



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 13, 2016 – 05:30 PM EDT

PDB ID : 4Y7C
Title : rat CYPOR mutant - G141del/E142N
Authors : Xia, C.; Kim, J.J.P.
Deposited on : 2015-02-13
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027790
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) : rb-20027790

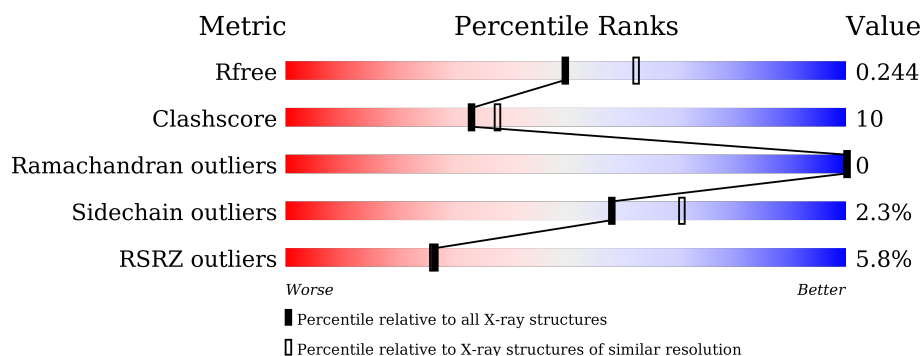
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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 $\leq 5\%$. 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	621	<div> <div>2%</div> <div>83%</div> <div>14%</div> <div>..</div> </div>
1	B	621	<div> <div>10%</div> <div>73%</div> <div>24%</div> <div>..</div> </div>

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 11097 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.

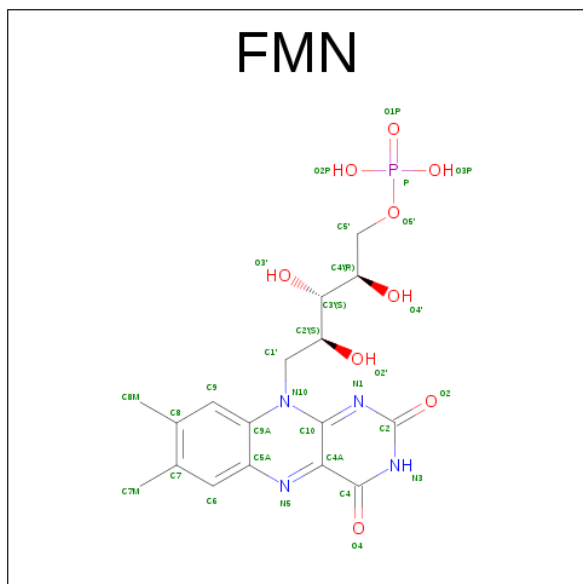
- Molecule 1 is a protein called NADPH–cytochrome P450 reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	611	Total	C	N	O	S	0	0	0
			4895	3101	844	927	23			
1	B	605	Total	C	N	O	S	0	0	0
			4831	3059	836	913	23			

There are 4 discrepancies between the modelled and reference sequences:

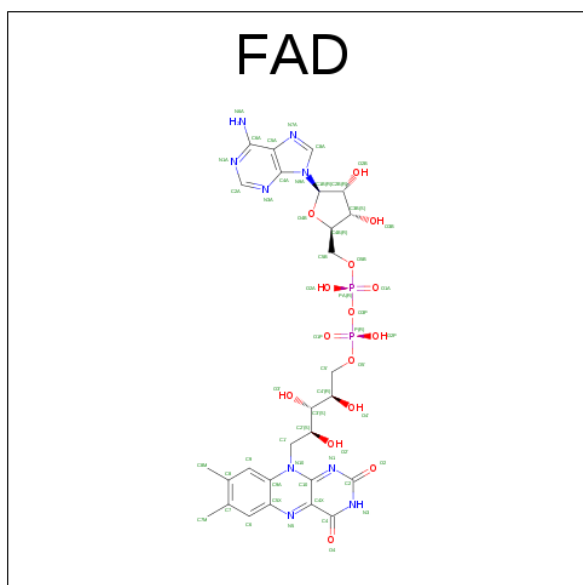
Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLY	deletion	UNP P00388
A	142	ASN	GLU	engineered mutation	UNP P00388
B	?	-	GLY	deletion	UNP P00388
B	142	ASN	GLU	engineered mutation	UNP P00388

- Molecule 2 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C₁₇H₂₁N₄O₉P).



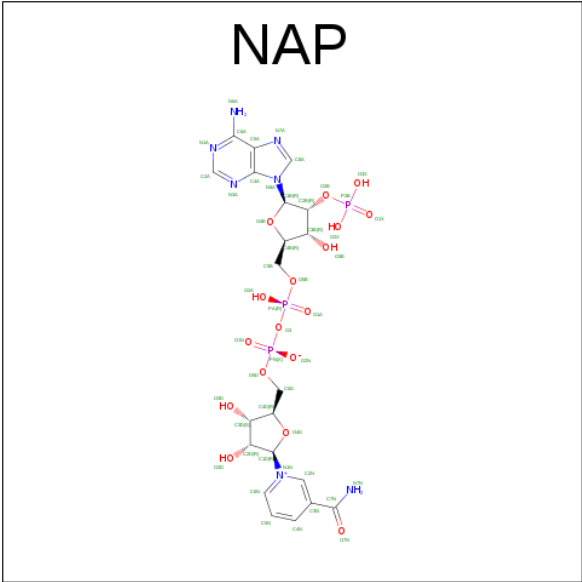
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



