



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 5, 2018 – 12:20 PM EST

PDB ID : 5URE
Title : Wild type rat CYPOR bound with NADP+ - reduced form
Authors : Xia, C.; Kim, J.J.
Deposited on : 2017-02-10
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030736
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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-20030736

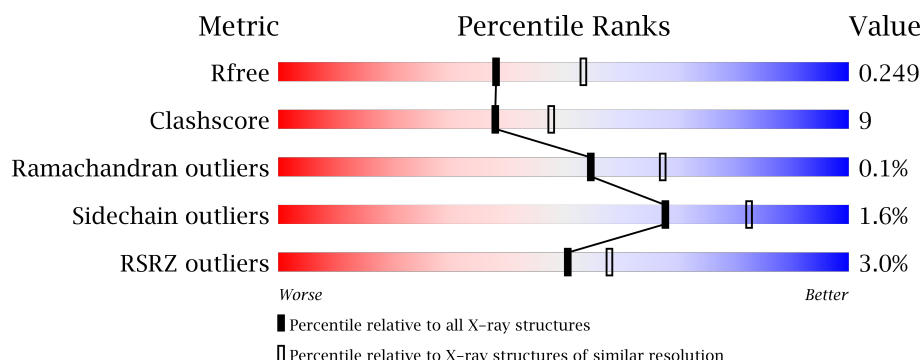
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	622	
1	B	622	

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	PO4	A	704	-	-	-	X

2 Entry composition [i](#)

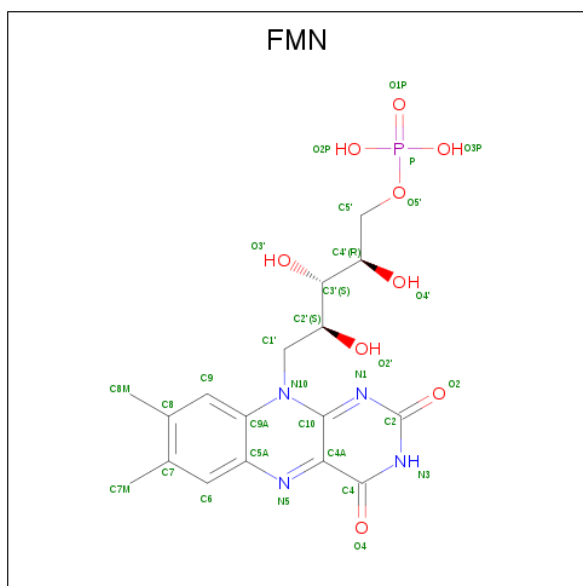
There are 6 unique types of molecules in this entry. The entry contains 10482 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	608	Total	C	N	O	S	0	0	0
			4875	3090	837	925	23			
1	B	607	Total	C	N	O	S	0	0	0
			4850	3072	836	919	23			

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



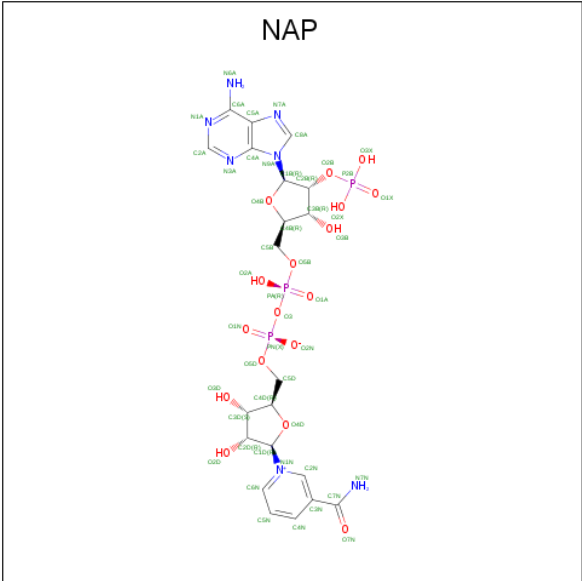
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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: C₂₁H₂₈N₇O₁₇P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

