:PHE:HE2	2.23	0.48
1:M:72:GLY:N	1:M:391:LEU:HD21	2.29	0.48
1:M:10:VAL:HG21	1:M:157:VAL:HG21	1.95	0.48
1:A:315:ASP:C	1:A:318:HIS:CE1	2.87	0.48
3:O:43:ILE:HD11	4:P:71:ILE:HG21	1.94	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:141:GLN:HB3	2:N:118:PRO:O	2.14	0.48
1:M:168:ARG:HG3	1:M:425:ILE:CG1	2.40	0.48
1:A:316:LEU:O	1:A:319:LEU:HB2	2.12	0.48
1:M:562:ARG:HG2	1:M:563:LEU:H	1.78	0.48
1:A:315:ASP:O	1:A:318:HIS:CE1	2.66	0.48
1:A:462:GLY:HA3	1:A:475:THR:OG1	2.13	0.48
1:A:342:ASP:C	1:A:344:VAL:H	2.17	0.48
2:N:241:LYS:H	2:N:242:PRO:HD2	1.78	0.48
1:A:356:TYR:CE2	1:A:390:ARG:HD3	2.49	0.48
2:B:116:ILE:HD13	2:B:176:ALA:HA	1.94	0.48
2:B:238:ALA:HA	2:B:241:LYS:HB2	1.94	0.48
2:B:78:LYS:HG2	2:B:78:LYS:O	2.14	0.47
3:C:33:VAL:HA	4:D:82:MET:CE	2.44	0.47
2:B:241:LYS:O	2:B:243:ARG:HG2	2.14	0.47
1:M:369:THR:OG1	1:M:374:LEU:O	2.25	0.47
1:M:53:ALA:H	1:M:394:ASN:CB	2.21	0.47
1:M:72:GLY:HA3	1:M:391:LEU:CD2	2.43	0.47
1:M:389:ASN:ND2	1:M:530:GLY:HA2	2.29	0.47
1:A:275:GLY:O	1:A:277:PRO:HD3	2.13	0.47
1:M:570:ILE:HG12	1:M:575:PRO:HG3	1.96	0.47
1:M:438:ASP:O	1:M:442:GLN:HB2	2.13	0.47
1:M:189:VAL:HA	1:M:375:PHE:HB2	1.97	0.47
1:M:226:MET:HB3	1:M:518:MET:HG2	1.96	0.47
4:D:6:LYS:HA	4:P:6:LYS:HG2	1.96	0.47
1:M:76:LEU:CD1	1:M:525:ARG:NH1	2.78	0.47
2:N:93:LEU:HG	2:N:156:ALA:HB2	1.95	0.47
4:P:22:MET:O	4:P:26:ILE:HD12	2.15	0.47
1:M:386:HIS:ND1	1:M:390:ARG:HG3	2.30	0.47
3:O:87:PHE:CE2	4:P:25:ALA:HB1	2.49	0.47
1:M:152:PHE:CD1	1:M:152:PHE:N	2.83	0.47
1:M:562:ARG:HG2	1:M:563:LEU:N	2.30	0.47
1:M:102:PRO:HB3	2:N:142:TYR:OH	2.15	0.47
1:M:522:ALA:HB1	1:M:532:HIS:CE1	2.50	0.47
1:M:553:ALA:HB1	1:M:561:THR:HG21	1.97	0.46
1:M:221:VAL:CG1	1:M:369:THR:HB	2.46	0.46
1:M:398:GLU:O	1:M:402:PHE:CB	2.62	0.46
3:O:128:LEU:HD22	4:P:45:PRO:HD2	1.98	0.46
4:P:33:LEU:HA	4:P:37:ILE:HD12	1.97	0.46
2:N:210:CYS:SG	2:N:221:ALA:HB2	2.55	0.46
1:M:520:HIS:HB3	1:M:563:LEU:HD21	1.96	0.46
1:A:10:VAL:HB	1:A:190:MET:CE	2.45	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:65:HIS:HD2	1:M:123:ARG:HH11	1.64	0.46
1:M:42:ARG:HD2	2:N:64:SER:OG	2.15	0.46
1:A:232:HIS:HD2	1:A:234:THR:H	1.64	0.46