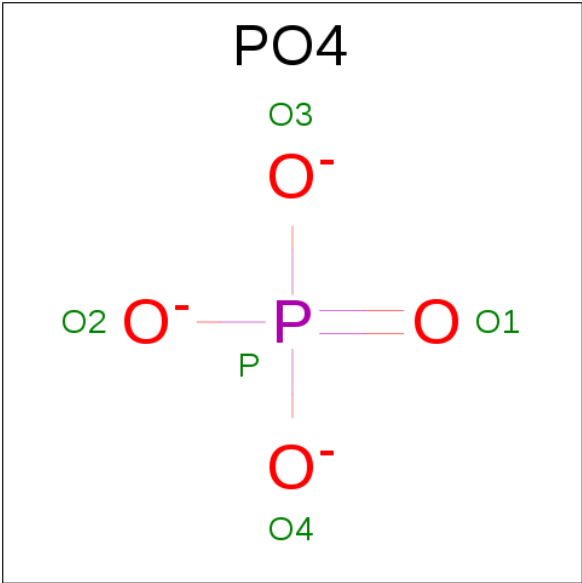
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 4 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	O	P	0	0
			5	4	1		

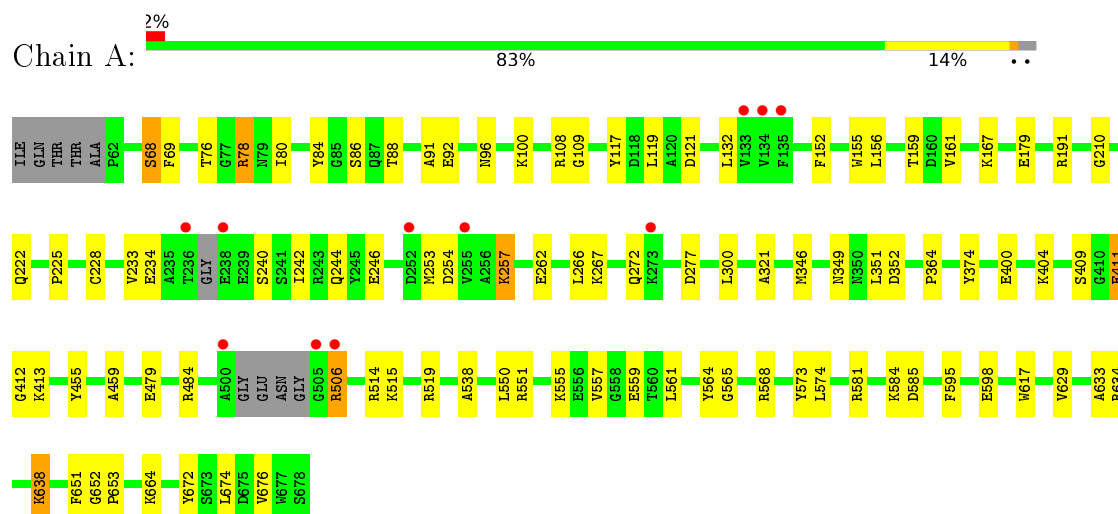
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	635	Total 635	O 635	0	0
6	B	501	Total 501	O 501	0	0

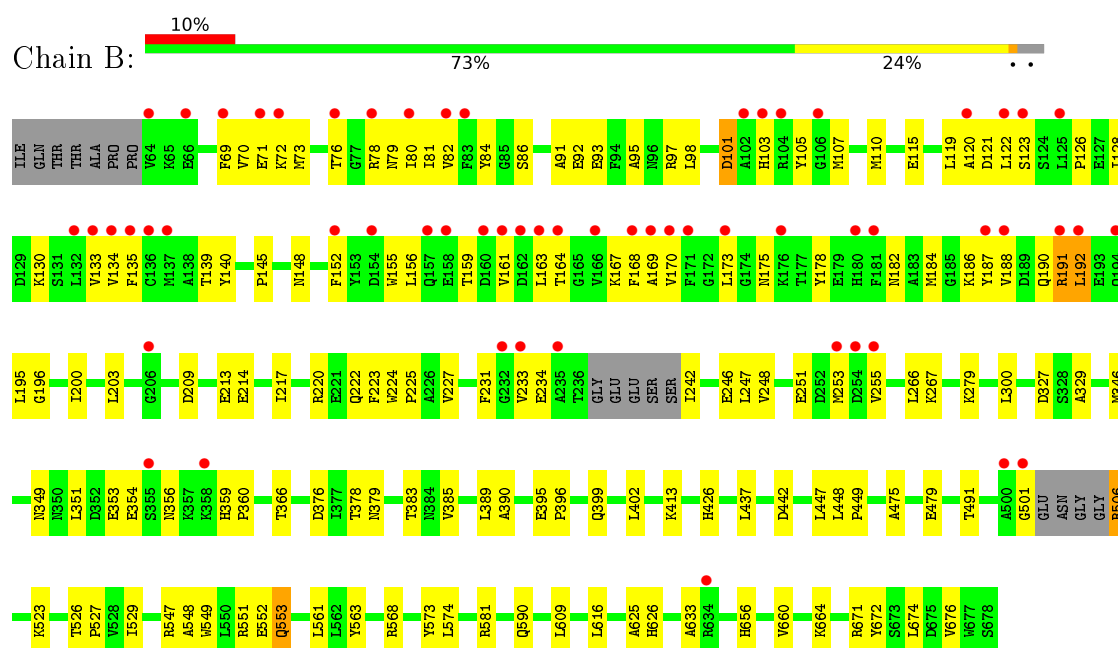
3 Residue-property plots

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: NADPH-cytochrome P450 reductase