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



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

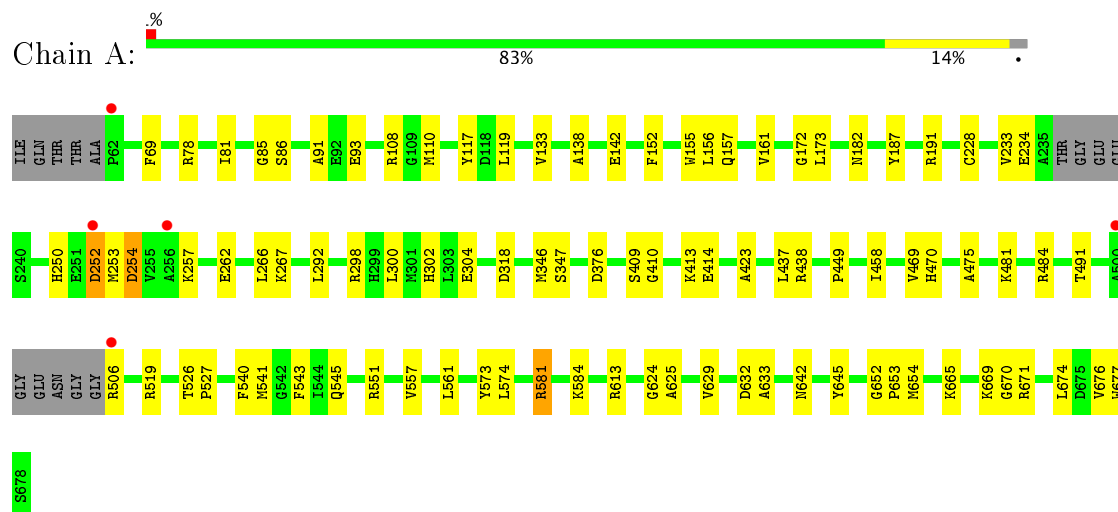
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	301	Total	O	0	0
			301	301		
6	B	182	Total	O	0	0
			182	182		

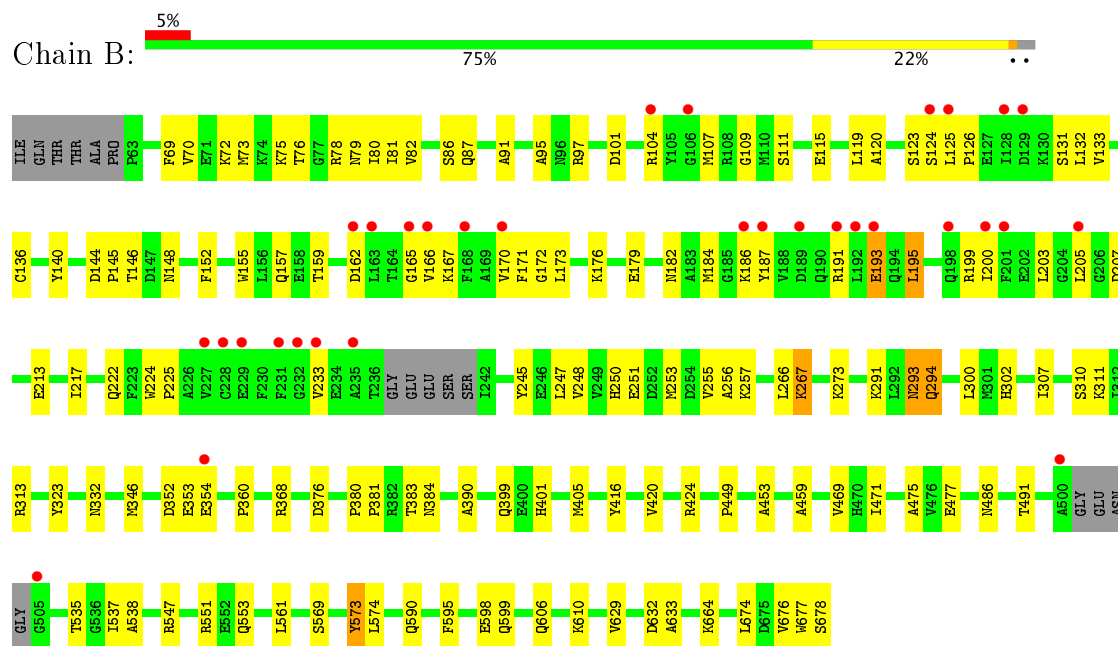
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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	102.09Å 114.98Å 118.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.86 – 2.30 46.86 – 2.28	Depositor EDS
% Data completeness (in resolution range)	94.3 (46.86-2.30) 93.1 (46.86-2.28)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 2.29Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.199 , 0.249 0.199 , 0.249	Depositor DCC
R_{free} test set	2974 reflections (5.05%)	DCC
Wilson B-factor (Å ²)	34.9	Xtriage
Anisotropy	0.551	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 30.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.012 for -h,l,k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10482	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.22% 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	0.37	0/4992	0.61	4/6755 (0.1%)
1	B	0.34	0/4966	0.62	4/6719 (0.1%)
All	All	0.36	0/9958	0.61	8/13474 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	193	GLU	CB-CA-C	-7.47	95.46	110.40
1	B	233	VAL	N-CA-C	6.88	129.57	111.00
1	A	253	MET	N-CA-CB	-6.12	99.59	110.60
1	B	195	LEU	N-CA-CB	-5.81	98.78	110.40
1	A	252	ASP	N-CA-C	5.68	126.35	111.00
1	B	233	VAL	N-CA-CB	-5.11	100.25	111.50
1	A	654	MET	CB-CA-C	5.05	120.51	110.40
1	A	85	GLY	N-CA-C	-5.01	100.56	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	4875	0	4722	56	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	4850	0	4677	109	0
2	A	31	0	19	0	0
2	B	31	0	19	0	0
3	A	53	0	31	1	0
3	B	53	0	31	1	0
4	A	48	0	25	4	0
4	B	48	0	25	8	0
5	A	5	0	0	0	0
5	B	5	0	0	0	0
6	A	301	0	0	3	0
6	B	182	0	0	3	0
All	All	10482	0	9549	169	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 9.