2:B:57:CYS:HB3	2:B:62:CYS:HB3	1.97	0.46
1:M:125:TRP:N	1:M:125:TRP:CD1	2.83	0.46
1:A:96:LEU:HD11	1:A:400:VAL:HG11	1.97	0.46
1:M:20:ALA:HB1	1:M:34:LEU:HD11	1.96	0.46
1:M:366:ASN:O	1:M:367:CYS:HB2	2.15	0.46
2:B:109:PHE:HE2	2:B:113:LEU:HD12	1.80	0.46
1:M:244:THR:CG2	1:M:331:ILE:HD11	2.46	0.46
2:B:204:CYS:SG	8:B:245:F3S:S1	3.13	0.46
1:M:75:TRP:CD1	1:M:575:PRO:HA	2.50	0.46
1:M:44:HIS:HB2	1:M:208:VAL:HG21	1.98	0.46
1:M:53:ALA:HB3	1:M:393:SER:HA	1.98	0.46
1:M:263:LEU:HD13	1:M:283:GLU:H	1.81	0.46
1:M:13:GLY:O	1:M:17:LEU:HG	2.16	0.45
1:M:215:MET:HG3	1:M:510:HIS:HE1	1.81	0.45
2:N:207:VAL:HG22	3:O:25:TYR:CZ	2.51	0.45
4:P:9:ASP:N	4:P:9:ASP:OD2	2.50	0.45
1:M:166:HIS:HE1	1:M:186:ASN:C	2.20	0.45
1:A:197:ARG:HB2	1:A:208:VAL:O	2.17	0.45
2:N:54:ARG:NH2	2:N:104:VAL:O	2.49	0.45
1:M:472:MET:HE3	1:M:523:MET:HG3	1.98	0.45
1:M:56:ALA:HB2	1:M:123:ARG:HA	1.98	0.45
2:N:120:ILE:C	2:N:121:ILE:HG13	2.37	0.45
2:B:50:ASP:O	2:B:100:ARG:NH2	2.48	0.45
1:A:122:GLU:N	1:A:122:GLU:OE2	2.50	0.45
1:A:356:TYR:CE1	1:A:379:GLU:HG3	2.51	0.45
1:M:168:ARG:HG3	1:M:425:ILE:CD1	2.46	0.45
1:A:237:PRO:O	1:A:308:ARG:HD2	2.16	0.45
1:M:550:HIS:HB2	1:M:566:SER:HB2	1.99	0.45
1:M:156:PHE:O	1:M:173:MET:N	2.41	0.45
1:M:12:ALA:HA	1:M:17:LEU:HD21	1.99	0.45
1:M:212:GLY:O	1:M:215:MET:HB2	2.17	0.45
1:M:33:ALA:HB1	1:M:152:PHE:CE1	2.52	0.45
1:M:76:LEU:HD11	1:M:525:ARG:NH1	2.31	0.45
2:N:6:LEU:N	2:N:30:TYR:CE2	2.85	0.44
1:A:232:HIS:CE1	1:A:242:LEU:HD11	2.52	0.44
1:A:363:THR:HB	1:A:367:CYS:HA	1.99	0.44
1:M:51:GLY:HA2	1:M:131:THR:HG21	2.00	0.44
2:B:164:ASN:OD1	2:B:166:GLU:N	2.50	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:601:FAD:H1'1	5:A:601:FAD:H9	1.81	0.44
1:M:197:ARG:HA	1:M:202:ASN:HD21	1.82	0.44
1:M:89:CYS:SG	1:M:401:VAL:HG21	2.58	0.44
1:M:536:ASP:O	1:M:540:THR:HG23	2.17	0.44
1:M:37:LYS:HA	1:M:155:HIS:H	1.81	0.44
1:M:571:THR:HG23	1:M:572:THR:N	2.33	0.44
1:M:510:HIS:O	1:M:514:VAL:HG23	2.18	0.44
1:A:127:ALA:HB3	1:A:131:THR:HA	2.00	0.44
1:A:529:ARG:NH2	1:A:548:LEU:HD13	2.32	0.44
1:M:115:ARG:HE	1:M:279:ASN:HD22	1.66	0.44
1:M:34:LEU:HD13	1:M:149:ILE:HG23	1.99	0.44
1:M:248:ARG:H	1:M:248:ARG:HG2	1.57	0.44