• Molecule 1: NADPH-cytochrome P450 reductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	101.48Å 115.64Å 118.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	23.54 – 2.20 23.54 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.2 (23.54-2.20) 96.2 (23.54-2.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.91 (at 2.19Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.192 , 0.244 0.192 , 0.244	Depositor DCC
R_{free} test set	3503 reflections (5.09%)	DCC
Wilson B-factor (Å ²)	29.3	Xtriage
Anisotropy	0.190	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 47.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.013 for -h,l,k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11097	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.89% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: FMN, PO4, NAP, 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	0.35	0/5012	0.57	1/6782 (0.0%)
1	B	0.32	0/4946	0.56	0/6695
All	All	0.34	0/9958	0.57	1/13477 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	210	GLY	N-CA-C	-5.37	99.67	113.10

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	4895	0	4739	69	0
1	B	4831	0	4642	132	0
2	A	31	0	19	0	0
2	B	31	0	19	0	0
3	A	53	0	31	0	0
3	B	53	0	31	0	0
4	A	31	0	11	0	0
4	B	31	0	11	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	5	0	0	0	0
6	A	635	0	0	18	0
6	B	501	0	0	16	0
All	All	11097	0	9503	201	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 10.

All (201) 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:B:81:ILE:HG23	1:B:133:VAL:HG23	1.42	0.97
1:B:155:TRP:O	1:B:159:THR:HG22	1.70	0.91
1:A:257:LYS:HA	1:A:266:LEU:HD21	1.54	0.90
1:B:191:ARG:HH11	1:B:195:LEU:HD11	1.35	0.89
1:B:86:SER:HB2	1:B:91:ALA:HB3	1.57	0.83
1:B:159:THR:OG1	1:B:161:VAL:HG13	1.81	0.81
1:B:167:LYS:HB3	1:B:200:ILE:HD11	1.62	0.81
1:B:155:TRP:O	1:B:159:THR:CG2	2.29	0.81
1:A:638:LYS:NZ	1:A:638:LYS:HA	1.99	0.77
1:A:550:LEU:HD22	1:A:555:LYS:HD2	1.67	0.77
1:A:633:ALA:HB2	1:A:676:VAL:HB	1.68	0.74
1:B:506:ARG:HB2	6:B:1074:HOH:O	1.88	0.72
1:B:214:GLU:OE1	1:B:217:ILE:HD12	1.90	0.71
1:B:81:ILE:CG2	1:B:133:VAL:HG23	2.20	0.70
1:B:222:GLN:O	1:B:225:PRO:HD2	1.92	0.69
1:B:190:GLN:HB3	6:B:932:HOH:O	1.92	0.68
1:B:175:ASN:HB3	1:B:178:TYR:HD2	1.57	0.68
1:A:86:SER:HB2	1:A:91:ALA:HB3	1.73	0.68
1:A:240:SER:O	1:A:242:ILE:HG13	1.96	0.66
1:B:145:PRO:HB3	1:B:184:MET:SD	2.37	0.65
1:A:506:ARG:HH11	1:A:506:ARG:HG2	1.61	0.65
1:A:638:LYS:HZ3	1:A:638:LYS:HA	1.62	0.63
1:A:515:LYS:HD2	6:A:1338:HOH:O	1.99	0.63
1:B:527:PRO:HB2	1:B:625:ALA:HB2	1.81	0.63
1:A:400:GLU:OE2	1:A:404:LYS:HE3	1.99	0.63
1:A:555:LYS:HE3	6:A:1383:HOH:O	1.98	0.62
1:B:123:SER:HA	6:B:1226:HOH:O	1.98	0.62
1:A:254:ASP:O	1:A:257:LYS:HG2	1.98	0.62
1:B:119:LEU:HG	1:B:152:PHE:CD1	2.35	0.62
1:B:501:GLY:H	1:B:506:ARG:NH1	1.98	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:551:ARG:HG3	1:A:557:VAL:HG21	1.83	0.61
1:B:164:THR:HA	1:B:196:GLY:O	2.01	0.60
1:B:123:SER:O	1:B:126:PRO:HD2	2.02	0.60
1:B:188:VAL:HG12	1:B:192:LEU:HD11	1.84	0.60
1:B:506:ARG:HA	1:B:506:ARG:HE	1.65	0.60
1:B:175:ASN:HB3	1:B:178:TYR:CD2	2.37	0.60
1:A:459:ALA:HA	1:A:538:ALA:O	2.02	0.60
1:A:514:ARG:HD2	6:A:1127:HOH:O	2.02	0.58
1:A:551:ARG:HG3	1:A:557:VAL:CG2	2.33	0.58
1:B:79:ASN:HD21	1:B:107:MET:CG	2.15	0.58
1:B:660:VAL:HG12	1:B:664:LYS:HE2	1.85	0.58
1:B:175:ASN:OD1	1:B:209:ASP:HB2	2.04	0.58
1:B:626:HIS:CD2	1:B:671:ARG:HG2	2.38	0.58
1:A:156:LEU:HB3	1:A:191:ARG:HG2	1.85	0.58
1:B:233:VAL:HG12	1:B:234:GLU:N	2.19	0.58
1:B:163:LEU:HA	6:B:1226:HOH:O	2.03	0.58