All (169) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:633:ALA:HB2	1:A:676:VAL:HB	1.49	0.95
1:B:193:GLU:HG2	1:B:193:GLU:O	1.72	0.89
1:B:293:ASN:HD22	1:B:293:ASN:H	1.30	0.79
1:A:257:LYS:HA	1:A:266:LEU:HD21	1.65	0.78
1:B:86:SER:HB2	1:B:91:ALA:HB3	1.68	0.75
1:B:294:GLN:NE2	1:B:294:GLN:H	1.85	0.74
1:B:266:LEU:HG	1:B:267:LYS:HD2	1.69	0.74
1:B:293:ASN:HD22	1:B:293:ASN:N	1.88	0.71
1:A:300:LEU:HD22	1:A:574:LEU:HD21	1.72	0.70
1:B:155:TRP:O	1:B:159:THR:HG22	1.92	0.69
1:B:595:PHE:HB3	1:B:598:GLU:HG3	1.74	0.69
1:A:86:SER:HB2	1:A:91:ALA:HB3	1.74	0.67
1:B:159:THR:HG23	1:B:159:THR:O	1.94	0.67
4:B:703:NAP:PA	4:B:703:NAP:H52N	2.35	0.67
1:B:70:VAL:HG21	1:B:124:SER:HB2	1.78	0.66
1:B:167:LYS:HB3	1:B:200:ILE:HD11	1.77	0.65
1:B:182:ASN:O	1:B:186:LYS:HG3	1.98	0.64
1:B:253:MET:HE1	1:B:257:LYS:HD2	1.81	0.63
1:B:632:ASP:HB2	4:B:703:NAP:O4D	1.98	0.63
1:B:125:LEU:HD23	1:B:166:VAL:HG13	1.81	0.63
1:B:561:LEU:HD22	1:B:590:GLN:HB2	1.80	0.62
1:A:506:ARG:HG3	1:A:506:ARG:HH11	1.65	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:LEU:HD12	1:B:167:LYS:O	2.00	0.62
1:B:678:SER:C	4:B:703:NAP:H5N	2.21	0.61
1:B:191:ARG:O	1:B:195:LEU:HB2	2.02	0.60
1:B:145:PRO:HB3	1:B:184:MET:SD	2.42	0.60
1:B:80:ILE:O	1:B:109:GLY:HA2	2.01	0.59
1:A:581:ARG:HH21	1:A:584:LYS:HD2	1.68	0.59
1:A:437:LEU:O	1:A:438:ARG:HD3	2.04	0.58
1:A:78:ARG:HH11	1:A:78:ARG:HG2	1.69	0.58
1:B:87:GLN:HG2	1:B:146:THR:HG22	1.84	0.58
1:B:273:LYS:NZ	1:B:273:LYS:HB3	2.19	0.58
3:A:702:FAD:H1'2	4:A:703:NAP:N7N	2.18	0.58
1:B:255:VAL:HG23	1:B:256:ALA:N	2.19	0.58
1:A:541:MET:O	1:A:545:GLN:HG3	2.03	0.57
1:B:390:ALA:O	1:B:399:GLN:HG3	2.04	0.57
1:A:119:LEU:HG	1:A:152:PHE:CD1	2.40	0.57
1:A:172:GLY:C	1:A:182:ASN:HD21	2.08	0.56
1:B:250:HIS:HB3	1:B:253:MET:HB2	1.88	0.56
1:B:401:HIS:O	1:B:405:MET:HG2	2.06	0.56
1:B:76:THR:HB	1:B:78:ARG:HG2	1.87	0.55
1:B:125:LEU:HB3	1:B:166:VAL:HG22	1.87	0.55
1:B:81:ILE:HG23	1:B:133:VAL:HG23	1.88	0.55
1:B:199:ARG:HB3	1:B:199:ARG:HH11	1.72	0.55
1:A:410:GLY:O	1:A:414:GLU:HG3	2.05	0.55
1:B:125:LEU:N	1:B:126:PRO:HD2	2.22	0.54
1:B:291:LYS:HZ2	1:B:293:ASN:HD21	1.55	0.54
1:A:228:CYS:HA	1:A:233:VAL:HG22	1.90	0.54
1:A:632:ASP:HB2	4:A:703:NAP:O4D	2.07	0.53
1:B:633:ALA:HB2	1:B:676:VAL:HB	1.90	0.53
1:A:633:ALA:CB	1:A:676:VAL:HB	2.30	0.52
1:B:70:VAL:HG11	1:B:124:SER:O	2.10	0.52
1:B:87:GLN:HG3	1:B:140:TYR:CG	2.45	0.52
1:B:255:VAL:HG23	1:B:256:ALA:H	1.74	0.52
1:A:629:VAL:HB	1:A:674:LEU:HD23	1.92	0.51
1:A:642:ASN:HA	1:A:645:TYR:CD2	2.45	0.51
1:A:409:SER:HA	1:A:413:LYS:HD3	1.93	0.51