1:M:10:VAL:HG13	5:M:601:FAD:N1A	2.32	0.43
3:C:50:LYS:HE2	3:C:50:LYS:HA	1.99	0.43
1:M:383:VAL:CG1	1:M:402:PHE:CE2	3.00	0.43
1:M:207:ILE:HG13	1:M:208:VAL:HG23	2.01	0.43
4:P:72:VAL:O	4:P:75:LEU:HB2	2.19	0.43
2:N:157:ALA:HB2	2:N:213:VAL:HG21	2.00	0.43
1:M:369:THR:HG21	1:M:375:PHE:HA	2.00	0.43
1:A:550:HIS:HB2	1:A:566:SER:OG	2.18	0.43
4:D:39:LEU:HB3	4:D:40:PRO:HD3	1.99	0.43
1:A:125:TRP:CD1	1:A:125:TRP:N	2.87	0.43
1:M:226:MET:HB2	1:M:517:CYS:C	2.39	0.43
1:M:74:ASP:N	1:M:74:ASP:OD1	2.52	0.43
1:M:162:VAL:CB	1:M:219:HIS:HE1	2.31	0.43
2:N:158:CYS:SG	2:N:160:GLN:HB2	2.59	0.43
3:O:33:VAL:HB	3:O:34:PRO:CD	2.47	0.43
2:N:155:TYR:HE1	2:N:171:ALA:HB3	1.84	0.43
1:A:54:ALA:HB3	1:A:125:TRP:NE1	2.33	0.43
1:M:176:MET:O	1:M:497:VAL:HG13	2.19	0.43
1:M:219:HIS:CD2	1:M:371:ILE:HD11	2.53	0.42
2:B:99:GLU:OE2	3:C:4:ARG:NH1	2.52	0.42
5:M:601:FAD:H9	5:M:601:FAD:H1'1	1.75	0.42
1:M:81:VAL:HG11	1:M:383:VAL:HB	2.01	0.42
2:B:65:CYS:SG	2:B:77:CYS:N	2.82	0.42
1:A:42:ARG:NH2	2:B:150:ASN:O	2.51	0.42
1:M:421:ASN:ND2	1:M:424:ALA:HB3	2.34	0.42
1:A:57:GLN:NE2	1:A:122:GLU:O	2.52	0.42
1:A:304:ILE:HD12	1:A:304:ILE:H	1.84	0.42
3:C:49:LEU:HB2	3:C:56:TRP:CE3	2.54	0.42
1:M:12:ALA:HB1	1:M:40:PRO:HA	2.00	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:368:GLU:HG3	1:M:375:PHE:CE2	2.55	0.42
1:M:499:ASN:O	1:M:503:LEU:HG	2.20	0.42
4:P:47:ASP:HB2	4:P:50:SER:HB3	2.01	0.42
1:M:159:ASP:OD2	1:M:432:VAL:HB	2.19	0.42
1:M:428:GLN:O	1:M:432:VAL:HG12	2.19	0.42
1:A:11:GLY:HA3	1:A:191:ALA:O	2.20	0.42
2:N:6:LEU:N	2:N:30:TYR:CD2	2.86	0.42
2:B:104:VAL:CG1	2:B:105:ASP:N	2.82	0.42
1:M:281:TYR:O	1:M:282:MET:CB	2.68	0.42
2:N:135:THR:HG22	2:N:136:PRO:HD2	2.02	0.42
3:O:28:ARG:HG3	3:O:85:THR:HG21	2.00	0.42
1:A:315:ASP:C	1:A:318:HIS:HE1	2.22	0.42
1:M:228:PHE:CZ	1:M:388:ALA:HA	2.55	0.42
2:N:188:LYS:HG3	2:N:188:LYS:H	1.63	0.42
2:N:117:LYS:N	2:N:118:PRO:HD3	2.34	0.42
1:M:491:ILE:HD13	1:M:502:LEU:HD12	2.01	0.42
1:A:154:GLU:OE2	2:B:54:ARG:NE	2.53	0.42
2:B:68:MET:HB2	2:B:91:GLU:HB2	2.02	0.42
1:M:574:PRO:HA	1:M:575:PRO:HD3	1.92	0.42
1:A:497:VAL:O	2:B:100:ARG:NH1	2.53	0.42
1:M:226:MET:C	1:M:518:MET:HA	2.40	0.41