1:B:279:LYS:HG3	6:B:1238:HOH:O	2.03	0.58
1:B:105:TYR:O	1:B:233:VAL:HG11	2.03	0.57
1:B:581:ARG:NH1	6:B:802:HOH:O	2.36	0.57
1:B:120:ALA:HA	1:B:155:TRP:CZ2	2.39	0.57
1:B:475:ALA:HA	1:B:491:THR:HB	1.86	0.57
1:B:506:ARG:NE	1:B:506:ARG:HA	2.19	0.57
1:B:222:GLN:C	1:B:225:PRO:HD2	2.25	0.57
1:B:86:SER:CB	1:B:91:ALA:HB3	2.31	0.56
1:B:396:PRO:HG2	6:B:863:HOH:O	2.06	0.56
1:B:266:LEU:O	1:B:267:LYS:HB2	2.06	0.56
1:A:638:LYS:HZ2	1:A:638:LYS:HA	1.71	0.55
1:A:506:ARG:N	1:A:506:ARG:HD3	2.21	0.55
1:A:277:ASP:HB2	6:A:1196:HOH:O	2.06	0.55
1:B:217:ILE:HD11	1:B:383:THR:HG21	1.89	0.55
1:B:633:ALA:HB2	1:B:676:VAL:HB	1.88	0.55
1:B:203:LEU:HB3	6:B:871:HOH:O	2.07	0.54
1:A:300:LEU:HD22	1:A:574:LEU:HD21	1.90	0.54
1:B:223:PHE:O	1:B:227:VAL:HG23	2.07	0.54
1:B:182:ASN:O	1:B:186:LYS:HG3	2.07	0.54
1:A:78:ARG:HE	1:A:108:ARG:NE	2.06	0.54
1:B:549:TRP:O	1:B:553:GLN:NE2	2.38	0.53
1:B:548:ALA:O	1:B:552:GLU:HG2	2.08	0.53
1:B:255:VAL:HG23	6:B:1032:HOH:O	2.07	0.53
1:B:93:GLU:O	1:B:97:ARG:HG3	2.08	0.53
1:A:634:ARG:HD2	6:A:1152:HOH:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:LYS:HA	1:B:231:PHE:CD1	2.44	0.53
1:B:390:ALA:O	1:B:399:GLN:HG3	2.10	0.52
1:A:257:LYS:HB3	1:A:257:LYS:NZ	2.26	0.51
1:B:479:GLU:HG2	6:B:1001:HOH:O	2.10	0.51
1:B:170:VAL:O	1:B:203:LEU:HD12	2.10	0.51
1:A:581:ARG:NH1	1:A:585:ASP:OD2	2.43	0.51
1:B:385:VAL:HG13	1:B:447:LEU:HB3	1.93	0.51
1:B:73:MET:HB3	1:B:78:ARG:HB2	1.93	0.51
1:A:228:CYS:HA	1:A:233:VAL:CG2	2.41	0.50
1:A:68:SER:HA	6:A:904:HOH:O	2.10	0.50
1:B:167:LYS:HB3	1:B:200:ILE:CD1	2.37	0.50
1:B:353:GLU:CD	1:B:353:GLU:H	2.14	0.50
1:B:214:GLU:OE1	1:B:214:GLU:HA	2.12	0.50
1:B:300:LEU:HD22	1:B:574:LEU:HD11	1.94	0.50
1:A:267:LYS:HA	6:A:1203:HOH:O	2.12	0.50
1:B:98:LEU:O	1:B:224:TRP:HZ2	1.95	0.50
1:B:70:VAL:HA	1:B:73:MET:HE3	1.93	0.50
1:B:159:THR:O	1:B:191:ARG:NH2	2.45	0.49
1:A:96:ASN:O	1:A:100:LYS:HG3	2.13	0.49
1:B:402:LEU:HD11	1:B:437:LEU:HD22	1.94	0.49
1:A:321:ALA:HB2	1:A:455:TYR:CE1	2.48	0.49
1:A:76:THR:OG1	1:A:78:ARG:HD3	2.13	0.49
1:B:195:LEU:HD12	1:B:195:LEU:N	2.27	0.49
1:A:595:PHE:HB3	1:A:598:GLU:HG3	1.95	0.48
1:B:233:VAL:HG13	6:B:1126:HOH:O	2.11	0.48
1:B:70:VAL:HG23	1:B:71:GLU:N	2.28	0.48
1:A:119:LEU:HG	1:A:152:PHE:CD1	2.49	0.48
1:A:84:TYR:CE2	1:A:92:GLU:HG3	2.48	0.48
1:B:119:LEU:O	1:B:122:LEU:HG	2.14	0.48
1:A:132:LEU:HD12	1:A:167:LYS:O	2.14	0.48
1:A:228:CYS:HA	1:A:233:VAL:HG22	1.96	0.48
1:B:135:PHE:HB2	1:B:170:VAL:HG13	1.96	0.48
1:B:242:ILE:CB	6:B:844:HOH:O	2.61	0.48
1:B:568:ARG:HB3	6:B:1124:HOH:O	2.14	0.48
1:B:84:TYR:HB3	1:B:95:ALA:HB2	1.95	0.48
1:A:262:GLU:HG2	6:A:1203:HOH:O	2.14	0.47
1:B:82:VAL:HG13	1:B:134:VAL:HB	1.96	0.47
1:A:80:ILE:O	1:A:109:GLY:HA2	2.15	0.47
1:B:139:THR:HG22	1:B:140:TYR:N	2.29	0.47
1:B:187:TYR:O	1:B:191:ARG:HB2	2.15	0.47
1:A:244:GLN:HG2	6:A:972:HOH:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:GLU:OE2	1:B:148:ASN:HA	2.15	0.47
1:B:660:VAL:CG1	1:B:664:LYS:HE2	2.44	0.47
1:A:584:LYS:HD3	6:A:835:HOH:O	2.14	0.46
1:B:69:PHE:HE1	1:B:121:ASP:HB2	1.80	0.46
1:B:169:ALA:HA	6:B:833:HOH:O	2.14	0.46
1:B:247:LEU:HD12	1:B:248:VAL:H	1.80	0.46
1:A:155:TRP:CZ2	1:A:161:VAL:HG11	2.50	0.46
1:B:70:VAL:HA	1:B:73:MET:CE	2.45	0.46
1:B:80:ILE:HD11	1:B:107:MET:SD	2.55	0.46
1:B:126:PRO:C	1:B:128:ILE:H	2.19	0.46
1:B:246:GLU:HB2	1:B:351:LEU:HD21	1.97	0.46
1:A:629:VAL:HB	1:A:674:LEU:HD23	1.98	0.46
1:A:272:GLN:HA	6:A:937:HOH:O	2.16	0.45
1:B:103:HIS:C	1:B:105:TYR:H	2.20	0.45
1:B:69:PHE:CE1	1:B:121:ASP:HB2	2.52	0.45
1:B:133:VAL:CG1	1:B:133:VAL:O	2.65	0.45
1:B:656:HIS:O	1:B:660:VAL:HG23	2.15	0.45