1:B:87:GLN:HG3	1:B:140:TYR:CD1	2.45	0.51
1:B:310:SER:O	1:B:311:LYS:HB2	2.09	0.51
1:B:678:SER:O	4:B:703:NAP:H5N	2.11	0.51
1:B:159:THR:CG2	1:B:159:THR:O	2.59	0.51
1:B:79:ASN:O	1:B:131:SER:HA	2.10	0.51
1:B:170:VAL:HG12	1:B:171:PHE:N	2.26	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:HIS:HE1	1:A:347:SER:OG	1.93	0.50
1:B:82:VAL:O	1:B:111:SER:HA	2.12	0.50
1:B:115:GLU:HB2	1:B:148:ASN:O	2.11	0.50
1:B:155:TRP:CE2	1:B:159:THR:HG21	2.47	0.50
1:B:294:GLN:HE21	1:B:294:GLN:H	1.60	0.50
1:A:292:LEU:HD11	1:A:302:HIS:HB2	1.94	0.50
1:B:424:ARG:HD3	6:B:967:HOH:O	2.09	0.50
1:B:213:GLU:O	1:B:217:ILE:HG13	2.11	0.49
1:A:458:ILE:HG23	1:A:469:VAL:HG13	1.95	0.49
1:B:217:ILE:HD11	1:B:383:THR:HG21	1.93	0.49
1:A:304:GLU:HG2	1:A:470:HIS:CD2	2.48	0.49
1:B:293:ASN:ND2	1:B:293:ASN:H	2.03	0.49
1:B:123:SER:O	1:B:126:PRO:HD2	2.11	0.49
1:B:179:GLU:OE1	1:B:664:LYS:HD2	2.12	0.49
1:B:173:LEU:N	1:B:173:LEU:HD12	2.28	0.49
1:B:245:TYR:CE2	1:B:360:PRO:HD3	2.48	0.49
1:B:97:ARG:CZ	1:B:384:ASN:HB3	2.43	0.49
1:A:228:CYS:HA	1:A:233:VAL:CG2	2.43	0.48
4:B:703:NAP:H52N	4:B:703:NAP:O5B	2.13	0.48
1:B:170:VAL:HB	1:B:203:LEU:HD13	1.95	0.48
1:A:632:ASP:HB2	4:A:703:NAP:C4D	2.43	0.48
1:A:157:GLN:HG2	1:A:187:TYR:OH	2.14	0.48
1:B:80:ILE:HD11	1:B:107:MET:SD	2.54	0.48
1:A:298:ARG:NH2	4:A:703:NAP:O1N	2.46	0.48
1:B:120:ALA:HA	1:B:155:TRP:CZ2	2.49	0.47
1:A:93:GLU:OE1	1:A:93:GLU:HA	2.14	0.47
1:B:302:HIS:HA	1:B:471:ILE:O	2.14	0.47
1:B:352:ASP:C	1:B:354:GLU:H	2.18	0.47
1:B:537:ILE:HG13	1:B:537:ILE:O	2.14	0.47
1:A:670:GLY:HA2	6:A:1044:HOH:O	2.15	0.47
1:B:245:TYR:CD2	1:B:360:PRO:HD3	2.51	0.46
1:B:376:ASP:HB3	1:B:449:PRO:HG2	1.96	0.46
1:B:222:GLN:C	1:B:225:PRO:HD2	2.35	0.46
1:A:561:LEU:HD12	1:A:561:LEU:N	2.31	0.45
1:B:205:LEU:N	1:B:205:LEU:HD22	2.31	0.45
1:B:475:ALA:HA	1:B:491:THR:HB	1.98	0.45
1:B:323:TYR:CE1	1:B:453:ALA:HB2	2.51	0.45
1:A:527:PRO:HB2	1:A:625:ALA:HB2	1.98	0.45
1:A:633:ALA:HB2	1:A:676:VAL:CB	2.35	0.45
1:B:86:SER:HA	1:B:146:THR:HG21	1.98	0.45
1:B:332:ASN:OD1	1:B:368:ARG:NH1	2.47	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:ASP:O	1:A:257:LYS:HG2	2.17	0.45
1:B:176:LYS:HZ2	1:B:207:ASP:HB2	1.81	0.45
1:B:75:LYS:HD2	1:B:75:LYS:O	2.17	0.45
1:A:262:GLU:HG2	6:A:1034:HOH:O	2.17	0.44
1:B:569:SER:HA	1:B:573:TYR:HB2	1.99	0.44
1:B:313:ARG:HA	6:B:851:HOH:O	2.17	0.44
1:B:547:ARG:O	1:B:551:ARG:HG3	2.17	0.44
1:A:78:ARG:HH11	1:A:108:ARG:HG2	1.83	0.44
1:A:581:ARG:HG2	6:A:1064:HOH:O	2.16	0.44
1:B:101:ASP:HB2	1:B:224:TRP:CZ2	2.52	0.44
1:B:76:THR:HG21	1:B:78:ARG:HE	1.81	0.44