1:M:377:VAL:HG23	1:M:402:PHE:CD1	2.55	0.41
2:B:100:ARG:O	2:B:101:ASP:C	2.58	0.41
1:A:54:ALA:O	1:A:123:ARG:O	2.38	0.41
3:O:19:LEU:HB2	3:O:20:PRO:HD2	2.02	0.41
4:D:24:SER:O	4:D:28:ALA:HB3	2.19	0.41
1:M:361:ILE:H	1:M:381:SER:HA	1.85	0.41
1:M:553:ALA:HA	1:M:562:ARG:O	2.20	0.41
1:A:366:ASN:O	1:A:367:CYS:HB2	2.21	0.41
2:N:170:PRO:HA	2:N:224:ILE:HD11	2.03	0.41
1:M:43:SER:OG	1:M:44:HIS:N	2.53	0.41
1:M:53:ALA:HA	1:M:124:THR:HA	2.03	0.41
3:C:63:LEU:HA	3:C:68:ILE:HG21	2.03	0.41
1:M:98:LEU:CD1	2:N:125:ARG:HD3	2.49	0.41
2:B:241:LYS:N	2:B:242:PRO:CD	2.84	0.41
1:M:525:ARG:NH2	1:M:549:LYS:O	2.54	0.41
1:M:554:PHE:O	1:M:561:THR:HA	2.21	0.41
1:A:543:ASP:OD2	1:A:546:ASN:HB2	2.21	0.41
1:M:485:ARG:O	1:M:489:VAL:HG23	2.20	0.41
1:M:232:HIS:HA	1:M:233:PRO:HD2	1.90	0.41
1:M:76:LEU:HD13	1:M:525:ARG:HH12	1.86	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:524:ALA:HB1	1:M:565:TYR:OH	2.21	0.41
4:P:28:ALA:N	4:P:29:PRO:HD2	2.36	0.41
1:M:146:PHE:HA	1:M:147:PRO:HD3	1.90	0.41
2:B:164:ASN:C	2:B:164:ASN:OD1	2.58	0.41
1:M:197:ARG:HD2	1:M:206:GLY:HA2	2.03	0.41
1:A:38:VAL:HG11	1:A:207:ILE:HG21	2.03	0.41
1:A:450:LYS:HA	1:A:450:LYS:HD3	1.85	0.41
1:M:223:LEU:HD23	1:M:360:GLY:HA2	2.03	0.41
1:A:451:ILE:HG23	1:A:482:LEU:HD22	2.02	0.41
2:B:241:LYS:O	2:B:243:ARG:N	2.53	0.41
1:A:448:TRP:CG	1:A:449:ALA:N	2.88	0.41
3:O:130:TRP:O	4:P:53:ARG:NH2	2.54	0.41
4:D:31:MET:HG3	4:D:70:MET:SD	2.61	0.41
1:M:395:SER:O	1:M:398:GLU:HB3	2.22	0.40
1:M:166:HIS:CE1	1:M:186:ASN:O	2.74	0.40
1:M:524:ALA:HB3	1:M:565:TYR:OH	2.20	0.40
2:N:72:VAL:HA	2:N:73:PRO:HD3	1.92	0.40
1:M:332:CYS:HA	1:M:343:PRO:HG2	2.02	0.40
1:M:41:MET:HB2	1:M:137:HIS:CE1	2.56	0.40
1:A:319:LEU:HD12	1:A:323:LYS:HD3	2.02	0.40
1:M:53:ALA:CB	1:M:392:GLY:O	2.69	0.40
2:N:106:MET:O	2:N:110:ILE:HG12	2.22	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	575/577 (100%)	562 (98%)	12 (2%)	1 (0%)	52 84
1	M	575/577 (100%)	542 (94%)	27 (5%)	6 (1%)	19 58
2	B	241/243 (99%)	224 (93%)	15 (6%)	2 (1%)	24 63

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	N	241/243 (99%)	230 (95%)	9 (4%)	2 (1%)	24	63