1:A:161:VAL:HG23	6:A:1303:HOH:O	2.15	0.45
1:A:479:GLU:HB3	6:A:1222:HOH:O	2.17	0.45
1:A:78:ARG:NH2	1:A:352:ASP:OD2	2.48	0.45
1:B:547:ARG:O	1:B:551:ARG:HG3	2.17	0.45
1:A:80:ILE:HG23	1:A:109:GLY:HA3	1.99	0.45
1:A:159:THR:OG1	1:A:161:VAL:HG12	2.16	0.45
1:B:561:LEU:HD22	1:B:590:GLN:HB2	1.98	0.44
1:B:73:MET:CB	1:B:78:ARG:HB2	2.47	0.44
1:A:349:ASN:HB3	6:A:1071:HOH:O	2.17	0.44
1:B:660:VAL:O	1:B:664:LYS:HG3	2.17	0.44
1:A:652:GLY:N	1:A:653:PRO:HA	2.33	0.44
1:B:152:PHE:CE2	1:B:156:LEU:HD11	2.53	0.44
1:A:411:GLU:HG3	1:A:412:GLY:N	2.32	0.44
1:B:130:LYS:HA	1:B:231:PHE:HD1	1.83	0.44
1:B:213:GLU:O	1:B:217:ILE:HG13	2.18	0.44
1:B:79:ASN:HD21	1:B:107:MET:HG2	1.83	0.44
1:B:152:PHE:O	1:B:156:LEU:HG	2.17	0.43
1:B:214:GLU:CD	1:B:413:LYS:HE3	2.37	0.43
1:B:246:GLU:HB2	1:B:351:LEU:CD2	2.48	0.43
1:A:664:LYS:HE2	6:A:1223:HOH:O	2.17	0.43
1:B:101:ASP:OD2	1:B:220:ARG:NH2	2.51	0.43
1:B:378:THR:O	1:B:426:HIS:HB3	2.18	0.43
1:A:568:ARG:NH1	6:A:811:HOH:O	2.50	0.43
1:B:133:VAL:HG12	1:B:168:PHE:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:PHE:HA	1:B:72:LYS:HB2	2.00	0.43
1:B:84:TYR:CG	1:B:92:GLU:HA	2.53	0.43
1:B:159:THR:HG1	1:B:161:VAL:HG13	1.81	0.43
1:A:246:GLU:HB3	1:A:351:LEU:HD21	2.01	0.42
1:B:366:THR:HG23	6:B:993:HOH:O	2.18	0.42
1:B:563:TYR:CE2	1:B:609:LEU:HD23	2.54	0.42
1:B:327:ASP:OD1	1:B:329:ALA:HB3	2.19	0.42
1:B:76:THR:HG21	1:B:354:GLU:HG2	2.02	0.42
1:B:173:LEU:N	1:B:173:LEU:HD12	2.34	0.42
1:A:633:ALA:HB2	1:A:676:VAL:CB	2.45	0.42
1:B:81:ILE:HD12	1:B:110:MET:O	2.20	0.42
1:B:349:ASN:OD1	1:B:359:HIS:CE1	2.72	0.42
1:B:188:VAL:CG1	1:B:192:LEU:HD11	2.47	0.42
1:B:224:TRP:HB2	1:B:225:PRO:HD3	2.02	0.42
1:B:233:VAL:HG12	1:B:234:GLU:H	1.82	0.42
1:A:506:ARG:NH1	1:A:506:ARG:HG2	2.29	0.42
1:B:395:GLU:HA	1:B:396:PRO:HD2	1.86	0.42
1:B:448:LEU:HA	1:B:449:PRO:HD3	1.92	0.42
1:B:81:ILE:HG23	1:B:81:ILE:O	2.20	0.42
1:A:253:MET:SD	1:A:364:PRO:HG3	2.59	0.42
1:B:186:LYS:O	1:B:190:GLN:NE2	2.50	0.42
1:B:385:VAL:O	1:B:389:LEU:HG	2.20	0.41
1:B:214:GLU:OE2	1:B:413:LYS:HG3	2.20	0.41
1:B:672:TYR:HE1	1:B:674:LEU:HD21	1.85	0.41
1:A:374:TYR:HA	6:A:1028:HOH:O	2.21	0.41
1:A:519:ARG:HG2	1:A:519:ARG:HH11	1.85	0.41
1:A:559:GLU:HB3	1:A:561:LEU:CD1	2.51	0.41
1:B:529:ILE:HD13	1:B:616:LEU:HD22	2.02	0.41
1:A:617:TRP:CD1	1:A:651:PHE:HB3	2.56	0.41
1:B:376:ASP:OD2	1:B:379:ASN:ND2	2.48	0.41
1:A:564:TYR:CG	1:A:565:GLY:N	2.88	0.41
1:B:191:ARG:CD	1:B:195:LEU:HD11	2.51	0.41
1:B:84:TYR:CD2	1:B:92:GLU:HB2	2.56	0.41
1:A:222:GLN:C	1:A:225:PRO:HD2	2.41	0.41
1:A:409:SER:HA	1:A:413:LYS:HD3	2.03	0.41
1:B:184:MET:O	1:B:188:VAL:HG23	2.20	0.41
1:B:523:LYS:NZ	6:B:828:HOH:O	2.54	0.41
1:A:155:TRP:HZ2	1:A:161:VAL:HG11	1.86	0.41
1:A:254:ASP:HB2	1:A:257:LYS:CD	2.51	0.41
1:A:69:PHE:HB3	1:A:117:TYR:CD1	2.56	0.40
1:A:68:SER:HB2	1:A:121:ASP:OD2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:VAL:HG13	1:B:133:VAL:O	2.20	0.40
1:B:359:HIS:HB3	1:B:360:PRO:HD2	2.03	0.40
1:B:526:THR:HA	1:B:527:PRO:HD3	1.92	0.40
1:A:581:ARG:NE	6:A:835:HOH:O	2.55	0.40
1:B:133:VAL:O	1:B:168:PHE:HA	2.22	0.40
1:B:233:VAL:CG1	1:B:234:GLU:N	2.85	0.40
1:B:79:ASN:ND2	1:B:107:MET:HG2	2.36	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	605/621 (97%)	586 (97%)	19 (3%)	0	100	100
1	B	599/621 (96%)	566 (94%)	33 (6%)	0	100	100
All	All	1204/1242 (97%)	1152 (96%)	52 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	522/531 (98%)	509 (98%)	13 (2%)	55	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	508/531 (96%)	497 (98%)	11 (2%)	60	72
All	All	1030/1062 (97%)	1006 (98%)	24 (2%)	58	71