1:A:376:ASP:HB3	1:A:449:PRO:HG2	1.99	0.44
1:A:665:LYS:HE2	1:A:669:LYS:HE3	1.99	0.44
1:B:133:VAL:HG13	1:B:133:VAL:O	2.17	0.44
1:B:222:GLN:O	1:B:225:PRO:HD2	2.17	0.44
1:B:91:ALA:HB1	1:B:136:CYS:O	2.18	0.44
1:B:247:LEU:HG	1:B:248:VAL:N	2.33	0.44
1:B:253:MET:CE	1:B:257:LYS:HD2	2.48	0.44
1:A:551:ARG:HG3	1:A:557:VAL:HG21	2.00	0.44
1:A:266:LEU:O	1:A:267:LYS:HB2	2.18	0.43
1:A:318:ASP:OD1	1:A:519:ARG:NH2	2.44	0.43
1:A:540:PHE:HA	1:A:543:PHE:HB2	1.99	0.43
1:A:173:LEU:N	1:A:182:ASN:HD21	2.15	0.43
1:B:352:ASP:O	1:B:354:GLU:N	2.52	0.43
1:A:652:GLY:N	1:A:653:PRO:HA	2.33	0.43
1:B:535:THR:HG23	4:B:703:NAP:O2N	2.19	0.43
1:B:307:ILE:HD13	1:B:469:VAL:HG23	2.01	0.43
1:A:78:ARG:CD	1:A:110:MET:HB3	2.49	0.42
1:B:172:GLY:HA3	1:B:182:ASN:HD21	1.83	0.42
1:B:82:VAL:HG11	1:B:95:ALA:HA	2.01	0.42
1:B:104:ARG:HB3	1:B:104:ARG:HH11	1.84	0.42
1:B:97:ARG:NH2	1:B:384:ASN:HB3	2.34	0.42
1:B:199:ARG:CB	1:B:199:ARG:NH1	2.82	0.42
1:B:266:LEU:O	1:B:267:LYS:HB2	2.18	0.42
1:A:138:ALA:HA	1:A:173:LEU:HB2	2.02	0.42
1:A:526:THR:HA	1:A:527:PRO:HD3	1.85	0.42
1:A:475:ALA:HA	1:A:491:THR:HB	2.00	0.42
1:B:300:LEU:HD22	1:B:574:LEU:HD11	2.02	0.42
1:B:459:ALA:HA	1:B:538:ALA:O	2.19	0.42
1:A:250:HIS:CE1	1:A:347:SER:OG	2.72	0.42
1:B:380:PRO:HA	1:B:381:PRO:HD3	1.93	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:599:GLN:CD	1:B:599:GLN:N	2.74	0.42
3:B:702:FAD:HM73	6:B:842:HOH:O	2.20	0.41
1:A:155:TRP:CZ2	1:A:161:VAL:HG11	2.55	0.41
1:B:291:LYS:NZ	1:B:293:ASN:HD21	2.17	0.41
1:B:629:VAL:HB	1:B:674:LEU:HD23	2.01	0.41
1:A:81:ILE:HG23	1:A:133:VAL:HG23	2.02	0.41
1:A:624:GLY:HA2	1:A:671:ARG:NH2	2.35	0.41
1:A:613:ARG:HG2	1:A:613:ARG:HH11	1.85	0.41
1:B:416:TYR:O	1:B:420:VAL:HB	2.20	0.41
1:B:69:PHE:O	1:B:73:MET:HG3	2.21	0.41
1:B:632:ASP:HB2	4:B:703:NAP:C4D	2.51	0.41
1:A:423:ALA:HA	1:A:481:LYS:HB2	2.03	0.41
1:B:119:LEU:HG	1:B:152:PHE:CD1	2.56	0.41
1:B:72:LYS:HE2	1:B:354:GLU:O	2.21	0.41
1:A:156:LEU:HB3	1:A:191:ARG:HG2	2.03	0.41
1:B:477:GLU:HA	1:B:486:ASN:O	2.21	0.41
1:B:610:LYS:HD2	1:B:610:LYS:HA	1.84	0.41
1:B:162:ASP:HA	1:B:195:LEU:O	2.21	0.40
1:B:157:GLN:NE2	1:B:187:TYR:OH	2.54	0.40
1:B:273:LYS:NZ	1:B:273:LYS:CB	2.85	0.40
1:A:252:ASP:CG	1:A:252:ASP:O	2.59	0.40
1:A:69:PHE:HB3	1:A:117:TYR:CD2	2.56	0.40
1:B:126:PRO:HB3	1:B:165:GLY:O	2.22	0.40
1:B:606:GLN:OE1	4:B:703:NAP:H2A	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	602/622 (97%)	581 (96%)	21 (4%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	601/622 (97%)	564 (94%)	36 (6%)	1 (0%)	51 63
All	All	1203/1244 (97%)	1145 (95%)	57 (5%)	1 (0%)	55 67