3	C	128/130 (98%)	126 (98%)	2 (2%)	0	100	100
3	O	128/130 (98%)	126 (98%)	2 (2%)	0	100	100
4	D	117/119 (98%)	114 (97%)	3 (3%)	0	100	100
4	P	117/119 (98%)	110 (94%)	7 (6%)	0	100	100
All	All	2122/2138 (99%)	2034 (96%)	77 (4%)	11 (0%)	34	72

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	M	43	SER
1	M	58	ASP
1	M	282	MET
2	N	189	LYS
2	B	101	ASP
1	M	373	GLY
2	N	101	ASP
1	M	206	GLY
2	B	242	PRO
1	M	220	GLY
1	A	343	PRO

### 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	460/460 (100%)	444 (96%)	16 (4%)	43	78
1	M	460/460 (100%)	435 (95%)	25 (5%)	27	64
2	B	205/205 (100%)	201 (98%)	4 (2%)	63	86
2	N	205/205 (100%)	198 (97%)	7 (3%)	44	79
3	C	111/111 (100%)	105 (95%)	6 (5%)	27	64
3	O	111/111 (100%)	108 (97%)	3 (3%)	52	82

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	97/97 (100%)	94 (97%)	3 (3%)	47	80
4	P	97/97 (100%)	94 (97%)	3 (3%)	47	80
All	All	1746/1746 (100%)	1679 (96%)	67 (4%)	40	76

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	42	ARG
1	A	74	ASP
1	A	93	MET
1	A	114	ARG
1	A	116	PHE
1	A	122	GLU
1	A	197	ARG
1	A	198	VAL
1	A	204	ASN
1	A	308	ARG
1	A	321	GLU
1	A	327	ARG
1	A	391	LEU
1	A	413	ARG
1	A	428	GLN
2	B	86	ASP
2	B	178	ARG
2	B	191	ARG
2	B	206	PHE
3	C	12	THR
3	C	24	PHE
3	C	26	MET
3	C	49	LEU
3	C	50	LYS
3	C	73	LEU
4	D	9	ASP
4	D	86	MET
4	D	113	ILE
1	M	10	VAL
1	M	27	ASN
1	M	35	ILE
1	M	41	MET
1	M	59	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	M	74	ASP
1	M	98	LEU
1	M	148	GLN
1	M	167	VAL
1	M	190	MET
1	M	197	ARG
1	M	203	THR
1	M	207	ILE
1	M	221	VAL
1	M	243	MET
1	M	248	ARG
1	M	255	VAL
1	M	281	TYR
1	M	319	LEU
1	M	321	GLU
1	M	362	GLU
1	M	383	VAL
1	M	472	MET
1	M	543	ASP
1	M	558	ASP
2	N	100	ARG
2	N	128	ASP
2	N	135	THR
2	N	206	PHE
2	N	210	CYS
2	N	226	GLN
2	N	240	LEU
3	O	19	LEU
3	O	39	SER
3	O	99	LYS
4	P	6	LYS
4	P	9	ASP
4	P	115	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	HIS
1	A	134	HIS
1	A	141	GLN
1	A	145	GLN
1	A	204	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	230	GLN
1	A	232	HIS
1	A	279	ASN
1	A	296	HIS
1	A	318	HIS
1	A	366	ASN
2	B	194	GLN
2	B	225	GLN
1	M	27	ASN
1	M	134	HIS
1	M	202	ASN
1	M	219	HIS
1	M	232	HIS
1	M	264	GLN