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	SER
1	A	78	ARG
1	A	88	THR
1	A	179	GLU
1	A	234	GLU
1	A	257	LYS
1	A	346	MET
1	A	411	GLU
1	A	484	ARG
1	A	506	ARG
1	A	573	TYR
1	A	638	LYS
1	A	672	TYR
1	B	101	ASP
1	B	191	ARG
1	B	192	LEU
1	B	251	GLU
1	B	253	MET
1	B	346	MET
1	B	356	ASN
1	B	442	ASP
1	B	506	ARG
1	B	553	GLN
1	B	573	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	359	HIS

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 ⓘ

7 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	FMN	A	701	-	32,33,33	2.97	15 (46%)	34,50,50	3.66	14 (41%)
3	FAD	A	702	-	52,58,58	2.14	11 (21%)	52,89,89	2.57	9 (17%)
4	NAP	A	703	-	28,33,52	1.55	3 (10%)	35,52,80	2.64	3 (8%)
2	FMN	B	701	-	32,33,33	2.96	13 (40%)	34,50,50	3.69	14 (41%)
3	FAD	B	702	-	52,58,58	2.14	11 (21%)	52,89,89	2.55	8 (15%)
4	NAP	B	703	-	28,33,52	1.55	3 (10%)	35,52,80	2.62	4 (11%)
5	PO4	B	704	-	4,4,4	1.40	0	6,6,6	0.23	0

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	FMN	A	701	-	-	0/18/18/18	0/3/3/3
3	FAD	A	702	-	-	0/30/50/50	0/6/6/6
4	NAP	A	703	-	-	0/17/37/67	0/3/3/5
2	FMN	B	701	-	-	0/18/18/18	0/3/3/3
3	FAD	B	702	-	-	0/30/50/50	0/6/6/6
4	NAP	B	703	-	-	0/17/37/67	0/3/3/5
5	PO4	B	704	-	-	0/0/0/0	0/0/0/0