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	353	GLU

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	521/531 (98%)	513 (98%)	8 (2%)	70 83
1	B	513/531 (97%)	504 (98%)	9 (2%)	64 79
All	All	1034/1062 (97%)	1017 (98%)	17 (2%)	68 82

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	142	GLU
1	A	234	GLU
1	A	254	ASP
1	A	346	MET
1	A	484	ARG
1	A	573	TYR
1	A	581	ARG
1	A	677	TRP
1	B	144	ASP
1	B	251	GLU
1	B	267	LYS
1	B	293	ASN
1	B	294	GLN
1	B	346	MET
1	B	553	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	573	TYR
1	B	677	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	182	ASN
1	A	250	HIS
1	A	359	HIS
1	A	399	GLN
1	A	403	HIS
1	A	470	HIS
1	B	157	GLN
1	B	293	ASN
1	B	294	GLN
1	B	399	GLN
1	B	583	HIS
1	B	641	GLN

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](#)

8 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	-	31,33,33	2.72	11 (35%)	38,50,50	3.36	19 (50%)
3	FAD	A	702	-	51,58,58	2.20	10 (19%)	54,89,89	2.34	10 (18%)
4	NAP	A	703	-	44,52,52	1.72	6 (13%)	51,80,80	2.14	6 (11%)
5	PO4	A	704	-	4,4,4	1.38	0	6,6,6	0.39	0
2	FMN	B	701	-	31,33,33	2.87	13 (41%)	38,50,50	3.41	16 (42%)
3	FAD	B	702	-	51,58,58	2.21	10 (19%)	54,89,89	2.29	10 (18%)
4	NAP	B	703	-	44,52,52	1.72	5 (11%)	51,80,80	2.11	6 (11%)
5	PO4	B	704	-	4,4,4	1.36	0	6,6,6	0.38	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	-	-	0/16/18/18	0/3/3/3
3	FAD	A	702	-	-	0/28/50/50	0/6/6/6
4	NAP	A	703	-	-	0/27/67/67	0/5/5/5
5	PO4	A	704	-	-	0/0/0/0	0/0/0/0
2	FMN	B	701	-	-	0/16/18/18	0/3/3/3
3	FAD	B	702	-	-	0/28/50/50	0/6/6/6
4	NAP	B	703	-	-	0/27/67/67	0/5/5/5
5	PO4	B	704	-	-	0/0/0/0	0/0/0/0

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	703	NAP	C3N-C7N	-7.10	1.39	1.50
4	A	703	NAP	C3N-C7N	-7.02	1.39	1.50
2	B	701	FMN	C8M-C8	-6.47	1.38	1.51
2	A	701	FMN	C8M-C8	-6.23	1.38	1.51
3	A	702	FAD	C8M-C8	-5.85	1.39	1.51
3	B	702	FAD	C8M-C8	-5.82	1.39	1.51
3	B	702	FAD	C7M-C7	-5.82	1.39	1.51
3	A	702	FAD	C7M-C7	-5.76	1.39	1.51
4	A	703	NAP	C5A-C4A	-3.14	1.33	1.40
3	B	702	FAD	C9A-N10	-3.09	1.34	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	702	FAD	C5A-C4A	-3.07	1.33	1.40
4	B	703	NAP	C5A-C4A	-3.00	1.33	1.40
3	B	702	FAD	C5A-C4A	-2.94	1.33	1.40
3	A	702	FAD	C9A-N10	-2.91	1.34	1.38
2	B	701	FMN	C1'-N10	-2.32	1.46	1.48
4	A	703	NAP	C6N-N1N	2.00	1.40	1.35
4	A	703	NAP	O4D-C1D	2.10	1.44	1.41
2	B	701	FMN	C4'-C3'	2.13	1.57	1.53
4	B	703	NAP	O4D-C1D	2.15	1.44	1.41
2	A	701	FMN	C4'-C3'	2.18	1.57	1.53
3	A	702	FAD	O4B-C1B	2.18	1.44	1.41
2	A	701	FMN	O2'-C2'	2.29	1.48	1.43
3	B	702	FAD	O4B-C1B	2.29	1.44	1.41
2	B	701	FMN	O2'-C2'	2.33	1.48	1.43
2	B	701	FMN	C7M-C7	2.34	1.55	1.51
2	B	701	FMN	C9A-C5A	2.66	1.48	1.42
2	A	701	FMN	C9A-C5A	2.67	1.48	1.42
2	A	701	FMN	C9-C9A	2.91	1.47	1.40
2	B	701	FMN	C9-C9A	3.14	1.47	1.40
2	B	701	FMN	C5A-N5	3.34	1.40	1.35
3	A	702	FAD	C2A-N1A	3.36	1.40	1.33
3	B	702	FAD	C2A-N1A	3.38	1.40	1.33
2	A	701	FMN	C5A-N5	3.38	1.40	1.35
4	B	703	NAP	C2A-N1A	3.39	1.40	1.33
4	A	703	NAP	C2A-N1A	3.43	1.40	1.33
2	A	701	FMN	C4-N3	3.72	1.39	1.33
2	B	701	FMN	C8-C7	3.79	1.50	1.41
2	A	701	FMN	C10-N1	3.88	1.38	1.33
2	A	701	FMN	C8-C7	3.89	1.50	1.41
2	B	701	FMN	C4-N3	3.89	1.40	1.33
3	B	702	FAD	C4-N3	4.00	1.40	1.33
3	A	702	FAD	C4-N3	4.02	1.40	1.33
2	B	701	FMN	C10-N1	4.49	1.39	1.33
3	A	702	FAD	C2A-N3A	4.90	1.40	1.32
4	B	703	NAP	C2A-N3A	4.95	1.40	1.32
3	B	702	FAD	C2A-N3A	4.96	1.40	1.32
4	A	703	NAP	C2A-N3A	5.01	1.40	1.32
3	B	702	FAD	C10-N1	5.09	1.40	1.33
3	A	702	FAD	C10-N1	5.14	1.40	1.33
2	A	701	FMN	C4A-N5	5.76	1.41	1.33
2	B	701	FMN	C4A-N5	5.91	1.41	1.33
2	A	701	FMN	C9A-N10	7.13	1.48	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	702	FAD	C8A-N7A	7.18	1.48	1.34
3	B	702	FAD	C8A-N7A	7.21	1.48	1.34
2	B	701	FMN	C9A-N10	7.68	1.48	1.38