1	M	292	GLN
1	M	296	HIS
1	M	510	HIS
2	N	95	ASN
2	N	160	GLN
2	N	225	GLN
4	P	80	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

9 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	FAD	A	601	-	48,58,58	0.85	1 (2%)	54,89,89	1.99	8 (14%)
6	3NP	A	602	-	2,5,7	2.02	1 (50%)	1,5,8	7.09	1 (100%)
7	FES	B	244	2	0,4,4	0.00	-	0,4,4	0.00	-
8	F3S	B	245	2	0,9,9	0.00	-	0,15,15	0.00	-
9	SF4	B	246	2	0,12,12	0.00	-	0,24,24	0.00	-
5	FAD	M	601	-	48,58,58	0.97	3 (6%)	54,89,89	2.14	9 (16%)
7	FES	N	244	2	0,4,4	0.00	-	0,4,4	0.00	-
8	F3S	N	245	2	0,9,9	0.00	-	0,15,15	0.00	-
9	SF4	N	246	2	0,12,12	0.00	-	0,24,24	0.00	-

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	FAD	A	601	-	-	0/30/50/50	0/6/6/6
6	3NP	A	602	-	-	0/1/3/5	0/0/0/0
7	FES	B	244	2	-	0/0/4/4	0/1/1/1
8	F3S	B	245	2	-	0/0/24/24	0/0/3/3
9	SF4	B	246	2	-	0/0/48/48	0/6/5/5
5	FAD	M	601	-	-	0/30/50/50	0/6/6/6
7	FES	N	244	2	-	0/0/4/4	0/1/1/1
8	F3S	N	245	2	-	0/0/24/24	0/0/3/3
9	SF4	N	246	2	-	0/0/48/48	0/6/5/5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	602	3NP	C3-N1	-2.83	1.36	1.48
5	M	601	FAD	O2B-C2B	-2.46	1.37	1.43
5	M	601	FAD	C9A-N10	2.30	1.41	1.38
5	A	601	FAD	C10-N10	2.41	1.42	1.39
5	M	601	FAD	C10-N10	2.49	1.42	1.39

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	601	FAD	N3A-C2A-N1A	-10.54	120.82	128.89
5	A	601	FAD	N3A-C2A-N1A	-10.44	120.90	128.89
5	M	601	FAD	P-O3P-PA	-3.37	123.27	132.73
5	M	601	FAD	C4X-C4-N3	-3.16	119.27	123.59
5	A	601	FAD	P-O3P-PA	-3.08	124.09	132.73
5	A	601	FAD	C4X-C4-N3	-2.51	120.16	123.59
5	A	601	FAD	C4A-C5A-N7A	-2.29	107.38	109.48
5	M	601	FAD	C4A-C5A-N7A	-2.14	107.51	109.48
5	A	601	FAD	O4B-C1B-N9A	2.01	112.30	108.10
5	M	601	FAD	C1'-C2'-C3'	2.35	116.54	109.82
5	A	601	FAD	C5X-C9A-N10	2.70	119.67	117.62
5	M	601	FAD	C4X-N5-C5X	3.40	120.67	116.76
5	M	601	FAD	C5X-C9A-N10	3.68	120.42	117.62
5	A	601	FAD	C4X-N5-C5X	3.85	121.20	116.76
5	M	601	FAD	C5B-C4B-C3B	3.90	130.69	115.21
5	A	601	FAD	C4-N3-C2	5.20	119.75	115.25
5	M	601	FAD	C4-N3-C2	6.22	120.63	115.25
6	A	602	3NP	C2-C3-N1	7.09	126.08	111.45