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	FMN	C8M-C8	-6.53	1.38	1.51
2	A	701	FMN	C8M-C8	-6.18	1.38	1.51
3	A	702	FAD	C8M-C8	-5.84	1.39	1.51
3	B	702	FAD	C8M-C8	-5.79	1.39	1.51
3	A	702	FAD	C7M-C7	-5.78	1.39	1.51
3	B	702	FAD	C7M-C7	-5.77	1.39	1.51
3	A	702	FAD	C10-N10	-4.11	1.34	1.39
3	B	702	FAD	C10-N10	-3.98	1.34	1.39
4	A	703	NAP	C5A-C4A	-3.04	1.33	1.40
4	B	703	NAP	C5A-C4A	-3.02	1.33	1.40
3	A	702	FAD	C9A-N10	-2.97	1.34	1.38
3	B	702	FAD	C9A-N10	-2.96	1.34	1.38
3	A	702	FAD	C5A-C4A	-2.94	1.33	1.40
3	B	702	FAD	C5A-C4A	-2.93	1.33	1.40
2	A	701	FMN	C1'-N10	-2.52	1.45	1.48
2	B	701	FMN	C1'-N10	-2.24	1.46	1.48
3	A	702	FAD	O4B-C1B	2.06	1.44	1.41
2	A	701	FMN	C6-C5A	2.10	1.45	1.41
3	B	702	FAD	O4B-C1B	2.13	1.44	1.41
2	A	701	FMN	C4'-C3'	2.17	1.57	1.53
2	B	701	FMN	C4'-C3'	2.23	1.57	1.53
2	A	701	FMN	C7M-C7	2.24	1.55	1.51
2	B	701	FMN	O2'-C2'	2.33	1.48	1.43
2	B	701	FMN	C10-N1	2.37	1.39	1.35
2	A	701	FMN	C10-N1	2.39	1.39	1.35
2	A	701	FMN	O2'-C2'	2.39	1.48	1.43
2	B	701	FMN	C9A-C5A	2.43	1.47	1.42
2	A	701	FMN	C9A-C5A	2.54	1.47	1.42
3	A	702	FAD	C10-N1	2.83	1.40	1.35
3	B	702	FAD	C10-N1	2.86	1.40	1.35
2	A	701	FMN	C9-C9A	2.97	1.47	1.40
2	B	701	FMN	C9-C9A	3.09	1.47	1.40
3	A	702	FAD	C2A-N1A	3.28	1.40	1.33
3	B	702	FAD	C2A-N1A	3.29	1.40	1.33
4	B	703	NAP	C2A-N1A	3.33	1.40	1.33
2	B	701	FMN	C5A-N5	3.34	1.40	1.35
4	A	703	NAP	C2A-N1A	3.34	1.40	1.33
2	A	701	FMN	C5A-N5	3.34	1.40	1.35
2	B	701	FMN	C8-C7	3.37	1.50	1.41
2	A	701	FMN	C8-C7	3.52	1.50	1.41
2	B	701	FMN	C4-N3	4.06	1.40	1.33
3	A	702	FAD	C4-N3	4.10	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	702	FAD	C4-N3	4.11	1.40	1.33
2	A	701	FMN	C4-N3	4.17	1.40	1.33
4	B	703	NAP	C2A-N3A	4.60	1.40	1.32
3	A	702	FAD	C2A-N3A	4.60	1.40	1.32
4	A	703	NAP	C2A-N3A	4.65	1.40	1.32
3	B	702	FAD	C2A-N3A	4.68	1.40	1.32
2	B	701	FMN	C4A-N5	5.79	1.42	1.33
2	A	701	FMN	C4A-N5	5.84	1.42	1.33
2	A	701	FMN	C9A-N10	6.43	1.47	1.38
2	B	701	FMN	C9A-N10	6.70	1.48	1.38
3	B	702	FAD	C8A-N7A	6.99	1.48	1.34
3	A	702	FAD	C8A-N7A	7.00	1.48	1.34
2	B	701	FMN	C10-N10	7.65	1.48	1.39
2	A	701	FMN	C10-N10	7.86	1.48	1.39