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	702	FAD	N3A-C2A-N1A	-13.21	117.36	128.86
3	B	702	FAD	N3A-C2A-N1A	-12.96	117.57	128.86
4	B	703	NAP	N3A-C2A-N1A	-12.69	117.80	128.86
4	A	703	NAP	N3A-C2A-N1A	-12.69	117.81	128.86
2	B	701	FMN	C4-C4A-C10	-5.91	115.18	119.96
2	B	701	FMN	C4A-C10-N10	-5.87	116.45	120.52
2	A	701	FMN	C4-C4A-C10	-5.84	115.24	119.96
2	A	701	FMN	C4A-C10-N10	-5.23	116.89	120.52
2	A	701	FMN	C4A-C4-N3	-4.91	116.49	123.48
2	B	701	FMN	C4A-C4-N3	-4.81	116.64	123.48
2	B	701	FMN	O3P-P-O5'	-4.33	95.21	106.73
4	A	703	NAP	C4B-O4B-C1B	-4.10	105.40	109.77
2	A	701	FMN	O3P-P-O5'	-3.95	96.21	106.73
4	B	703	NAP	C4B-O4B-C1B	-3.93	105.59	109.77
3	A	702	FAD	C4B-O4B-C1B	-3.45	106.09	109.77
3	B	702	FAD	C4B-O4B-C1B	-3.34	106.21	109.77
2	B	701	FMN	C6-C5A-N5	-3.24	115.16	118.97
2	B	701	FMN	C5A-C9A-N10	-3.20	115.28	117.66
2	B	701	FMN	C4'-C3'-C2'	-3.11	106.72	113.41
2	A	701	FMN	C6-C5A-N5	-2.99	115.45	118.97
2	B	701	FMN	O4'-C4'-C3'	-2.96	101.75	109.09
2	A	701	FMN	O4'-C4'-C3'	-2.90	101.90	109.09
4	A	703	NAP	C4D-O4D-C1D	-2.86	106.72	109.77
2	A	701	FMN	C5A-C9A-N10	-2.71	115.64	117.66
2	A	701	FMN	C4A-N5-C5A	-2.69	113.92	116.76
4	A	703	NAP	O4B-C1B-C2B	-2.67	101.93	106.59
2	A	701	FMN	C4'-C3'-C2'	-2.64	107.72	113.41
3	A	702	FAD	C4X-C10-N10	-2.56	118.74	120.52
4	A	703	NAP	C3B-C2B-C1B	-2.55	97.77	102.75
3	B	702	FAD	C4X-C4-N3	-2.52	119.89	123.48
3	A	702	FAD	C4X-C4-N3	-2.45	120.00	123.48
3	B	702	FAD	C2B-C3B-C4B	-2.40	97.94	102.62
3	A	702	FAD	C2B-C3B-C4B	-2.31	98.12	102.62
4	B	703	NAP	C4D-O4D-C1D	-2.28	107.34	109.77
4	B	703	NAP	C3N-C7N-N7N	-2.25	115.21	117.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	FMN	C4A-N5-C5A	-2.24	114.40	116.76
4	B	703	NAP	C3B-C2B-C1B	-2.24	98.37	102.75
4	A	703	NAP	C3N-C7N-N7N	-2.12	115.35	117.77
2	A	701	FMN	C8M-C8-C9	-2.11	115.05	120.34
3	A	702	FAD	C5A-C6A-N6A	-2.07	116.25	120.47
3	B	702	FAD	C5A-C6A-N6A	-2.05	116.29	120.47
4	B	703	NAP	O4B-C1B-C2B	-2.05	103.01	106.59
3	B	702	FAD	C4X-C10-N10	-2.03	119.11	120.52
2	A	701	FMN	O4'-C4'-C5'	-2.02	105.50	110.00
2	A	701	FMN	C7M-C7-C6	-2.00	115.32	120.34
2	B	701	FMN	C1'-N10-C9A	2.10	120.28	118.35
2	B	701	FMN	O2P-P-O1P	2.30	119.48	110.50
2	A	701	FMN	C1'-N10-C9A	2.33	120.48	118.35
3	A	702	FAD	C5X-C9A-N10	2.37	119.42	117.66
2	A	701	FMN	O2P-P-O1P	2.47	120.16	110.50
3	B	702	FAD	C5X-C9A-N10	2.51	119.52	117.66