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 42 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	601	FAD	5	0
8	B	245	F3S	3	0
9	B	246	SF4	4	0
5	M	601	FAD	20	0
7	N	244	FES	2	0
8	N	245	F3S	5	0
9	N	246	SF4	3	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	577/577 (100%)	-0.28	2 (0%) 94 88	42, 56, 89, 117	0
1	M	577/577 (100%)	1.17	120 (20%) 1 0	87, 137, 155, 180	0
2	B	243/243 (100%)	-0.30	3 (1%) 81 64	41, 60, 86, 314	0
2	N	243/243 (100%)	0.46	25 (10%) 9 3	77, 113, 151, 159	0
3	C	130/130 (100%)	-0.36	0 100 100	61, 73, 102, 131	0
3	O	130/130 (100%)	-0.13	6 (4%) 36 17	59, 85, 144, 150	0
4	D	119/119 (100%)	-0.43	1 (0%) 87 75	61, 72, 95, 122	0
4	P	119/119 (100%)	-0.38	1 (0%) 87 75	67, 80, 122, 156	0
All	All	2138/2138 (100%)	0.19	158 (7%) 17 6	41, 82, 150, 314	0

All (158) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	373	GLY	9.5
1	M	571	THR	7.8
1	M	411	THR	7.7
1	M	169	GLY	7.4
1	M	172	ALA	6.6
1	M	188	VAL	5.9
1	M	393	SER	5.8
1	M	376	ALA	5.7
1	M	218	SER	5.2
1	M	490	ARG	5.0
1	M	6	ASP	4.9
2	N	98	ILE	4.9
1	M	225	ASP	4.7
1	M	489	VAL	4.6
1	M	189	VAL	4.6
1	M	386	HIS	4.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	M	380	CYS	4.3
1	M	179	THR	4.3
1	M	500	THR	4.2
1	M	572	THR	4.2
1	M	8	ALA	4.1
1	M	573	LEU	4.0
1	M	219	HIS	4.0
1	M	281	TYR	3.9
2	N	33	THR	3.9
1	M	79	GLN	3.8
1	M	370	ARG	3.8
1	M	484	GLU	3.8
1	M	250	GLU	3.7
1	M	475	THR	3.7
1	M	357	THR	3.7
1	M	229	VAL	3.7
1	M	366	ASN	3.6
1	M	367	CYS	3.6
2	N	29	PRO	3.5
1	M	419	ASN	3.5
1	M	59	HIS	3.5
1	M	7	LEU	3.5
1	M	108	ASP	3.5
1	M	227	GLU	3.5
1	M	494	THR	3.4
1	M	194	GLY	3.4
1	M	325	HIS	3.4
1	M	537	GLU	3.4
1	M	377	VAL	3.4
1	M	480	ALA	3.4
1	M	491	ILE	3.4
1	M	193	GLY	3.3
1	M	270	PRO	3.3
2	N	15	PRO	3.3
2	N	8	ILE	3.3
1	M	147	PRO	3.3
1	M	80	ASP	3.3
2	N	26	TYR	3.3
1	M	392	GLY	3.3
2	N	2	GLU	3.3
1	M	170	LEU	3.2
1	M	413	ARG	3.2

*Continued on next page...*



*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	M	165	GLY	3.2
1	M	385	LEU	3.2
1	M	358	MET	3.2
3	O	1	THR	3.1
1	M	422	GLU	3.1
1	M	191	ALA	3.1
1	M	429	ALA	3.1
1	M	9	ILE	3.1
1	M	378	GLY	3.1
1	M	161	LEU	3.1
1	M	549	LYS	3.1
1	M	220	GLY	3.0
1	M	192	THR	3.0
1	M	548	LEU	3.0
1	M	575	PRO	3.0