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	702	FAD	N3A-C2A-N1A	-14.76	117.28	128.87
3	B	702	FAD	N3A-C2A-N1A	-14.54	117.45	128.87
4	A	703	NAP	N3A-C2A-N1A	-14.07	117.82	128.87
4	B	703	NAP	N3A-C2A-N1A	-14.03	117.85	128.87
2	B	701	FMN	C4-C4A-C10	-7.93	114.87	119.94
2	A	701	FMN	C4-C4A-C10	-7.81	114.95	119.94
2	B	701	FMN	N3-C2-N1	-6.58	116.61	127.69
2	A	701	FMN	N3-C2-N1	-6.49	116.75	127.69
2	A	701	FMN	C4A-C10-N10	-5.49	116.53	120.52
2	B	701	FMN	C4A-C10-N10	-5.48	116.54	120.52
2	A	701	FMN	C4A-C4-N3	-5.45	116.40	123.52
2	B	701	FMN	C4A-C4-N3	-5.33	116.56	123.52
3	A	702	FAD	N3-C2-N1	-4.79	119.63	127.69
3	B	702	FAD	N3-C2-N1	-4.72	119.74	127.69
2	A	701	FMN	O4'-C4'-C3'	-3.34	100.36	108.96
3	A	702	FAD	C4B-O4B-C1B	-3.33	106.11	109.64
2	B	701	FMN	O4'-C4'-C3'	-3.31	100.44	108.96
3	B	702	FAD	C4B-O4B-C1B	-3.16	106.29	109.64
4	A	703	NAP	C4B-O4B-C1B	-3.08	106.38	109.64
3	B	702	FAD	C4X-C4-N3	-2.94	119.67	123.52
2	B	701	FMN	C6-C5A-N5	-2.86	115.36	118.92
2	B	701	FMN	C5A-C9A-N10	-2.80	115.48	117.58
3	A	702	FAD	C4X-C4-N3	-2.72	119.97	123.52
2	A	701	FMN	C6-C5A-N5	-2.71	115.53	118.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	703	NAP	C4B-O4B-C1B	-2.63	106.86	109.64
3	B	702	FAD	C2B-C3B-C4B	-2.54	97.44	102.64
2	A	701	FMN	C5A-C9A-N10	-2.53	115.68	117.58
2	B	701	FMN	O3P-P-O5'	-2.32	99.96	106.72
2	A	701	FMN	C4A-N5-C5A	-2.26	114.06	116.72
2	B	701	FMN	C4A-N5-C5A	-2.25	114.07	116.72
4	A	703	NAP	C3B-C2B-C1B	-2.24	98.35	102.63
4	B	703	NAP	C3B-C2B-C1B	-2.18	98.45	102.63
2	A	701	FMN	O4'-C4'-C5'	-2.13	105.44	110.09
4	B	703	NAP	C1B-N9A-C4A	-2.13	124.43	126.81
3	A	702	FAD	C2B-C3B-C4B	-2.07	98.39	102.64
2	A	701	FMN	O3P-P-O5'	-2.05	100.75	106.72
2	B	701	FMN	O4'-C4'-C5'	-2.01	105.71	110.09
3	A	702	FAD	C1'-N10-C9A	2.04	121.19	118.83
2	B	701	FMN	C8M-C8-C7	2.47	126.05	120.73
2	A	701	FMN	C8M-C8-C7	2.53	126.17	120.73
3	A	702	FAD	C4X-N5-C5X	2.61	119.80	116.72
2	A	701	FMN	C9A-C5A-N5	2.73	126.62	122.18
3	B	702	FAD	C4X-N5-C5X	2.74	119.95	116.72
2	B	701	FMN	C9A-C5A-N5	2.77	126.68	122.18
3	B	702	FAD	C5X-C9A-N10	2.80	119.67	117.58
2	A	701	FMN	O2P-P-O1P	2.81	119.80	110.63
2	B	701	FMN	O2P-P-O1P	2.83	119.88	110.63
3	A	702	FAD	C5X-C9A-N10	3.00	119.83	117.58
3	A	702	FAD	C4-N3-C2	5.96	120.13	115.16
3	B	702	FAD	C4-N3-C2	6.03	120.18	115.16
2	B	701	FMN	C4-N3-C2	14.73	127.45	115.16
2	A	701	FMN	C4-N3-C2	14.74	127.46	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	611/621 (98%)	-0.34	11 (1%) 71 70	15, 28, 46, 86	0
1	B	605/621 (97%)	0.29	59 (9%) 10 8	16, 35, 86, 99	0
All	All	1216/1242 (97%)	-0.03	70 (5%) 26 26	15, 30, 82, 99	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	133	VAL	7.7
1	B	135	PHE	7.2
1	B	134	VAL	6.8
1	B	254	ASP	4.9
1	B	233	VAL	4.8
1	B	82	VAL	4.6
1	B	137	MET	4.5
1	B	501	GLY	4.4
1	B	136	CYS	4.4
1	B	120	ALA	4.4
1	B	160	ASP	4.3
1	B	188	VAL	4.3
1	A	505	GLY	4.2
1	B	166	VAL	4.1
1	B	64	VAL	4.0
1	B	106	GLY	4.0
1	B	500	ALA	3.9
1	A	506	ARG	3.8
1	B	181	PHE	3.8
1	A	238	GLU	3.8
1	B	187	TYR	3.8
1	A	500	ALA	3.7
1	B	132	LEU	3.5
1	B	232	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	71	GLU	3.4
1	B	173	LEU	3.4
1	B	158	GLU	3.3
1	B	103	HIS	3.3
1	B	72	LYS	3.3
1	B	235	ALA	3.2
1	B	76	THR	3.2
1	B	176	LYS	3.1
1	A	252	ASP	3.1
1	B	83	PHE	3.1
1	B	123	SER	3.1
1	B	168	PHE	2.9
1	B	192	LEU	2.9
1	B	163	LEU	2.9
1	B	162	ASP	2.8
1	B	80	ILE	2.8
1	B	170	VAL	2.7
1	B	194	GLN	2.7
1	A	255	VAL	2.6
1	B	152	PHE	2.5
1	A	236	THR	2.5
1	A	134	VAL	2.5
1	B	255	VAL	2.5
1	B	161	VAL	2.5
1	B	102	ALA	2.5
1	A	273	LYS	2.5
1	B	164	THR	2.4
1	B	253	MET	2.4
1	B	355	SER	2.4
1	B	180	HIS	2.4
1	B	122	LEU	2.3
1	B	104	ARG	2.3
1	B	157	GLN	2.3
1	B	66	GLU	2.3
1	B	69	PHE	2.2
1	B	358	LYS	2.2
1	B	169	ALA	2.2
1	B	125	LEU	2.1
1	A	133	VAL	2.1
1	B	191	ARG	2.1
1	B	634	ARG	2.1
1	B	171	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	154	ASP	2.1
1	B	78	ARG	2.1
1	A	135	PHE	2.1
1	B	206	GLY	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	FMN	A	701	31/31	0.94	0.13	0.27	29,35,39,40	0
2	FMN	B	701	31/31	0.87	0.20	-0.04	57,73,74,74	0
4	NAP	B	703	31/48	0.97	0.09	-0.42	17,21,43,48	0
3	FAD	B	702	53/53	0.97	0.09	-0.53	12,19,25,29	0
4	NAP	A	703	31/48	0.98	0.08	-0.84	17,20,44,50	0
3	FAD	A	702	53/53	0.97	0.08	-0.91	16,20,28,30	0
5	PO4	B	704	5/5	0.73	0.30	-	98,99,99,99	0

6.5 Other polymers [i](#)

There are no such residues in this entry.