2	B	701	FMN	C8M-C8-C7	2.54	126.04	120.72
2	A	701	FMN	C8M-C8-C7	2.74	126.48	120.72
3	A	702	FAD	C4X-N5-C5X	2.93	119.86	116.76
3	B	702	FAD	C4X-N5-C5X	2.94	119.86	116.76
2	B	701	FMN	C9A-C5A-N5	2.94	126.62	122.24
2	A	701	FMN	C9A-C5A-N5	2.96	126.65	122.24
2	B	701	FMN	P-O5'-C5'	3.19	127.09	118.30
3	A	702	FAD	C1'-N10-C9A	3.31	121.38	118.35
2	A	701	FMN	P-O5'-C5'	3.39	127.63	118.30
3	B	702	FAD	C1'-N10-C9A	3.44	121.50	118.35
2	A	701	FMN	C10-C4A-N5	5.68	127.12	120.59
2	B	701	FMN	C10-C4A-N5	5.71	127.16	120.59
3	B	702	FAD	C4-N3-C2	5.76	120.19	115.16
3	A	702	FAD	C4-N3-C2	5.82	120.25	115.16
2	A	701	FMN	C4-N3-C2	13.76	127.20	115.16
2	B	701	FMN	C4-N3-C2	13.81	127.23	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	702	FAD	1	0
4	A	703	NAP	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	702	FAD	1	0
4	B	703	NAP	8	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, 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	608/622 (97%)	-0.41	5 (0%) 86 89	25, 36, 52, 78	0
1	B	607/622 (97%)	-0.01	32 (5%) 27 34	24, 44, 86, 103	0
All	All	1215/1244 (97%)	-0.21	37 (3%) 51 58	24, 39, 81, 103	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	166	VAL	5.5
1	B	163	LEU	4.9
1	B	231	PHE	4.1
1	B	227	VAL	4.0
1	A	252	ASP	4.0
1	B	505	GLY	3.7
1	B	125	LEU	3.7
1	B	168	PHE	3.6
1	B	193	GLU	3.5
1	B	232	GLY	3.5
1	B	205	LEU	3.4
1	B	106	GLY	3.2
1	B	129	ASP	3.2
1	B	200	ILE	3.1
1	A	500	ALA	3.1
1	B	192	LEU	3.0
1	B	233	VAL	2.9
1	A	506	ARG	2.9
1	B	162	ASP	2.7
1	B	165	GLY	2.7
1	B	201	PHE	2.7
1	A	256	ALA	2.6
1	B	235	ALA	2.6
1	B	354	GLU	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	170	VAL	2.5
1	B	187	TYR	2.4
1	B	191	ARG	2.3
1	A	62	PRO	2.3
1	B	124	SER	2.3
1	B	128	ILE	2.2
1	B	104	ARG	2.2
1	B	186	LYS	2.1
1	B	229	GLU	2.1
1	B	228	CYS	2.1
1	B	198	GLN	2.0
1	B	500	ALA	2.0
1	B	189	ASP	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
5	PO4	A	704	5/5	0.86	0.17	6.71	101,102,103,103	0
2	FMN	A	701	31/31	0.95	0.15	1.54	24,36,38,39	0
4	NAP	B	703	48/48	0.96	0.14	0.60	33,44,77,78	0
4	NAP	A	703	48/48	0.98	0.11	0.06	29,36,55,57	0
2	FMN	B	701	31/31	0.94	0.14	0.03	57,70,72,73	0
3	FAD	A	702	53/53	0.98	0.11	-0.44	24,29,39,40	0
3	FAD	B	702	53/53	0.98	0.11	-0.44	25,30,38,39	0
5	PO4	B	704	5/5	0.94	0.11	-	75,76,77,77	0

6.5 Other polymers [i](#)

There are no such residues in this entry.