2	B	241	LYS	3.0
1	M	555	ARG	3.0
1	M	428	GLN	3.0
1	M	395	SER	3.0
1	M	216	ALA	2.9
1	M	451	ILE	2.9
1	M	274	LEU	2.9
2	N	128	ASP	2.8
1	M	187	ALA	2.8
1	M	546	ASN	2.8
1	M	102	PRO	2.8
1	M	212	GLY	2.8
1	M	574	PRO	2.8
1	M	409	GLN	2.8
1	M	58	ASP	2.8
1	M	375	PHE	2.7
2	N	6	LEU	2.7
2	N	241	LYS	2.7
1	M	100	GLY	2.7
3	O	8	VAL	2.7
1	M	513	ASN	2.7
1	M	121	ILE	2.7
2	N	4	LYS	2.7
1	M	168	ARG	2.6
2	N	1	ALA	2.6
2	N	40	LEU	2.6
2	N	52	SER	2.6

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	M	223	LEU	2.6
1	M	221	VAL	2.6
2	N	16	GLU	2.6
1	M	183	ILE	2.6
1	M	545	VAL	2.6
1	M	355	HIS	2.5
1	M	77	CYS	2.5
1	M	384	GLY	2.5
1	M	163	ASP	2.5
1	M	401	VAL	2.5
2	N	27	GLU	2.5
1	M	493	ASP	2.4
1	M	44	HIS	2.4
1	M	415	ALA	2.4
1	M	16	GLY	2.4
1	M	32	ILE	2.4
1	M	91	THR	2.4
1	M	379	GLU	2.4
4	D	0	MET	2.4
3	O	96	ILE	2.4
1	M	538	GLY	2.4
2	N	24	ALA	2.4
1	M	399	LEU	2.4
1	M	280	LYS	2.3
2	B	243	ARG	2.3
2	B	1	ALA	2.3
2	N	130	GLY	2.3
1	M	576	ALA	2.3
1	M	84	TYR	2.3
1	M	356	TYR	2.3
1	M	203	THR	2.3
2	N	124	SER	2.3
1	M	553	ALA	2.2
1	M	552	LEU	2.2
1	M	295	TRP	2.2
2	N	56	SER	2.2
2	N	47	LEU	2.2
3	O	103	MET	2.2
2	N	25	PHE	2.2
1	M	162	VAL	2.2
3	O	98	VAL	2.2
4	P	0	MET	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	299	ARG	2.1
1	M	210	GLY	2.1
1	M	180	LEU	2.1
1	A	576	ALA	2.1
3	O	106	GLU	2.1
1	M	305	SER	2.1
1	M	228	PHE	2.1
2	N	51	LEU	2.1
1	M	381	SER	2.1
1	M	438	ASP	2.1
1	M	471	LEU	2.1
1	M	389	ASN	2.1
2	N	125	ARG	2.0
1	M	342	ASP	2.0
2	N	3	MET	2.0
1	M	99	TRP	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<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
5	FAD	A	601	53/53	0.96	0.39	2.40	60,65,75,76	0
6	3NP	A	602	6/8	0.88	0.28	2.06	74,76,76,77	0
8	F3S	B	245	7/7	0.98	0.27	1.67	100,101,102,102	0
9	SF4	B	246	8/8	0.98	0.25	1.16	79,79,80,80	0
7	FES	B	244	4/4	0.98	0.27	1.09	59,60,61,61	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
8	F3S	N	245	7/7	0.94	0.24	0.54	124,124,125,126	0
5	FAD	M	601	53/53	0.81	0.42	0.45	124,134,143,143	0
7	FES	N	244	4/4	0.94	0.25	0.01	105,105,105,106	0
9	SF4	N	246	8/8	0.97	0.20	-0.69	97,97,97,98	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.